Journal of Statistical Physics, Vol. 1, No. 1, 1969

Pattern Recognition and Statistical Mechanics

John M. Richardson[1]

Received March 27, 1969

A mathematical connection is established between classes of problems in pattern recognition and in statistical mechanics. More explicitly, the former class embraces problems arising from the decision-theoretic approach to the automatic recognition of certain properties of patterns containing many targets. The latter class contains almost all problems involving the statistical mechanics of classical systems of interacting particles. The usefulness of the mathematical connection lies in the fact that it provides a bridge for the transfer of approximation methodologies from one area to the other. As examples of such a transfer this paper presents applications of a least mean square approximation method, which is well known in pattern recognition, to two problems in classical statistical mechanics, namely, the one-dimensional Ising problem and the one-component plasma problem. These problems were chosen because their solutions are well understood (the exact solution of the one-dimensional Ising model and the solution of the one-component plasma that is exact in the low concentration limit are both very well known) and consequently they are appropriate as "test beds" for the new approximation method. The simplest nontrivial approximate trial functions were used for the calculation of the average values of certain observables and the results were in agreement with the corresponding exact results for the Ising model in the limit of high temperature and for the one-component plasma in the limit of low concentration.

KEY WORDS: Decision theory; Ising model; Least square estimation; Pattern recognition; Plasmas; Statistical mechanics.

1. INTRODUCTION

The decision-theoretic treatment of the recognition (or estimation) of a prescribed property of patterns involving many targets with additive noise yields *a posteriori* distribution functions (conditioned by the observation of the pattern density function) that are mathematically identical to the configurational distribution functions arising

[1] Science Center, North American Rockwell Corporation, Thousand Oaks, California 91360.

in the statistical mechanics of classical systems of interacting particles with arbitrary external forces. This mathematical connection between two different classes of problems in unrelated fields provides an interdisciplinary bridge for the transfer of approximation techniques from one field to the other. The main emphasis in the present paper is the application of the least mean square method for computing conditional averages (a well-known procedure in pattern recognition) to the treatment of mathematically isomorphic problems in classical statistical mechanics.

2. RECOGNITION OF MULTIPLE TARGET PATTERNS

Consider a class of patterns each of which contains N identical targets of known structure, but unknown positions, orientations, etc., against a noise-like background. We assume that the possible observed pattern densities are given by the stochastic model

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \sigma(\mathbf{r} - \mathbf{s}_i , \alpha_i) + \nu(\mathbf{r}) \tag{1}$$

where $\mathbf{r}$ and the $\mathbf{s}_i$ are vectors in the p-dimensional space in which the pattern is exhibited. The function $\sigma(\mathbf{r} - \mathbf{s}_i , \alpha_i)$ is the contribution to the pattern density of a target centered at the position $\mathbf{s}_i$. The symbol α_i, an n-dimensional vector, gives the internal state of target i, e.g., the orientation (if not circularly or spherically symmetric), the nature of the illumination, etc. We assume that the *a priori* distribution of the $\mathbf{s}_i$ and α_i is given by the distribution function[2]

$$P(\{\mathbf{s}_i , \alpha_i\}) \tag{2}$$

which may, for example, contain a statistical bias against targets overlapping to a significant degree. A particularly simple assumption is that the target position and internal states are completely random with no bias against overlap, in which case $P(\{\mathbf{s}_i , \alpha_i\})$ is a constant. The function $\nu(\mathbf{r})$ representing the remainder of the pattern is assumed here to be a stationary (spatially) Gaussian random process defined by the relations

$$E\nu(\mathbf{r}) = 0 \tag{3a}$$

$$E\nu(\mathbf{r})\,\nu(\mathbf{r}') = C(\mathbf{r} - \mathbf{r}') \tag{3b}$$

where E is the averaging operator and where $C(\mathbf{r} - \mathbf{r}')$ is the correlation function. One might be tempted to give a positive value to $E\nu(\mathbf{r})$ such that the probability of $\rho(\mathbf{r})$ becoming negative at any point can be made arbitrarily small. This is immaterial since we can assume that $\rho(\mathbf{r})$ is related to the physical representation of the pattern (e.g., light intensity from the face of a cathode ray tube, local transmission coefficient

[2] We will use the curly brackets { } to denote "set of." For example, $[\mathbf{s}_i , \alpha_i]$ denotes the set $\mathbf{s}_1 , \ldots, \mathbf{s}_N , \alpha^1 , \ldots, \alpha_N$. We will use $\{\rho(\mathbf{r})\}$ to denote the continuous set of values of $\rho(\mathbf{r})$ for all $\mathbf{r}$ in an appropriate domain to be defined later. It will usually be clear what parameter or variable labels the members of the set.

of a photographic transparency, etc.) by an appropriate point-to-point transformation.

We assume that the observed pattern is confined to a rectangular region Ω of $\mathbf{r}$-space. For the sake of analytic simplicity we will assume that $\sigma(\mathbf{r}, \alpha_i)$ and $\nu(\mathbf{r})$ are periodic in the entire $\mathbf{r}$-space with a period Ω. The periodicity of $\nu(\mathbf{r})$ implies of course that the correlation function $C(\mathbf{r})$ is periodic in the same sense. Although the target positions $\mathbf{s}_i$ are confined to the region Ω, the distribution function must reflect the same statistical bias (if any) against the overlap of a target with the periodic replication of a second target as against the overlap of the targets themselves. These assumptions are equivalent in every way to the periodic boundary conditions widely employed in theoretical physics.

