OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...

SIMULATED ANNEALING. (The process of "annealing" is studied in thermodynamics and concerns the cooling process of materials driven by energy minimization. SIMULATED annealing, in our context, is a cost function optimization method adapted to classification system optimization.) For classification performance function optimization, a simulated annealing algorithm can be summarized at a high level as follows:

- define an initial value of the parameter vector W;
- define an initial value of the temperature T;
- compute $p(W) = performance(W)$;
- WHILE ($p(W)$ "not good enough" AND noIterations < maxIterations)
  - determine a random perturbation ΔW, where $\Delta W = \Delta W(T, p(W), \ldots)$;
  - set $W := W + \Delta W$;
  - compute $p(W)$;
  - IF ($p(W)$ has improved)
    - accept the new W value;

    ELSE
    - accept the new W value with a probability (<1) depending on T (and...);
  - IF ("time to reduce T")
    - reduce T value;
- return values of W and $p(W)$;

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

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We now explain this algorithm in more detail, with a focus on material classification. The essential (hyper-) parameter values of the classification system define the values of the **parameter vector** $\mathbb{W}$ to be optimized. The annealing-specific **temperature** T, with monotonically decreasing value, is crucially important for "not getting stuck" in a local optimum. Temperature can be used in various way to allow the algorithm to explore $\mathbb{W}$'s domain space. Most importantly, smaller values of T imply lower probabilities for a new $\mathbb{W}$-value to be accepted when $p(\mathbb{W}_{new})$ is worse than $p(\mathbb{W}_{old})$. Further, one can also use the T-value to scale the magnitude/length of the perturbation vector $\Delta\mathbb{W}$: a large (small) value of T should imply a large (small) perturbation vector $\Delta\mathbb{W}$. The calculation of the system's **performance** $p(\mathbb{W})$ is the computationally most expensive part of the algorithm. The computation of $p(\mathbb{W})$ for a new parameter value setting makes it necessary to calculate new values for the relative occurrences of the classification result types, i.e., $\bar{n}_{0,0}, \bar{n}_{1,0}, \ldots, \bar{n}_{c,0}, \ldots, \bar{n}_{0,c}, \ldots, \bar{n}_{c,c}$, involving substantial data processing of material samples in the sample database with known ground truth information.

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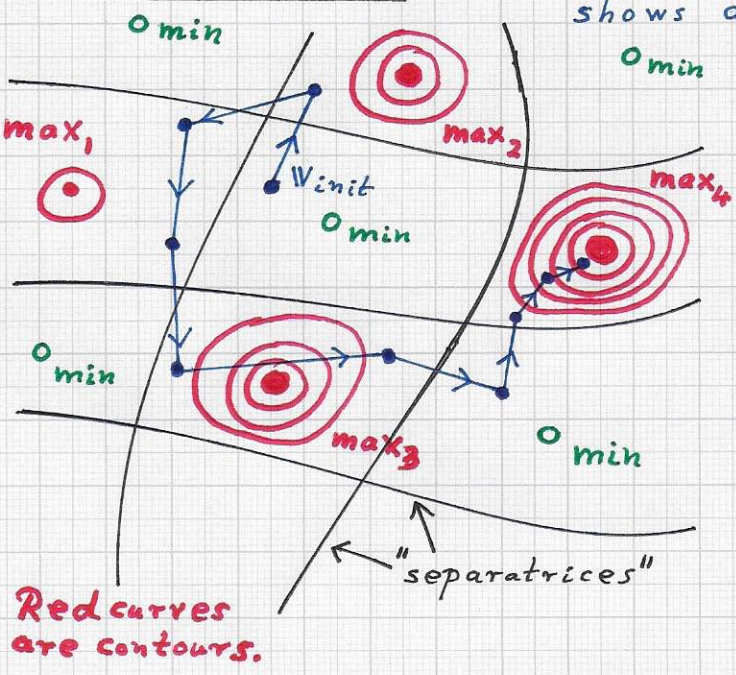
OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks: ...



