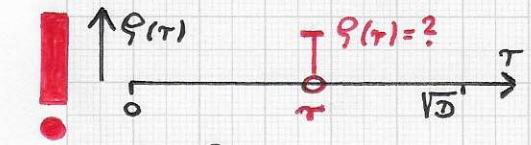
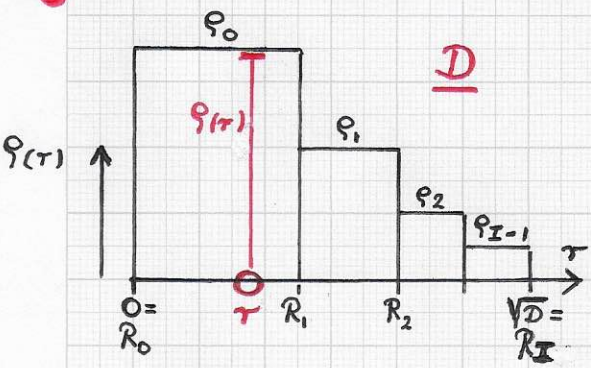
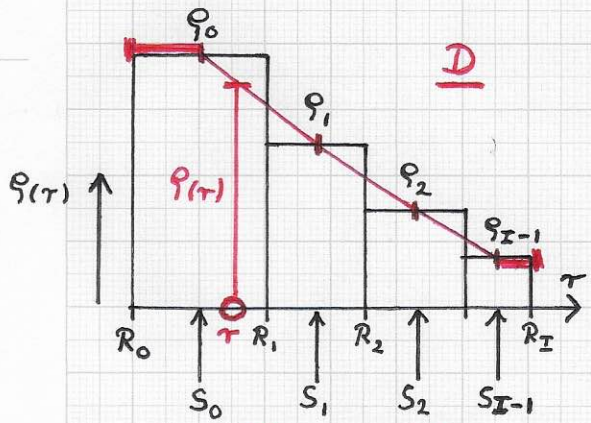
■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...







$S_i = (R_i + R_{i+1}) / 2$, $i = 0 \ldots (I-1)$

$\delta_i = S_{i+1} - S_i$, $i = 0 \ldots (I-2)$

⇒ Piecewise linear function:

$$\varrho(r) = \begin{cases} \dfrac{S_{i+1} - r}{\delta_i}\,\varrho_i + \dfrac{r - S_i}{\delta_i}\,\varrho_{i+1}, & \text{if } S_0 \le r < S_{I-1}; \\ \varrho_0, & \text{if } 0 \le r < S_0; \\ \varrho_{I-1}, & \text{if } S_{I-1} \le r < R, \end{cases}$$

$i = 0 \ldots (I-2)$.

We use a constructed normalized probability density function to compute a PROBABILITY VALUE FOR A GIVEN r-VALUE — to establish the probability of a material associated with this r-value to belong to the material class with this specific density function $\varrho(r)$.

The left figures provide illustrations. Here, we assume that $\varrho = {}^{D}\varrho$, i.e., the density is a density relative to a D-dimensional domain, and that $\varrho(r)$ is the described normalized piecewise constant function defined as

$$\varrho(r) = \begin{cases} \varrho_i, & \text{if } r \in [R_i, R_{i+1}), \; i = 0 \ldots (I-1) \\ 0, & \text{if } r \ge R_I \end{cases}.$$

Thus, the simplest method to determine a probability value for a given r-value, $r \ge 0$, uses the $\varrho(r)$-value of the piecewise constant function.

An alternative is the use of a piecewise linear function (left).

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...

• **Note.** One must keep the following important facts in mind:

(i) Only the discontinuous piecewise constant (step-) function $\varrho(r)$ as defined on the previous page is the PROPERLY NORMALIZED probability density function based on the given data. The "alternative function," i.e., the described piecewise linear function, can only be viewed as an APPROXIMATION of the discontinuous (step-) function, considered merely to have available a simple continuous alternative function — understanding that this piecewise linear function is NOT the result of a normalization process.

(ii) Assuming that the classification decision must be binary ($1 \hat{=}$ yes, $0 \hat{=}$ no), one must define an optimal, or near-optimal, value of a threshold ϱ_t. In other words, if $\varrho(r) \geq \varrho_t$, the decision will be '1'; and if $\varrho(r) < \varrho_t$, the decision will be '0'. The objective is to define the ϱ_t-value in such a way that the value of overall classification performance is maximized. As discussed, the performance function depends on the numbers of true negative, true positive, false negative, false positive and mis-classification outcomes.