Now the problem we wish to solve is: given an observation of the pattern density $\rho(\mathbf{r})$, what is the best estimate in a mean square sense of the value of a prescribed function of the target positions and internal states $\{\mathbf{s}_i, \alpha_i\}$? To be more explicit, let us denote the observed pattern density by $\tilde{\rho}(\mathbf{r})$ [using the language of mathematical statistics, $\tilde{\rho}(\mathbf{r})$ is a sample function of the random proces $\rho(\mathbf{r})$]. Let us assume that the prescribed function is

$$\phi(\{\mathbf{s}_i, \alpha_i\}) \tag{4}$$

and let the estimator be

$$\hat{\phi}(\{\tilde{\rho}(\mathbf{r})\}) \tag{5}$$

which is as yet an arbitrary functional of the observed pattern density $\tilde{\rho}(\mathbf{r})$. The problem of choosing the optimal form of $\hat{\phi}(\{\tilde{\rho}(\mathbf{r})\})$ involves minimizing the difference between $\hat{\phi}$ and ϕ in some sense. In order that $\hat{\phi}$ and ϕ deviate from each other as little as possible for a large number of reasonably probable cases, we will minimize the mean square error

$$E[\hat{\phi}(\{\rho(\mathbf{r})\}) - \phi(\{\mathbf{s}_i, \alpha_i\})]^2 \tag{6}$$

in which we have substituted the random process $\rho(\mathbf{r})$ given by (1) for $\tilde{\rho}(\mathbf{r})$. The averaging operation involves of course all random variables and random processes, i.e., $\{\mathbf{s}_i, \alpha_i\}$ and $\nu(\mathbf{r})$.

3. EXACT SOLUTION OF THE RECOGNITION PROBLEM

The minimization problem (6) has a solution that is well known in decision theory,[3] namely, that the optimal $\hat{\phi}$ is given by

$$\hat{\phi}(\{\tilde{\rho}(\mathbf{r})\}) = E(\phi(\{\mathbf{s}_i, \alpha_i\}) \mid \{\tilde{\rho}(\mathbf{r})\}) \tag{7}$$

[3] See, for example, T. S. Ferguson, *Mathematical Statistics, A Decision Theoretic Approach*, Academic Press, New York and London (1967).

where $E(\phi \mid \{\tilde{\rho}\})$ is the *a posteriori* average of ϕ conditioned by the observation of the function $\rho(\mathbf{r})$ for all $\mathbf{r} \in \Omega$. We can rewrite (7) in the form

$$\hat{\phi}(\{\tilde{\rho}\}) = \int \prod_{i=1}^{N} d\mathbf{s}_i \, d\alpha_i \phi(\{\mathbf{s}_i , \alpha_i\}) \, P(\{\mathbf{s}_i , \alpha_i\} \mid \{\tilde{\rho}\}) \tag{8}$$

where $P\{\mathbf{s}_i , \alpha_i\} \mid \{\tilde{\rho}\})$ is the *a posteriori* distribution of the target positions and internal states $\{\mathbf{s}_i , \alpha_i\}$ conditioned by the inequality $\mid \rho(\mathbf{r}) - \tilde{\rho}(\mathbf{r})\mid < \delta$, $\mathbf{r} \in \Omega$.

In order to write this distribution in a compact form it is necessary to introduce additional notation. We will define the inner product of two quadratically integrable functions $u(\mathbf{r})$ and $v(\mathbf{r})$ by

$$(u, v) = \int_{\Omega} d\mathbf{r} \int_{\Omega} d\mathbf{r}' u(\mathbf{r}) \, D(\mathbf{r} - \mathbf{r}') \, v(\mathbf{r}') \tag{9}$$

where $D(\mathbf{r} - \mathbf{r}')$ is the inverse correlation function defined by

$$\int_{\Omega} d\mathbf{r}' C(\mathbf{r} - \mathbf{r}') \, D(\mathbf{r} - \mathbf{r}'') = \delta(\mathbf{r} - \mathbf{r}'') \tag{10}$$

where $\delta(\mathbf{r} - \mathbf{r}'')$ is the δ-function in the p-dimensional $\mathbf{r}$ space. The norm corresponding to (u, v) is of course defined by

$$\| u \| = (u, u)^{1/2} \tag{11}$$

The Gaussian distribution function $P(\{\nu(\mathbf{r})\})$ (unnormalized in the function space) can now be written:

$$\log P(\{\nu(\mathbf{r})\}) = -\tfrac{1}{2} \| \nu \|^2 \tag{12}$$

To obtain the *a posteriori* distribution function of $\{\mathbf{s}_i , \alpha_i\}$ we perform a functional integration of $P(\{\nu(\mathbf{r})\}) \, P(\{\mathbf{s}_i , \alpha_i\})$ on $\nu(\mathbf{r})$ constrained by the condition $\mid \rho - \tilde{\rho} \mid < \delta$, $\mathbf{r} \in \Omega$, finally obtaining (after $\delta \to 0$)

$$\log P(\{\mathbf{s}_i , \alpha_i\} \mid \{\tilde{\rho}\}) = -\frac{1}{2} \left\| \tilde{\rho} - \sum_{i=1}^{N} \sigma_i \right\|^2 + \log P(\{\mathbf{s}_i , \alpha_i\}) + \log A \tag{13}$$

where A is determined by the normalization condition

$$\int \prod d\mathbf{s}_i \, d\alpha_i P(\{\mathbf{s}_i , \alpha_i\} \mid \{\rho\}) = 1 \tag{14}$$

The symbol σ_i is an abbreviated notation for $\sigma(\mathbf{r} - \mathbf{s}_i , \alpha_i)$.