The sketch included here (left) shows a two-dimensional system parameter space V. Nine sub-regions are associated with five locations "min" where the performance value of $p(V)$ is a local minimum. Of interest are the four locations "max_1", "max_2", "max_3" and "max_4" where the $p(V)$ function has local maxima. It is assumed that $p(max_4)$ is the globally maximal value of p, and that the location "max_4" must be found. (The so-called "separatrices" define the topological neighborhood relationship between the minimum- and maximum-regions. "Separatrices" are shown simply to provide structure.) The super-imposed blue polygon with directed edges visualizes a possible progression of V-tuples during the iterative simulated annealing process — starting with V_{init} and ending very close to "max_4". In this example, the algorithm performs as desired, i.e., it does not "get stuck" at local optima but it finds the global maximum — involving 10 $p(V)$ computations.

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■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

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The **WHILE loop** of the simulated annealing algorithm will always terminate since only a finite number of iterations (**maxIterations**) is permitted. The **p(W) "not good enough"** part of the termination condition can be defined in a variety of ways, for example: p(W) is not yet larger than the expected / required p_{min}-value, i.e., $p(W) \not> p_{min}$; or, considering the set of the most recently computed p(W)-values, one cannot observe a "trend" of generally improving, i.e., generally increasing, p(W)-values (keeping in mind that strict monotonically increasing p(W)-value behavior is NOT required by simulated annealing — where it is in fact permitted to accept decreasing p(W)-values. In the W parameter space, one "moves" from a current location to a new location via a **random perturbation ΔW** serving as an offset/propagation vector, i.e., $W \mapsto W + \Delta W$. Again, one can consider several possibilities to define and compute a ΔW-value: In the early stage of the simulated annealing process, at relatively higher temperature, one should permit relatively large magnitudes of ΔW-values; in the late stage, one should permit only relatively small magnitudes of ΔW-values.

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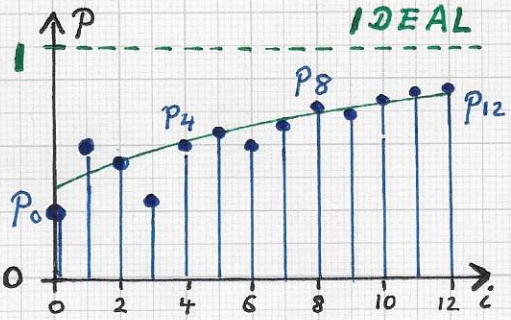
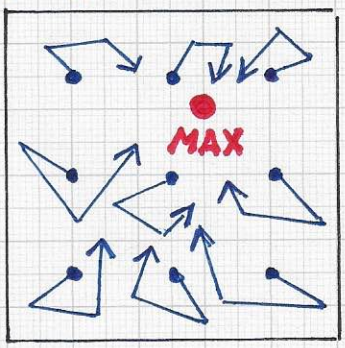
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



One can consider the values of the current temperature T, the current performance p(W), the current location of W (in the finite, bounded parameter space domain) and other values to compute ΔW. (The figure (top-Left) sketches a hypothetical, desirable progression of p_i-values, as a function of iteration index i. The general "trend" is asymptotic convergence towards the ideal p-value of one.) We compute $p(W_{new}) = p(W+\Delta W)$ and must decide whether to **accept the new W value** (or not). Simulated annealing always accepts the new W value if $p(W+\Delta W) > p(W)$; if $p(W+\Delta W) \leq p(W)$, then the new W value will be **accepted with a probability (<1)** that decreases – often in an exponentially decreasing fashion – during the progression of simulated annealing. Usually the temperature value is most important for the definition of this probability. At certain stages, one must (monotonically) **reduce the T value** ("annealing schedule"). The output will be the **values of W and p(W)**, for the best, largest value of p obtained.



Using multiple initial locations '•' to start simulated annealing.

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