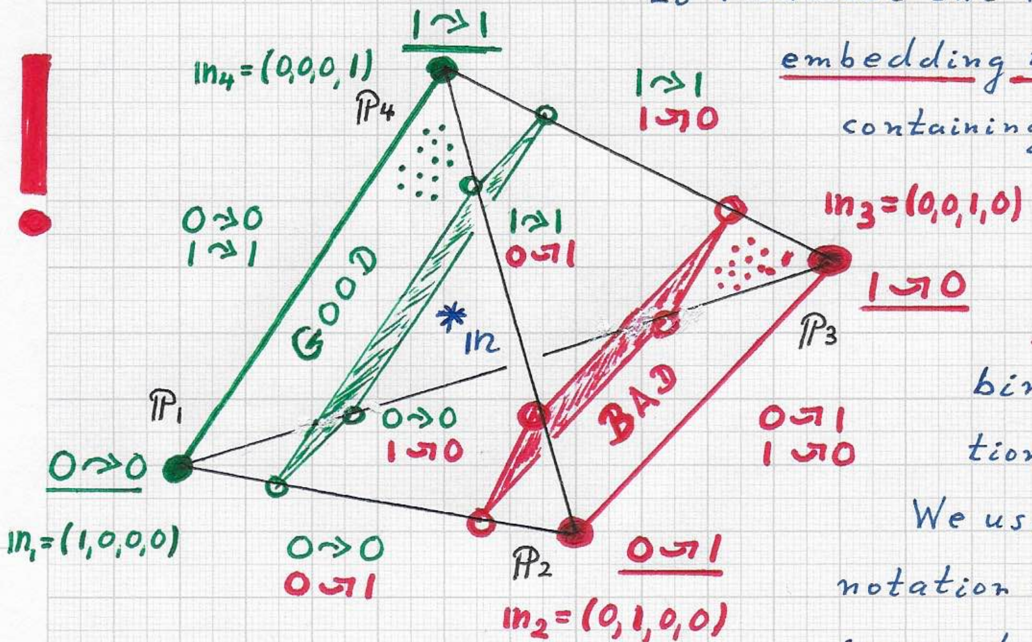
Stratovan

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• *Laplacian eigenfunctions and neural networks:...*



The figure shown here is an attempt to visualize the regions in the embedding tetrahedron – containing all allowable $\mathbb{m}$-tuples $\mathbb{m}$ – that define GOOD and BAD binary classification performance.

We use the following notation for correct and incorrect classifications:

Correct classifications, classifying class 0 as class 0 and class 1 as class 1, are written as 0→0 and 1→1. Incorrect classifications, classifying class 0 as class 1 and class 1 as class 0, are written as 0⇁1 and 1⇁0. Points on the edge $\overline{\mathbb{P}_1\mathbb{P}_4}$ reflect perfect classification performance, where 0→0 and 1→1 holds. Points on the edge $\overline{\mathbb{P}_2\mathbb{P}_3}$ reflect worst classification performance, where 0⇁1 and 1⇁0 holds. As indicated in the figure, one can define a region in the tetrahedron that is close to the edge $\overline{\mathbb{P}_1\mathbb{P}_4}$ as a GOOD performance region – ~~and~~ a region close to the edge $\overline{\mathbb{P}_2\mathbb{P}_3}$ as a BAD performance region. The figure shows point, $\mathbb{m}$-tuple "clouds" {·} and {·} in these two regions.

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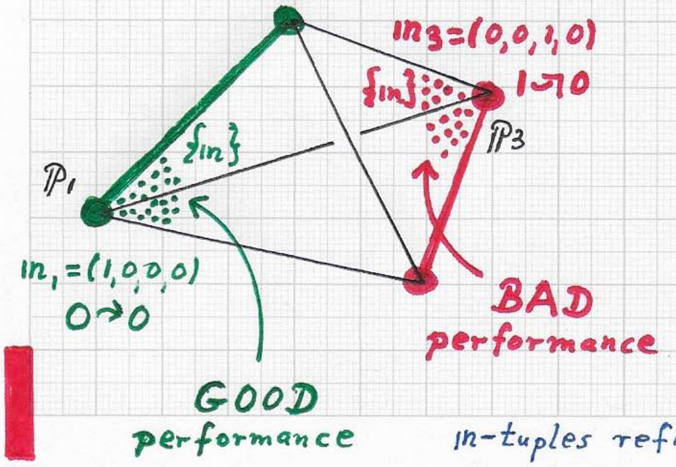
OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