4. DIRECT VARIATIONAL APPROACH

When the exact solution (7) cannot be reduced to a form that is computable in a practical sense (this is unfortunately almost always the case), approximate approaches must be employed. There are two possible kinds of approaches. One is to apply approximation methods to the exact solution (7). The other kind of approach—the

one to be emphasized in the present paper—is to go back to the problem of minimizing the mean square error and employ direct variational methods.

A typical procedure is to consider a limited class of possible estimators labeled by a vector parameter γ, say $\phi(\{\tilde{\rho}\}, \gamma)$, and then minimize the corresponding mean square error

$$E[\hat{\phi}(\{\rho\}, \gamma) - \phi(\{\mathbf{s}_i , \alpha_i\})]^2 \tag{15}$$

with respect to γ.

From a practical calculational point of view it is desirable to consider equivalent forms of the variational problem (6). One equivalent form is the minimization of

$$Ew(\{\rho\})[\hat{\phi}(\{\rho\}) - \phi(\{\mathbf{s}_i , \alpha_i\})]^2 \tag{16}$$

where the weighting functional $w(\{\rho\})$ is positive. It can be readily proved that the exact solution of the minimization of (16) is independent of w and therefore it is given by (7). It is possible to make w depend on the form of $\hat{\phi}$, but only *after* the minimization has been carried out. The above equivalent variations of the original minimization problem provide a much broader basis for approximation techniques.

5. THE CLASSICAL STATISTICAL MECHANICS OF INTERACTING PARTICLES

In the present section we will show that the exact solution of the problem of the recognition of multiple target patterns discussed in the previous sections is mathematically identical to the problem of calculating the average value of a certain observable in a canonical ensemble of classical systems of interacting particles. We will demonstrate this by further analysis of $P(\{\mathbf{s}_i , \alpha_i\} \mid \{\tilde{\rho}\})$ given by (13). For the sake of simplicity let us confine our discussion to the case in which the *a priori* distribution of the target positions and internal states, i.e., $P(\{\mathbf{s}_i , \alpha_i\})$ is constant. Equation (13) can now be written as

$$\log P(\{\mathbf{s}_i , \alpha_i\} \mid \{\tilde{\rho}\}) = -\frac{1}{2}\sum_{ij}{}' (\sigma_i , \sigma_j) + \sum_i (\sigma_i , \tilde{\rho}) + f \tag{17}$$

where

$$f = -\frac{1}{2}\sum_i \| \sigma_i \|^2 - \frac{1}{2}\| \tilde{\rho} \|^2 + B \tag{18}$$

where in turn B is a constant independent of ρ and $\{\mathbf{s}_i , \alpha_i\}$. The prime on the summation denotes the avoidance of terms for which $i = j$.

Now let us further examine the terms in the above expression. The terms (σ_i , σ_j) can be written more fully in the form

$$\begin{aligned}(\sigma_i , \sigma_j) &= \int_\Omega d\mathbf{r} \int_\Omega d\mathbf{r}' \sigma(\mathbf{r} - \mathbf{s}_i , \alpha_i)\, D(\mathbf{r} - \mathbf{r}')\, \sigma(\mathbf{r}' - \mathbf{s}_j , \alpha_j) \\ &= \int_\Omega d\mathbf{r} \int_\Omega d\mathbf{r}' \sigma(\mathbf{r}, \alpha_i)\, D(\mathbf{r} - \mathbf{r}')\, \sigma(\mathbf{r}' - \mathbf{s}_j + \mathbf{s}_i , \alpha_j) \\ &\equiv v^{(2)}(\mathbf{s}_i - \mathbf{s}_j , \alpha_i , \alpha_j)\end{aligned} \tag{19}$$

The dependence of $v^{(2)}$ on the functional forms of D and σ are not explicitly noted. This result was obtained by replacing $\mathbf{r}$ and $\mathbf{r}'$ by $\mathbf{r} + \mathbf{s}_i$ and $\mathbf{r}' + \mathbf{s}_i$, respectively, and by using the fact that $D(\mathbf{r})$ and $\sigma(\mathbf{r})$ are periodic with period Ω. It is clear that $v^{(2)}(\mathbf{s}_i - \mathbf{s}_j, \alpha_i, \alpha_j)$ is a periodic function of $\mathbf{s}_i - \mathbf{s}_j$ with the same period. Although it is impossible for a periodic function to be isotropic (i.e., spherically symmetric), it is nevertheless possible for $v^{(2)}$ to be isotropic in a limited region if that region is contained within the region Ω. It is obvious that $\| \sigma_i \|^2 = (\sigma_i, \sigma_i)$ is independent of $\mathbf{s}_i$, but in general depends on α_i. The term $(\sigma_i, \tilde{\rho})$ can be written

$$\begin{aligned}(\sigma_i, \tilde{\rho}) &= \int_\Omega d\mathbf{r} \int_\Omega d\mathbf{r}' \sigma(\mathbf{r} - \mathbf{s}_i, \alpha_i)\, D(\mathbf{r} - \mathbf{r}')\, \tilde{\rho}(\mathbf{r}') \\ &= \int_\Omega d\mathbf{r} \int_\Omega d\mathbf{r}' \sigma(\mathbf{r}, \alpha_i)\, D(\mathbf{r} - \mathbf{r}')\, \tilde{\rho}(\mathbf{r}' + \mathbf{s}_i) \\ &\equiv -v^{(1)}(\mathbf{s}_i, \alpha_i)\end{aligned} \tag{20}$$

using procedures similar to those used in (19). We can now write (17) in the form

$$\log P(\{\mathbf{s}_i, \alpha_i\} \mid \{\rho\}) = -\frac{1}{2}{\sum_{ij}}' v^{(2)}(\mathbf{s}_i - \mathbf{s}_j, \alpha_i, \alpha_j) - \sum_i v^{(1)}(\mathbf{s}_i, \alpha_i) + f \tag{21}$$

