OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:… The detailed discussion of density function construction from discrete, finite data relates to the goal of determining a continuously defined density from $(s_1, \ldots, s_c)$-tuple data. (See pp. 16-20, from 9/4/2022 to 9/5/2022.) By having access to pre-computed and stored continuous density functions – or by being able to compute density functions in "real time" – one can effectively use them as WEIGHT FUNCTIONS. The purpose of these density functions is the proper association of weights to the individual elements of a material sample/training data set. It can and must generally be assumed that such a data set does not cover the material-class-associated region(s) in feature space in a uniform, nearly constant-density fashion. In other words, "certain allowable sample types" of a specific material might arise seldom, being quasi-outliers, far away in feature space from the vast majority of the samples. This non-uniform distribution of samples in feature space can be captured via a density function that describes sample density variation continuously in feature space.

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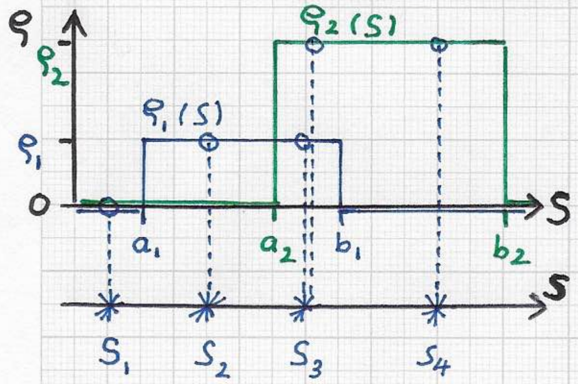
OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...



We consider increasingly complex examples to explain the value and use of these density functions for the calculation of classification probabilities that take into account (i) the relative total numbers of material samples across all classes of interest and (ii) the relative distributions/densities of all material samples per class, for all material classes. The figure (top) illustrates a first, simple scenario: Two piecewise-constant density functions (box functions) are given, reflecting uniform distributions:

$$\rho_1(S) = \begin{cases} \rho_1, & S \in [a_1, b_1] \\ 0, & \text{otherwise} \end{cases}, \quad \rho_2(S) = \begin{cases} \rho_2, & S \in [a_2, b_2] \\ 0, & \text{otherwise} \end{cases}.$$

$\rho_1(S)$ and $\rho_2(S)$ must only satisfy the condition $\rho_i(S) \geq 0$.

We consider four locations/values of an unclassified sample, i.e., S_1, S_2, S_3 and S_4. The density functions $\rho_1(S)$ and $\rho_2(S)$ are associated with material classes 1 and 2, respectively. In this simple setting, one obtains the following class-membership probability tuples (P_1, P_2): $S_1: (0, 0)$, $S_2: (1, 0)$, $S_3: (\rho_1/(\rho_1+\rho_2), \rho_2/(\rho_1+\rho_2))$, and $S_4: (0, 1)$.

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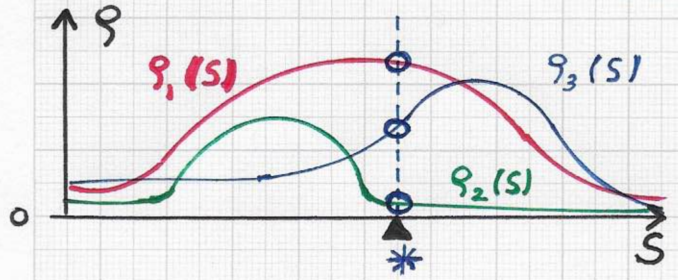
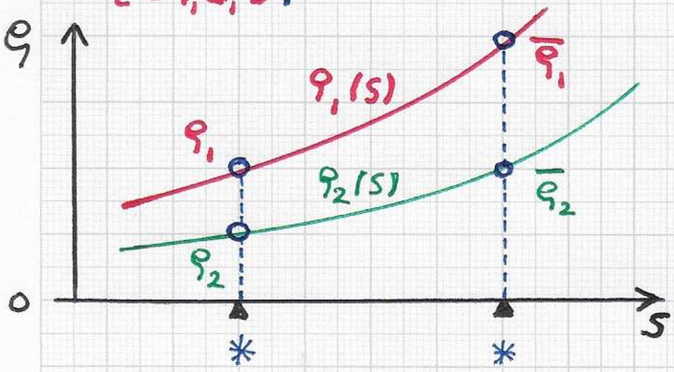
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks:... Thus, the individual class probabilities are $P_i = \rho_i / (\rho_1 + \rho_2)$, $\rho_1 + \rho_2 \neq 0$ and $i = 1, 2$. More precisely, P_i's value is

