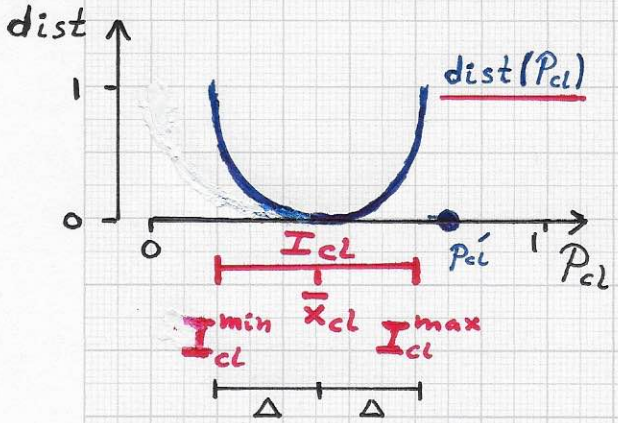
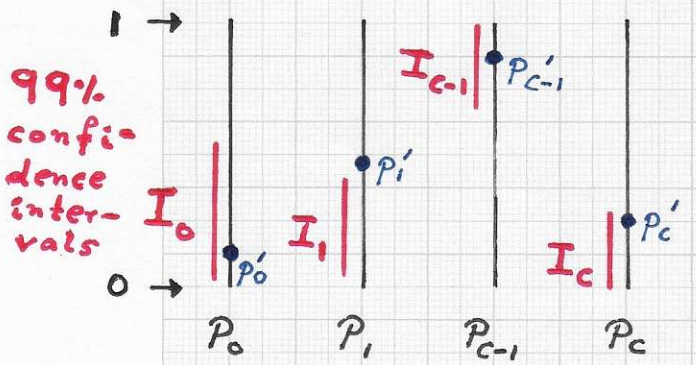
■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks: ...



Sketch of high-degree polynomial distance function $dist(P_{cl})$. Its value for p_{ci}' is

$$dist(p_{ci}') = (|p_{ci}' - \bar{x}_{cl}| / \Delta)^n .$$



Parallel coordinates plot of class-(C-1) signature with p_{ci}'-values of unclassified material. The sum of the individual $dist(P_{cl})$ values yields

$$D_{C-1} = \sum_{cl=0}^{C} dist(p_{ci}') .$$

We can compute C values for $D_1, D_2, \ldots, D_C$. Further, we can sort these values: We use the values and their relative magnitudes and order for classification.

Distance/similarity measures are crucially important at this late stage of material classification. First, we focus in more detail on the distance between a single p_{ci}'-value of an unclassified material segment and associated "confidence interval" on the P_{cl}-axis, see left figure. (On page 19, 10/13/2022, a simple distance $|\bar{x}_{cl} - p_{ci}'|$ is suggested.) A more sophisticated distance is suggested here: One can argue that all values of p_{ci}' that satisfy $I_{cl}^{min} < p_{ci}' < I_{cl}^{max}$ should imply a very low distance to the interval $[I_{cl}^{min}, I_{cl}^{max}]$; p_{ci}'-values outside this interval: distances should be large. This objective is achieved, for example, by using a function of the kind

$$dist(P_{cl}) = (|P_{cl} - \bar{x}_{cl}| / \Delta)^n , \quad n \in \{1, 2, 3, \ldots\} .$$

The figure sketches a polynomial function of this kind.

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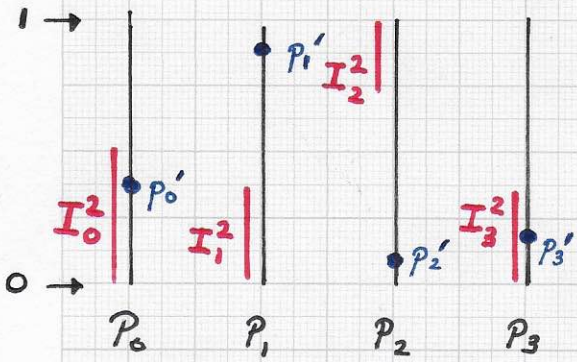
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



Scenario where tuple (p_0', p_1', p_2', p_3') is compared with the class-2 signature. Thus, one should assign higher significance to the value of $dist(p_2')$.