The quantity f given by (18) contains the term

$$-\frac{1}{2}\sum_i \| \sigma_i \|^2 \tag{22}$$

which, as we have already stated, is independent of the $\mathbf{s}_i$ but may in some cases depend on the α_i.

The reader will note that (21) is identical to the configurational distribution function associated with the canonical distribution of classical particles involving binary interactions and acted upon by an arbitrary external force. From this point of view $\beta^{-1}v^{(2)}(\mathbf{s}_i - \mathbf{s}_j, \alpha_i, \alpha_j)$ can be regarded as the interaction potential between particles i and j located at positions $\mathbf{s}_i$ and $\mathbf{s}_j$, and having internal states α_i and α_j. In the expression above $\beta^{-1} = kT$, where k is the Boltzmann factor and T is the absolute temperature. Similarly, $\beta^{-1}v^{(1)}(\mathbf{s}_i, \alpha_i)$ can be regarded as the contribution of the external force to the potential energy of particle i having position $\mathbf{s}_i$ and internal state α_i.

It is quite possible that, if the interaction energy $\beta^{-1}v^{(2)}$ is chosen in advance without any concern for the corresponding pattern recognition problem, it may be inconsistent with (19). A necessary and sufficient condition that a $v^{(2)}$ chosen in advance be consistent with (19) is that $v^{(2)}$ be positive indefinite in the sense that

$$\int d\mathbf{s}_1\, d\alpha_1 \int d\mathbf{s}_2\, d\alpha_2 u(\mathbf{s}_1, \alpha_1)\, v^{(2)}(\mathbf{s}_1 - \mathbf{s}_2, \alpha_1, \alpha_2)\, u(\mathbf{s}_2, \alpha_2) \geqslant 0 \tag{23}$$

for any real function $u(\mathbf{s}, \alpha)$. An equivalent condition is that the spatial Fourier transform of $v^{(2)}$ be nonnegative definite with respect to the variables α_1 and α_2.

We hasten to remark that such a condition does not imply that $v^{(2)}$ must be non-negative everywhere. It is possible that $v^{(2)}$ can represent a typical potential with mutual attraction for large and repulsion for small separation distances. The non-negativity of the Fourier transform of $v^{(2)}$ is achieved by having the potential sufficiently large and positive for small distances, Wherever $v^{(2)} \gg 1$, i.e., $\beta^{-1}v^{(2)} \gg kT$, it does not matter how large it is. For example, if $v^{(2)} = 10$ for a certain configuration given by the position $\mathbf{s}_1$ and $\mathbf{s}_2$, then the corresponding probabilities will be e^{10} times smaller than at another configuration where $v^{(2)} \simeq 0$. Increasing $v^{(2)}$ by a factor of 2, say, at the former configuration makes very little difference since a relative probability of e^{-10} is already so small that a revised value of e^{-20} would make essentially no difference in any averaged observable of physical significance.

In statistical mechanics we will also be interested in cases of *a priori* distributions other than $P(\{\mathbf{s}_i, \alpha_i\}) = \text{const}$. For example, if we wish to localize each particle to a lattice site x_i, we would write

$$P(\{\mathbf{s}_i, \alpha_i\}) = P(\{\alpha_i\}) \prod_{\delta} \delta(\mathbf{s}_j - \mathbf{x}_j) \tag{24}$$

Another case is one where hard sphere repulsion is to be accounted for without allowing $v^{(2)}$ to become unbounded. Here, for example, one could take

$$\begin{aligned} P(\{\mathbf{s}_i, \alpha_i\}) &= \text{const}, \qquad |\mathbf{s}_i - \mathbf{s}_j| \geqslant a, \qquad \text{for all pairs } ij, \qquad i \neq j \\ &= 0 \quad \text{otherwise} \end{aligned} \tag{25}$$

Other examples involve special assumptions concerning the parameters α_i. For instance, if one wishes to cancel out the terms $\sum \| \sigma_i \|^2$ in f given by (22), one can include a compensating factor in $P(\{\mathbf{s}_i, \alpha_i\})$, namely, $\exp(\frac{1}{2} \sum \| \sigma_i \|^2)$. In this way one can eliminate potential self-energies dependent on the α_i. Such a factor may destroy the normalizability of this distribution; however, this is unimportant since all that actually matters is the normalizability of $P(\{\mathbf{s}_i, \alpha_i\} \mid \{\tilde{\rho}\})$ and existence of the corresponding average value of ϕ.

If the statistical mechanical objective is the calculation of the average value of some observable $\phi(\{\mathbf{s}_i, \alpha_i\})$, we have a problem with mathematically the same end objective as in the pattern recognition case. In the latter case the problem is to calculate the conditional average of the property ϕ, namely, $E(\phi \mid \{\rho\})$, and in the former it is to calculate the average of ϕ using the distribution function given in (21). Since the distribution function is actually $P(\{\mathbf{s}_i, \alpha_i\} \mid \{\rho\})$ using the notation pertaining to the pattern recognition case, it is clear that the averages of ϕ in the statistical mechanics and pattern recognition cases are identical if the proper correspondences have been made between the basic quantities in the two cases.