$$P_i = \begin{cases} \rho_i / (\rho_1 + \rho_2), & \rho_1 + \rho_2 \neq 0 \\ 0, & \text{otherwise} \end{cases}, \quad i = 1, 2.$$



The left figure shows an example of three density functions $\rho_i(S)$, $i=1,2,3$, where the functions indicate non-uniform density and have non-zero positive values in the entire S-domain. In this scenario, one could define a class-membership probability as $P_i(*) = \rho_i(*) / (\rho_1(*) + \rho_2(*) + \rho_3(*))$, $i = 1, 2, 3$.



We should, must consider an additional aspect, sketched in the figure (left): The ratios of the two density functions $\rho_1(S)$ and $\rho_2(S)$ are equal at the two locations indicated as '$*$', i.e., $\rho_1 : \rho_2 = \bar{\rho}_1 : \bar{\rho}_2$. Nevertheless, the values $\bar{\rho}_1$ and $\bar{\rho}_2$ indicate a higher probability of belonging to class 1 and 2, respectively, as $\bar{\rho}_1 > \rho_1$ and $\bar{\rho}_2 > \rho_2$. This fact can be captured by defining

$$P_i(*) = \frac{\sum_{j=1}^{2} \rho_j(*)}{M} \, \rho_i(*) / \sum_{j=1}^{2} \rho_j(*), \quad i = 1, 2.$$

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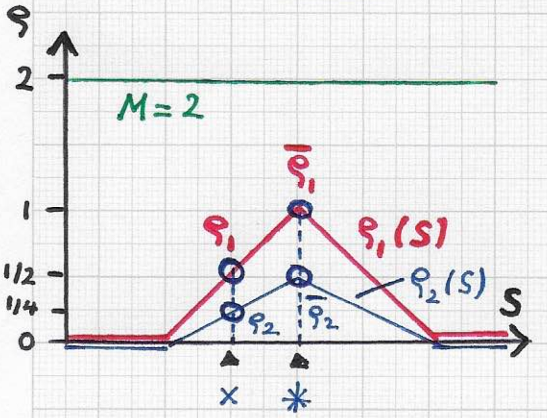
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



One can understand this definition of P_i as a product of a scaling factor s and a fraction f_i, i.e., one can write P_i as

$$P_i(*) = s(*) \cdot f_i(*) \quad ,$$

where one defines (for $i = 1,2$)

$$s(*) = 1/M \cdot \Sigma_{j=1}^{2} \varrho_j(*) \, ,$$

$$f_i(*) = \varrho_i(*) / \Sigma_{j=1}^{2} \varrho_j(*) \, .$$

Thus, the scaling factor s ensures that the resulting values of $P_i(*)$ properly capture the absolute values, the magnitudes of the density functions $\varrho_i(S)$, i.e., the "scaled probability" of a material to belong to material class i. The figure (top, left) illustrates a numerical example, and we use it to perform exemplery calculations. We define an "upper limit," a "maximal value" $M = 2$. The value of M must be viewed as a data-dependent value that has to be "learned" from classified material samples — and the M-value should optimize classification. We use two density functions, and they satisfy the equation $\varrho_1(S) = 2\varrho_2(S)$ in the entire S-domain. We calculate probability values for $S = 'x'$ and $S = '*'$:

• $S = 'x'$: $\varrho_1(x) = \varrho_1$, $\varrho_2(x) = \varrho_2$, $s(x) = 1/2 \cdot (1/2 + 1/4) = 3/8$
  $S = '*'$: $\varrho_1(*) = \bar{\varrho}_1$, $\varrho_2(*) = \bar{\varrho}_2$, $s(*) = 1/2 \cdot (1 + 1/2) = 3/4$

(Since $1 = \bar{\varrho}_1 = 2\varrho_1 = 2 \cdot \frac{1}{2}$ and $\frac{1}{2} = \bar{\varrho}_2 = 2\varrho_2 = 2 \cdot \frac{1}{4}$, we obtain the ratio $s(x) : s(*) = 1 : 2 = 3/8 : 3/4$.)

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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks:... Next, we compute the values of the fractions; we obtain:
  - $S = \text{'x'}$: $f_1(x) = 1/2 : 3/4 = \rho_1 / (\rho_1 + \rho_2) = 2/3$,

    $f_2(x) = 1/4 : 3/4 = \rho_2 / (\rho_1 + \rho_2) = 1/3$

    $S = \text{'*'}$: $f_1(*) = 1 : 3/2 = \bar{\rho}_1 / (\bar{\rho}_1 + \bar{\rho}_2) = 2/3$,

    $f_2(*) = 1/2 : 3/2 = \bar{\rho}_2 / (\bar{\rho}_1 + \bar{\rho}_2) = 1/3$

Thus, the resulting class-membership probabilities are:

- $S = \text{'x'}$: $P_1(x) = s(x) \cdot f_1(x) = 3/8 \cdot 2/3 = 1/4$,

  $P_2(x) = s(x) \cdot f_2(x) = 3/8 \cdot 1/3 = 1/8$

  $S = \text{'*'}$: $P_1(*) = s(*) \cdot f_1(*) = 3/4 \cdot 2/3 = 1/2$,

  $P_2(*) = s(*) \cdot f_2(*) = 3/4 \cdot 1/3 = 1/4$

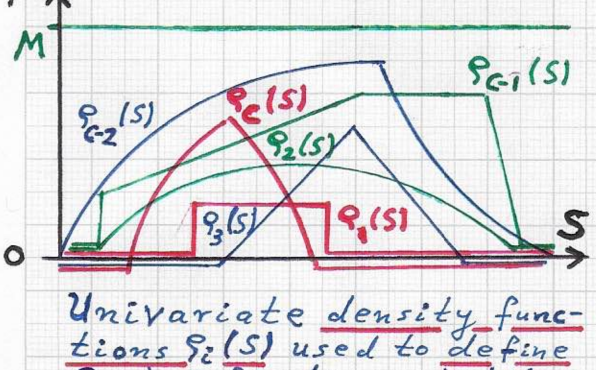
These probability values have ratios as desired for the considered two density functions:

$$P_1(x) = 2\,P_2(x), \quad P_1(*) = 2\,P_2(*)$$

and

$$P_1(x) = 1/2\,P_1(*), \quad P_2(x) = 1/2\,P_2(*).$$

The general case involving C class-membership probabilities is therefore defined as follows:



Univariate density functions $\rho_i(S)$ used to define C classification probabilities $P_i(S)$, $i = 1, \ldots, C$.

$$\mathbb{P}(S) = (P_1(S), \ldots, P_C(S)),$$

where

$$P_i(S) = \begin{cases} s(S) \cdot f_i(S), & \text{if } \sum_{j=1}^{C} \rho_j(S) \neq 0 \\ 0, & \text{otherwise} \end{cases},$$

and

$$s(S) = 1/M \cdot \sum_{j=1}^{C} \rho_j(S),$$

$$f_i(S) = \rho_i(S) \Big/ \sum_{j=1}^{C} \rho_j(S).$$

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