- Laplacian eigenfunctions and neural networks:... The other four edges of the tetrahedron, i.e., edges $\overline{\mathbb{P}_1\mathbb{P}_2}$, $\overline{\mathbb{P}_1\mathbb{P}_3}$, $\overline{\mathbb{P}_2\mathbb{P}_4}$ and $\overline{\mathbb{P}_3\mathbb{P}_4}$ represent $\mathbb{m}$-tuples with two coordinates/components different from zero: one of these two coordinates reflects the relative occurrence of correct classifications, $0 \to 0$ or $1 \to 1$, while the other one of these two coordinates reflects the relative occurrence of incorrect classifications, $0 \to 1$ or $1 \to 0$. Similarly, one can describe the meaning of a point/$\mathbb{m}$-tuple in the interior of one of the four faces of the tetrahedron.

Thus, the classification performance evaluation of the system — and one specific setting of its parameters — produces one $\mathbb{m}$-tuple, one point in the tetrahedron, when evaluating system performance for a material set consisting of L materials.



The figure (left) shows an example with two $\mathbb{m}$-tuple/point clouds representing drastically different classification performance. The GOOD (BAD) cloud consists of $\mathbb{m}$-tuples reflecting that class-0 (class-1) material sets are leading, with great probability, to correct $0 \to 0$ (incorrect $1 \to 0$) results. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The characterization of classification performance via normalized, "barycentric" m-tuples defining the relative occurrences of classification result types (and an effective visualization of these m-tuples) allows one to perform various system evaluation methods:

(1) One evaluates one system and one of its parameter value settings for one set of to-be-classified materials (possibly a stream of "subsequently incoming" materials), where one number of materials is used, L.

(2) One evaluates MULTIPLE SYSTEMS, each system tested for MULTIPLE PARAMETER VALUE SETTINGS, for MULTIPLE DIFFERENT SETS of to-be-classified materials (possibly SEVERAL STREAMS of "subsequently incoming" materials), where MULTIPLE DIFFERENT NUMBERS OF MATERIALS are used, $L_1, L_2, L_3, \ldots$

These two system evaluation possibilities, (1) and (2), are the two "extreme methods" to be considered. Method (1), producing just a single m-tuple, is not sufficient. Method (2) is practically not viable, due to time and cost constraints that apply to an affordable protocol and procedure for evaluation. One must devise a compromise.

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■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The ultimate goal is the implementation of ONE system with an optimal – a near-optimal – setting of its performance-defining parameter values. Therefore, a practically viable evaluation approach that supports this goal should be based on this principle:

- **One evaluates ONE SYSTEM and a viable number of DIFFERENT PARAMETER VALUE SETTINGS, for MULTIPLE SETS of to-be-classified materials – using DIFFERENT INCREASING NUMBERS $L_1, L_2, L_3, \ldots$ of set cardinality (to understand extrapolated convergence behavior for $L \to \infty$).**

As discussed before, the performance (cost) function to be optimized could be a scalar-valued function (e.g., based on an average) or a vector-valued function (e.g., based on several averages and/or performance of the system for several specific classification result types). Further, this function might involve both absolute numbers and relative "barycentric" numbers of result type occurrences, and the weights for the various result types as described and explained above.

SYSTEM PERFORMANCE OPTIMIZATION IS A SUPREMELY IMPORTANT, CRUCIAL TIME- AND COMPUTING-INTENSIVE "PRE-PROCESSING STEP."

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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... • **Note.** Considering the ultimate purpose of the classification system — DETECTION OF DANGEROUS MATERIALS AND OBJECTS TO **SAVE LIVES** — one should be willing to invest substantial computational resources to ensure that the deployed system delivers best-possible performance. OPTIMIZATION OF THE PERFORMANCE-DEFINING SYSTEM (HYPER-) PARAMETER VALUES IS THE MOST CHALLENGING AND TIME-INTENSIVE STEP IN PRE-DEPLOYMENT SYSTEM EVALUATION AND "FINE-TUNING." The parameter space of the system is multi-/high-dimensional. Further, it is generally not possible to assume or postulate that the system's performance function satisfies specific "nice and desirable properties" — like continuity behavior; monotonicity (in part of the domain); number and locations of the function's maxima (or minima); or the function's "value characteristic," i.e., being a scalar-valued or a vector-valued function. Thus, traditional and standard function minimization/maximization methods must generally be viewed as insufficient for our purposes; nevertheless, they could be used in conjunction with more general approaches. SIMULATED ANNEALING AND EVOLUTIONARY ALGORITHMS SHOULD BE CONSIDERED.

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