6. COMMENTS

We have thus established a mathematical connection between two apparently unrelated groups of problems, one group lying in the pattern recognition field, and

the other in the classical statistical mechanics field. With very few exceptions the problems in each group are equally insoluble.

The two fields have hitherto evolved completely idependently of each other, so that at the present time two sets of approximation methodologies have been built up with rather little overlap. The value of the mathematical connection is to make the approximation methodologies of each field available to the other. As an example of methodological transfer, we present in the next two sections examples of the application of the approximate mean square optimization of estimators, a very well known technique in pattern recognition, to two problems in statistical mechanics: the one-dimensional Ising model and the system of charged particles in a uniform background of compensating charge.

7. THE ONE-DIMENSIONAL ISING MODEL

The one-dimensional Ising model[4] is perhaps the simplest system of interacting particles amenable to exact treatment. In this system particles are situated at the discrete set of points labeled by n. The particle at the point n has two internal states $\alpha_n = \pm 1$. The energy of the system is assumed to be

$$U = \epsilon \sum_{n=1}^{N} \alpha_n \alpha_{n+1} + \sum_{n=1}^{N} b_n \alpha_n \tag{26}$$

where it is understood that $\alpha_{N+1} = \alpha_1$.

The partition function is given by

$$\sum_{\{\alpha_n\}} \exp(-\beta U) \equiv Z(\beta, \{b_n\}) \tag{27}$$

where, of course, the summation is over all values $\alpha_1 = \pm 1$, $\alpha_2 = \pm 1$,..., $\alpha_N = \pm 1$. The partition function can be evaluated by rewriting (27) in terms of the matrix $M(\beta, b)$ whose elements are given by

$$\langle \alpha_n \mid M(\beta, b) \mid \alpha_{n+1} \rangle = \exp[-\beta(\epsilon \alpha_n \alpha_{n+1} + b\alpha_n)] \tag{28}$$

in which case (27) reduces to

$$Z(\beta, \{b_n\}) = \operatorname{Tr} M(\beta, b_1)\, M(\beta, b_2) \cdots M(\beta, b_N) \tag{29}$$

If all of the b_i are assigned the common value b, the partition function is easy to evaluate by going over to a representation in which $M(\beta, b)$ is diagonal. In particular, for $b = 0$, we obtain for N large

$$Z(\beta, \{0\}) = (2 \cosh \beta\epsilon)^N \tag{30}$$

[4] For a comprehensive review of investigations of the Ising model, see G. F. Newell and E. W. Montroll, *Rev. Mod. Phys.* **25**:353–389 (1953).

One can use somewhat more elaborate matrix techniques to evaluate the average of α_n due to an external force acting only at m (i.e., $b_m \neq 0$, $b_n = 0$ for $n \neq m$). We obtain for large N

$$E\alpha_n = -(-\tanh \beta\epsilon)^{|m-n|} \tanh \beta b_m \tag{31}$$

This result is valid in the form given if m is large compared with the correlation length $(-\log | \tanh \beta\epsilon |)^{-1}$. If both $\beta\epsilon$ and βb_m are small compared with unity, the last result reduces to

$$E\alpha_n = -(-\beta\epsilon)^{|m-n|}\beta b_m \tag{32}$$

a result we will later reproduce using an approximation technique imported from the pattern recognition domain.

As a preliminary to the accomplishment of the last objective we consider the relation

$$\rho(x) = \sum_{n=1}^{N} \alpha_n \sigma(x - n) + \nu(x) \tag{33}$$

where the α_n are independent random variables each assuming the values ± 1 with equal *a priori* probability. The function $\nu(x)$ is a stationary Gaussian random process defined by the relations

$$E\nu(x) = 0, \qquad E\nu(x)\,\nu(x') = \beta^{-1}\delta(x - x') \tag{34}$$

We require $\nu(x)$ and $\sigma(x)$ to be periodic with period N.

Equation (33) is a special case of (7) if we assume that $p = 1$ and $C(x - x') = \beta^{-1}\delta(x - x')$, and that the distribution function (8) is given by

$$P(\{s_n\,,\, \alpha_n\}) = 2^{-N} \prod_n \delta(s_n - n)[\delta(\alpha_n - 1) + \delta(\alpha_n + 1)] \tag{35}$$

We will define the inner product of two arbitrary functions $u(x)$ and $v(x)$ by

$$(u, v) = \beta \int_0^N dx\, u(x)\, v(x) \tag{36}$$

and the corresponding norm by

$$\| u \| = (u, u)^{1/2} \tag{37}$$

The *a posteriori* or conditional distribution of the $\{\alpha_i\}$, given that $\rho = \tilde{\rho}$, can be written

$$\begin{aligned} \log P(\{\alpha_n\} \mid \{\tilde{\rho}(x)\}) &= \frac{1}{2} \left\| \tilde{\rho}(x) - \sum_n \alpha_n \sigma(x - n) \right\|^2 \\ &= -\beta \left(\frac{1}{2} \sum_{mn}{}' \epsilon_{mn}\alpha_m\alpha_n + \sum_n b_n\alpha_n \right) + g \end{aligned} \tag{38}$$