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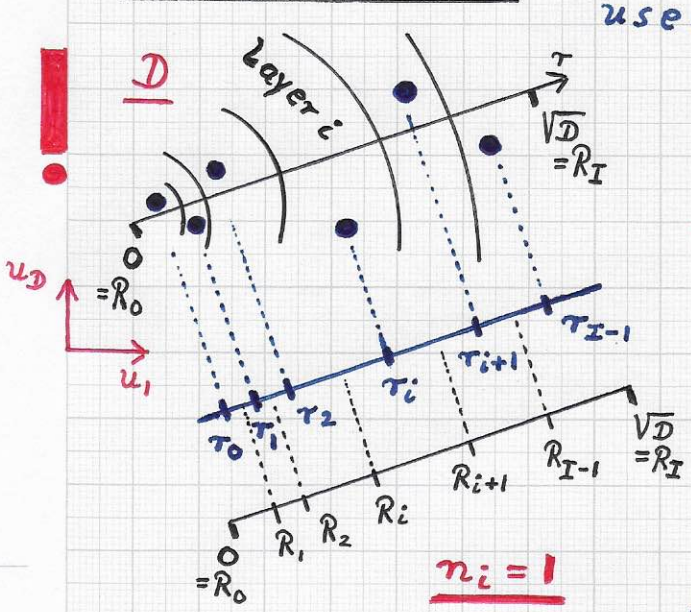
■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:... (iii) We have no knowledge of an exact, analytically defined normalized probability density function per se. We only have access to a discrete, finite data set of points in a D-dimensional domain in the described "experimental and practical context." The best normalized probability density function we can construct using the presented technique is a function that is based on all available points in D-space and where each individual point implies a layer, "the single point's layer," with an associated "layer thickness." Considering our technique, "layer thickness" can be understood as an interval on the radial r-line, i.e., an interval $[R_i, R_{i+1})$. In this limit case, the resulting normalized probability density function $\rho(r)$ is a step-function where the number of points in D-space is equal to the number of steps – assuming that all point-associated r-values are mutually different from each other. We describe a viable construction of such a SINGLE-POINT-BASED NORMALIZED PROBABILITY FUNCTION, representing the limit case in the following. (In fact, when only a very small, spare point data set is given, one should consider this single-point-based construction.)...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...



The construction principle used for a possible definition of a SINGLE-POINT-BASED NORMALIZED PROBABILITY DENSITY FUNCTION is sketched in the left figure for the general D-dimensional setting. We are given I points '•' in the D-dimensional domain space. (The value of I is 6 for the example used in the figure.) Each point i has a specific (radial) distance r_i from the origin of the normalized u-space coordinate system. In other words, point i lies on the hyper-sphere with radius r_i, with u = 0 as its center. When sorting the r_i-values of all points, we obtain the sequence $r_0 < r_1 < \ldots < r_{I-2} < r_{I-1}$. For each pair (r_i, r_{i+1}), we compute the average $R_i = (r_{i-1} + r_i)/2$, $i = 1 \ldots (I-1)$. One can consider R_i also as midpoint — the "bisecting midpoint" — of two consecutive r_i-values. In addition, one defines R_0 and R_I as before, i.e., $R_0 = 0$ and $R_I = \sqrt{D}$. Thus, layer i is the hyper-volume bounded by the two hyper-spheres with radii R_i and R_{i+1}, see figure above. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...

Based on this definition of R_i-values and the underlying constant number of points for each layer – $n_i=1$, $i = 0 \ldots (I-1)$ – it is now possible to calculate the value of $\|\cdot\|_\Omega$ for the constructed piecewise constant function. This value is:

$$\|\cdot\|_\Omega = \left(\frac{1}{V(D,\Omega)} \int_\Omega (\text{hyper\_layer\_densities})^2 \, dv \right)^{1/2}$$

$$= \left(\frac{1}{c_D \cdot D^{D/2}} \sum_{i=0}^{I-1} \int_{\Omega_i} \frac{1}{(c_D (R_{i+1}^D - R_i^D))^2} \, dv \right)^{1/2}$$

$$= \frac{1}{c_D^{1/2} \cdot D^{D/4}} \left(\sum_{i=0}^{I-1} \frac{1}{c_D (R_{i+1}^D - R_i^D)} \right)^{1/2}$$

$$= \frac{1}{c_D \, D^{D/4}} \left(\sum_{i=0}^{I-1} \frac{1}{R_{i+1}^D - R_i^D} \right)^{1/2}.$$

The original not-yet-normalized density value associated with layer i, containing only the one point i, is defined by the corresponding hyper-volume-based ratio $q_i = \left(1 / (R_{i+1}^D - R_i^D) \right)$, $i=0 \ldots (I-1)$. These original values must be divided by the value of $\|\cdot\|_\Omega$, i.e., the value of the original and therefore not-yet-normalized metric value of the single-point-based density function. The result of the division, i.e., normalization, is the desired discontinuous, piecewise constant (step-) function that represents the "maximal-resolution probability-density function", reflecting each given point.

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