For example, one could use a weight for $dist(p_2')$. In this specific case, one could consider the weighted sum

$$D_2 = w_2 \cdot dist(p_2') + \sum_{\substack{cl=0 \\ cl \neq 2}}^{3} dist(p_{cl}')$$

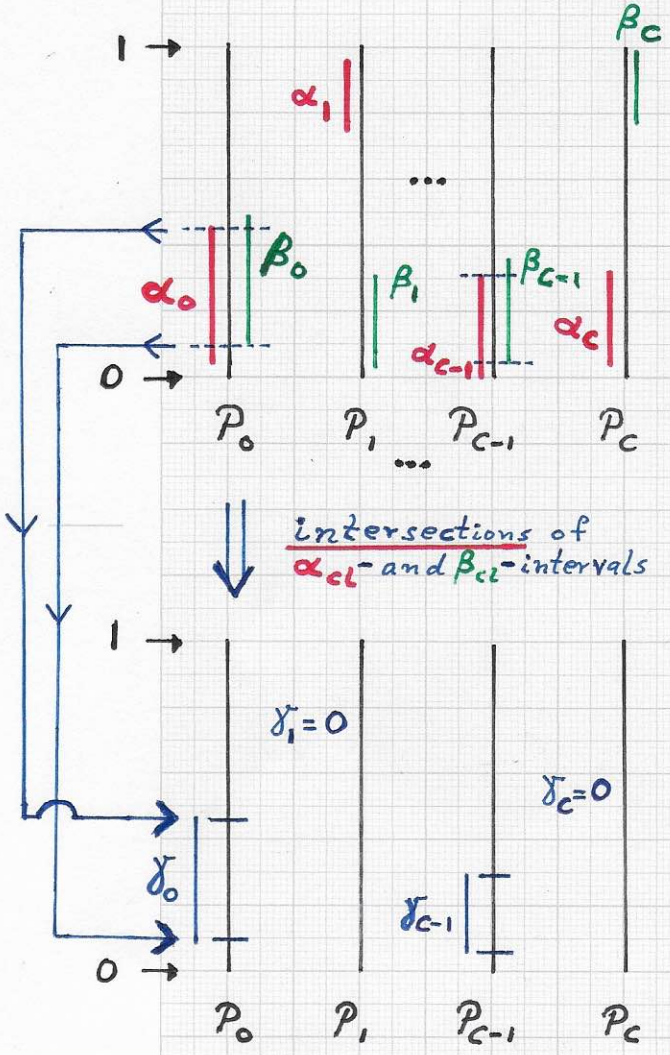
as the measure of total distance between the given unclassified tuple and the class-2 signature. (Here, the tuple most likely is a class-1 tuple, given the large value of p_1'.) It can only be decided via experiment how to define a near-optimal value of weight w_2.

• Note. We compute C distance values $D_1, D_2, ..., D_C$ for an unclassified material tuple $(p_0', p_1', ..., p_C')$. These distances $D_1, ..., D_C$ should be sorted, from smallest to largest distance value. If, for example, $D_1 < D_2 < ... < D_C$, then class 1 is interpreted as the class to which the given tuple belongs. The actual value of D_1 can be viewed as "certainty measure": The smaller the value of D_1, the higher the certainty about class match. Various "ambiguous cases" must be handled, e.g.: (i) the value of D_1 (the smallest value) is NOT "close to zero," and the certainty about class match is low; (ii) the values of both D_1 and D_2 are "close to zero" and nearly equal, and one must determine whether class 1 or class 2 is the best match.

• Note. When comparing the given tuple $(p_0', ..., p_C')$ with the class-cl signature, then the P_{cl}-axis distance value, will be most important, $dist(P_{cl})$; $dist(P_{cl})$ should have larger weight. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: ...



Top: Lengths of P_{cl}-axis "confidence intervals" of two material signatures to be compared. The distance between two signatures should be based on the overlap of α_{cl}- and β_{cl}-intervals.

Bottom: The intersection of "confidence intervals" generates intersection interval lengths γ_{cl}.

In addition, one computes the values of an appropriate distance measure for the signatures of material classes. The left figure illustrates the relevant parameters for such a signature distance measure. The first signature has "confidence intervals $I^{\alpha}_{cl} = [{}^{\alpha}I^{min}_{cl}, {}^{\alpha}I^{max}_{cl}]$, and the second signature has "confidence intervals $I^{\beta}_{cl} = [{}^{\beta}I^{min}_{cl}, {}^{\beta}I^{max}_{cl}]$. The lengths of these intervals are $\alpha_0, \ldots, \alpha_C$ and $\beta_0, \ldots, \beta_C$, respectively, as sketched in the figure. For each P_{cl}-axis, we compute the intersections of two "confidence intervals," i.e., we calculate $I^{\alpha}_{cl} \cap I^{\beta}_{cl}$, $cl = 0 \ldots C$. The resulting (intersection) intervals have lengths $\gamma_0, \ldots, \gamma_C$, also shown in the figure. Next, we compute the sums of these lengths: $A = \sum_{cl=0}^{C} \alpha_{cl}$, $B = \sum_{cl=0}^{C} \beta_{cl}$, $C_{\cap} = \sum_{cl=0}^{C} \gamma_{cl}$.