where

$$\epsilon_{mn} = \int_0^N dx\, \sigma(x - m)\, \sigma(x - n) \tag{39}$$

$$b_n = -\int_0^N dx\, \sigma(x - n)\, \tilde{\rho}(x) \tag{40}$$

The summations involve all values n, $m - 1,\ldots, N$ except for the fact that the prime on the double summation denotes the elimination of terms for which $m = n$. The additional quanity is given by

$$g = -\frac{1}{2} \| \tilde{\rho} \|^2 - \frac{1}{2} \sum_n \| \sigma(x - n) \|^2 + B \tag{41}$$

where B is a normalization constant. It is obvious that g is independent of the α_n and therefore it can be treated as an alternative normalization constant. It is further clear that (38) is the distribution function corresponding to the canonical ensemble of systems where energy U is given by (26) if

$$\begin{aligned} \epsilon_{nm} &= \epsilon, \qquad | n - m | = 1 \\ &= 0, \qquad | n - m | > 1 \end{aligned} \tag{42a}$$

with the exception that when $n = 1$, $m = N$, and *vice versa*, we assume

$$\epsilon_{1N} = \epsilon_{N1} = \epsilon \tag{42b}$$

In this case we obtain

$$\frac{1}{2} \sum{}' \epsilon_{mn} \alpha_m \alpha_n = \epsilon \sum_{n=1}^{N} \alpha_n \alpha_{n+1} \tag{43}$$

where it is understood that $\alpha_{N+1} = \alpha_1$. Thus it is clear that aside from a multiplicative constant $P(\{\alpha_n\} \mid \{\rho\})$ given by (38) and $\exp(-\beta U\}$ with U given by (26) are equal. It is to be noted that ϵ_{nn} does not enter the problem. We cannot take $\epsilon_{nn} = 0$, because this would be inconsistent with (39).

In the problem of least mean square estimation we attempt to estimate the observables α_n of interest and denote by $\hat{\alpha}_n = \hat{\alpha}_n(\{\rho\})$ the corresponding estimators. By inspection of (38) we see that the average value of any function of the α_n must dependend on $\tilde{\rho}(x)$ only through the discrete set of quantities b_n given by (40). Therefore, we will henceforth consider only estimators of the form $\hat{\alpha}_n = \hat{\alpha}_n(\{b_n\})$. In the minimization of the mean square deviation of $\hat{\alpha}_n$ from α_n, i.e.,

$$E(\hat{\alpha}_n - \alpha_n)^2 \tag{44}$$

where it is understood that in $\hat{\alpha}_n$ the b_m entail the substitution of $\tilde{\rho}(x)$ by $\rho(x)$ and where the *a priori* averaging operator E involves the random variables $\{\alpha_n\}$ and the random process $\nu(x)$ with no conditioning by $\tilde{\rho}(x)$. As we have already stated in Section 3, the exact solution of the minimization problem is obtained by setting $\hat{\alpha}_n$

equal to the *a posteriori* (conditional) average of α_n, namely, $\hat{\alpha}_n = E(\alpha_n \mid \{\tilde{\rho}\})$, which is the same as averaging α_n using the distribution (38).

We now consider this minimization problem using an approximate form of $\hat{\alpha}_n$ with adjustable parameters. Let us assume

$$\hat{\alpha}_n = c_n + \beta \sum_m a_{nm} b_m \tag{45}$$

and attempt to minimize (44) with respect to the adjustable parameters c_n and a_{nm}. We obtain the moment equations

$$\begin{aligned} E(\hat{\alpha}_n - \alpha_n) &= 0 \\ E(\hat{\alpha}_n - \alpha_n)\, b_p &= 0 \end{aligned} \tag{46}$$

from which we obtain

$$c_n = 0 \tag{47}$$

and

$$\sum_n a_{nm} \left(\beta \sum_q \epsilon_{mq} \epsilon_{qp} + \epsilon_{mp} \right) = -\epsilon_{np} \tag{48}$$

Multiplying (48) on the right by the inverse of the matrix ϵ_{nm} we obtain

$$\sum_m a_{nm} (\beta \epsilon_{mp} + \delta_{mp}) = -\delta_{np} \tag{49}$$

Using the invariance to translations (in the sense of periodic boundary conditions) by integral steps, it is clear that ϵ_{nm}, and hence a_{nm}, can be diagonalized by going over to a representation defined by the basis vectors

$$N^{-1/2} e^{ikn} \tag{50}$$

where $k = 2\pi\mu/N$, $\mu = 0, \ldots, N-1$. Defining

$$\begin{aligned} a_k &= N^{-1} \sum_{mn} e^{-ikm}\, a_{mn}\, e^{ikn} \\ \epsilon_k &= N^{-1} \sum_{mn} e^{-ikm}\, \epsilon_{mn}\, e^{ikn} \end{aligned} \tag{51}$$

we then obtain the inverse equations

$$\begin{aligned} a_{mn} &= N^{-1} \sum_k e^{ikm}\, a_k\, e^{-ikn} \\ \epsilon_{mn} &= N^{-1} \sum_k e^{ikm}\, \epsilon_k\, e^{-ikn} \end{aligned} \tag{52}$$

If we use a_{mn} and ϵ_{mn} given by (52), Eq. (49) reduces to

$$a_k(\beta \epsilon_k + 1) = -1 \tag{53}$$

from which we finally obtain

$$a_{mn} = -N^{-1} \sum_k e^{ikm}(\beta\epsilon_k + 1)^{-1} e^{-ikn} \tag{54}$$

the desired answer. From (39) it follows that ϵ_{mn} is symmetric, and hence (49) implies that a_{mn} is also symmetric. Therefore, (54) can be rewritten as

$$a_{mn} = -N^{-1} \sum e^{ik|m-n|}(\beta\epsilon_k + 1)^{-1} \tag{55}$$

Thus the response at the point m due to a force at n depends only on the magnitude of the distance from n to m, i.e., $| m - n |$, as one would expect.

In the limit $N \to \infty$, k becomes a continuous variable and the summation is replaced by an integration, whereupon (54) reduces to

$$a_{mn} = -\frac{1}{2\pi} \int_0^{2\pi} dk e^{ik|m-n|}(1 + \epsilon_k)^{-1} \tag{56}$$

It is convenient to introduce the complex variable $z = e^{ik}$ with a corresponding introduction of a new function $\epsilon(z) = \epsilon_k$. In terms of the new variable we can write

$$a_{mn} = -\frac{1}{2\pi i} \int_\Gamma dz\, z^{|m-n|-1}(\beta\epsilon(z) + 1)^{-1} \tag{57}$$

where Γ denotes the unit circle in the complex z-plane.

Let us consider the case where ϵ is positive. It is easy to verify that if we assume

$$\sigma(x) = \epsilon^{1/2} \sum_{q=-\infty}^{\infty} \Lambda(x - qN) \tag{58}$$

where

$$\begin{aligned} \Lambda(x) &= 1, \qquad | x | \leqslant 1 \\ &= 0, \qquad | x | > 1 \end{aligned} \tag{59}$$

then (39) yields ϵ_{mn} in agreement with the assumptions (42a) and (42b). We then obtain

$$\begin{aligned} \epsilon_k &= 2\epsilon(1 + \cos k) \\ &= \epsilon(2 + z + z^{-1}) \end{aligned} \tag{60}$$

Substitution of (60) into (57) yields

$$a_{mn} = -\frac{1}{\sqrt{1 + 4\beta\epsilon}} (z_+)^{|m-n|} \tag{61}$$

where

$$\begin{aligned} z_+ &= -\frac{1}{2\beta\epsilon}(1 + 2\beta\epsilon - \sqrt{1 + 4\beta\epsilon}) \\ &= -\beta\epsilon + o(\beta^2\epsilon^2) \end{aligned} \tag{62}$$

When $\beta\epsilon \ll 1$, Eq. (61) reduces to

$$a_{mn} = -(-\beta\epsilon)^{|m-n|} \tag{63}$$

Thus in this limit we obtain

$$\begin{aligned} E\alpha_n &= \beta \sum_m a_{nm} b_m \\ &= -\sum_m (-\beta\epsilon)^{|m-n|} \beta b_m \end{aligned} \tag{64}$$

In the special case in which all of the b_p's vanish except for b_m, Eq. (64) reduces to

$$E\alpha_n = (-\beta\epsilon)^{|m-n|} \beta b_m \tag{65}$$

in perfect agreement with the exact result when $\beta\epsilon$ and βb_m are small compared with unity, namely, Eq. (32).

The case of negative ϵ can be treated by replacing $\Lambda(x)$ defined in (59) by another function $M(x)$, where

$$\begin{aligned} M(x) &= 1, \qquad 0 < x \leqslant 1 \\ &= -1, \qquad -1 \leqslant x \leqslant 0 \\ &= 0, \qquad |x| > 1 \end{aligned} \tag{66}$$

It is not correct simply to change the sign of ϵ in (60).

8. ONE-COMPONENT CLASSICAL PLASMA

We consider a classical system of charged particles of one kind with a uniform smear of compensating charge. Let us assume that a particle at the origin is modeled by an extended charge distribution $\tau(\mathbf{r})$, where $\mathbf{r}$ is a three-dimensional position vector. If the total charge of each particle is e, we require

$$\int d\mathbf{r}\, \tau(\mathbf{r}) = e \tag{67}$$

The interaction potential for two isolated particles and positions $\mathbf{s}_1$ and $\mathbf{s}_2$ is then

$$\int d\mathbf{r}_1 \int d\mathbf{r}_2\, \tau(\mathbf{r}_1 - \mathbf{s}_1)\, |\, \mathbf{r}_1 - \mathbf{r}_2\, |^{-1}\, \tau(\mathbf{r}_2 - \mathbf{s}_2) \tag{68}$$

However, this is not the whole story. We wish to introduce periodic boundary conditions. Let us assume that the system is confined to the cubic volume Ω defined by the inequalities $0 \leqslant x_i \leqslant L$, $i = 1, 2, 3$, where the x_i are the components of $\mathbf{r}$, i.e., $\mathbf{r} = (x_1, x_2, x_3)$. Let us consider the lattice of points $\mathbf{R}$ defined by

$$\mathbf{R} = (Ln_1, Ln_2, Ln_3) \tag{69}$$

where each n_i assumes all integral values (positive and negative). In order to achieve both periodicity and a uniform compensating charge, we associate with each particle the charge distribution

$$\sigma(r) = \sum_R \tau(\mathbf{r} - \mathbf{R}) - e\Omega^{-1} \tag{70}$$

where the symbol Ω is also used to denote the volume of the region Ω (i.e., $\Omega = L^3$). It is easy to show that

$$\int_\Omega d\mathbf{r}\, \sigma(\mathbf{r}) = 0 \tag{71}$$

thus, each particle carries its own compensating uniform distribution. The expression (68) is now to be replaced by

$$\begin{aligned} &\int_\Omega d\mathbf{r}_1 \int_\infty d\mathbf{r}_2\, \sigma(\mathbf{r}_1 - \mathbf{s}_1) \mid \mathbf{r}_1 - \mathbf{r}_2 \mid^{-1} \sigma(\mathbf{r}_2 - \mathbf{s}_2) \\ &\quad = \int_\Omega d\mathbf{r}_1 \int_\Omega d\mathbf{r}_2\, \sigma(\mathbf{r}_1 - \mathbf{s}_1) \sum_R \mid \mathbf{r}_1 - \mathbf{r}_2 - \mathbf{R} \mid^{-1} \sigma(\mathbf{r}_2 - \mathbf{s}_2) \qquad (72 \\ &\quad \equiv v^{(2)}(\mathbf{s}_1 - \mathbf{s}_2) \end{aligned}$$