• **Our overall goal is to obtain a small distance when $C_{\cap}$ is large and a large distance when $C_{\cap}$ is small.**

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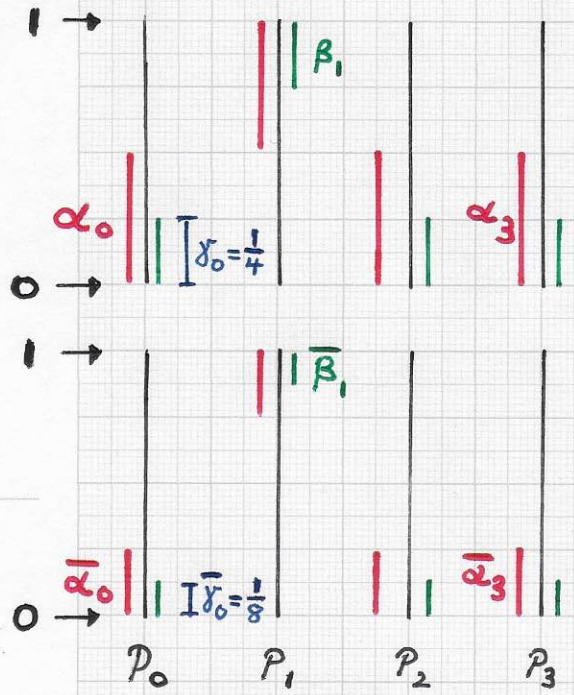
OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...



Two pairs of signatures are being compared and their distances computed.

Top: $A=2, B=1, C_n=1$

$\Rightarrow d = 1/3$

Bottom: $\bar{A}=1, \bar{B}=\frac{1}{2}, \bar{C}_n=\frac{1}{2}$

$\Rightarrow \bar{d} = 1/3$

In this case, the signature distance formula for d (right, bottom) yields the same value of distance for the top and bottom pair of signatures.

It might be desirable to include a scaling factor in the definition of d, to obtain different values.

First, we calculate the sum-of-lengths ratio

$$2C_n/(A+B) .$$

The range of this relative length measure is the interval $[0, 1]$. When the signatures of two materials have empty ($\emptyset$) intersection intervals on every P_{cl}-axis, this ratio is 0; when two signatures are identical, this ratio is 1. (The value of $A+B$ must not be zero. The upper bound for the value of $A+B$ is $(C+1)+(C+1) = 2(C+1)$ — since we consider $(C+1)$ P_{cl}-axes, and the maximal length of a "confidence interval is one.) We must map the ratio value 0 to an (initial) distance value 1 and the ratio value 1 to an (initial) distance value 0, i.e.,

$$\frac{2C_n}{A+B} \longmapsto 1 - \frac{2C_n}{A+B} = d.$$

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks: ...

cl \ cl	1	2	...	C-1	C
1	0	$d_{1,2}$	...	$d_{1,C-1}$	$d_{1,C}$
2	_	0	...	$d_{2,C-1}$	$d_{2,C}$
⋮	_	_	0	⋮	⋮
C-1	_	_	_	0	$d_{C-1,C}$
C	_	_	_	_	0

Matrix representation of signature distances for all signature pairs.

cl \ i	(i1)	i2	...	iC-1	iC
1	(1)	4	...	9	3
⋮	⋮	⋮	⋮	⋮	⋮
C	(C)	5	...	8	2

Table of indices of classes ordered by signature distance for each class, cl = 1 ... C. For class cl (row cl) the table provides the C indices of the classes when sorted by increasing signature distance relative to class cl's signature. For example, the sorted set of classes relative to class 1 is the set {cl 1, cl 4, ..., cl 9, cl 3}.

Using sorted tuple distances D_{cl} and sorted class signature distances $d_{i1,i2}$ can improve classification.

A potentially desirable scaling factor can be included in this definition, to "assign weights" to the "confidence interval" lengths as follows:

$$d = \frac{A+B}{2(C+1)} \cdot \left(1 - \frac{2C_n}{A+B}\right).$$

Considering the two signature pairs from the previous page, the scaling factor $(A+B)/(2(C+1))$ has the values $3/8$ (top pair) and $3/16$ (bottom pair). The ability to compute and store distances for all class signature pairs can and should be used to confirm or change an initial classification of a given unclassified material segment: On p. 21 (10/15/2022), it is discussed how a (sorted) set of distance values $D_1, \ldots, D_C$ is used to classify a tuple $(p'_0, p'_1, \ldots, p'_C)$ initially. Knowing class-to-class signature distances $d_{i1,i2}$, one can use them to potentially change the tuple's initial classification.

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