Although the above integral converges, the kernel does not converge by itself. However, one can construct another function

$$\Delta(\mathbf{r}_1 - \mathbf{r}_2) = \frac{4\pi}{\Omega} \sum_{\mathbf{k}}{}' k^{-2} e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}^2)} \tag{73}$$

that does exist and can replace $\sum_R \mid \mathbf{r}_1 - \mathbf{r}_2 - \mathbf{R} \mid^{-1}$ in the integral on the second line of (72) withput changing its value. In (73) the summation is over all integral values of m_1, m_2, and m_3 in

$$\mathbf{k} = \left(\frac{2\pi m_1}{L}, \frac{2\pi m_2}{L}, \frac{2\pi m_3}{L}\right) \tag{74}$$

and the prime on the summation denotes the absence of the $\mathbf{k} = 0$ term. Therefore we will henceforth use the definition

$$v^{(2)}(\mathbf{s}_1 - \mathbf{s}_2) \equiv \int_\Omega d\mathbf{r}_1 \int_\Omega d\mathbf{r}_2\, \sigma(\mathbf{r}_1 - \mathbf{s}_1)\, \Delta(\mathbf{r}_1 - \mathbf{r}_2)\, \sigma(\mathbf{r}_2 - \mathbf{s}_2) \tag{75}$$

in all further work.

The contribution of an arbitrary external potential $\psi(\mathbf{r})$, not necessarily a solution of Laplace's equation, to the potential energy of a particle at $\mathbf{s}$ can be written as

$$\int_\Omega d\mathbf{r}\, \tau(\mathbf{r} - \mathbf{s})\, \psi(\mathbf{r}) \tag{76}$$

If ψ is periodic with period Ω, the last expression differs from

$$\int_{\Omega} d\mathbf{r}\, \sigma(\mathbf{r} - \mathbf{s})\, \psi(\mathbf{r}) \equiv v^{(1)}(\mathbf{s}) \tag{77}$$

by a constant independent of $\mathbf{s}$.

The total potential energy of a system of N particles is clearly

$$U = \frac{1}{2} \sum_{i,j=1}^{N}{}' v^{(2)}(\mathbf{s}_i - \mathbf{s}_j) + \sum_{i=1}^{N} v^{(1)}(\mathbf{s}_i) \tag{78}$$

and the corresponding canonical distribution function is proportional to $\exp(-\beta U)$.

To proceed with our approximation method, we consider

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \sigma(\mathbf{r} - \mathbf{s}_i) + \nu(\mathbf{r}) \tag{79}$$

where $\sigma(\mathbf{r})$ is defined by (70). We assume that the positions $\mathbf{s}_i$ are uniformly distributed in the region Ω. The function $\nu(\mathbf{r})$ is a stationary (spatially) Gaussian random process that is periodic with period Ω. We have defined $\sigma(\mathbf{r})$ in such a way that

$$\int_{\Omega} d\mathbf{r}\, \sigma(\mathbf{r}) = 0 \tag{80}$$

We now impose the same condition on $\nu(\mathbf{r})$, namely,

$$\int_{\Omega} d\mathbf{r}\, \nu(\mathbf{r}) = 0 \tag{81}$$

We further assume that

$$\begin{aligned} E\nu(\mathbf{r}) &= 0 \\ E\nu(\mathbf{r})\, \nu(\mathbf{r}') &= C(\mathbf{r} - \mathbf{r}') \\ &= -\frac{1}{4\pi\beta} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \end{aligned} \tag{82}$$

for $\mathbf{r}, \mathbf{r}' \in \Omega$. In calculating the inverse correlation function we must allow for the fact that all functions are subject to constraints of the type (80) and (81); in other words, the uniform functions have been projected out of function space. Therefore, the inverse correlation function $D(\mathbf{r})$ is given by

$$\int_{\Omega} d\mathbf{r}' C(\mathbf{r} - \mathbf{r}')\, D(\mathbf{r}' - \mathbf{r}'') = \delta(\mathbf{r} - \mathbf{r}'') - \Omega^{-1} \tag{83}$$

reflecting the fact that the uniform part of the δ-function has been projected out. With $C(\mathbf{r} - \mathbf{r}')$ given by (82), we obtain the solution

$$D(\mathbf{r}) = \beta \Delta(\mathbf{r}) \tag{84}$$

where $\Delta(\mathbf{r})$ is defined by (73).

Let us define the inner product

$$(u, v) = \int_{\Omega} d\mathbf{r} \int_{\Omega} d\mathbf{r}' u(\mathbf{r})\, D(\mathbf{r} - \mathbf{r}')\, v(\mathbf{r}') \tag{85}$$

with the corresponding norm $\| u \| = (u, u)^{1/2}$. It is easy to show that the *a posteriori* distribution function given by

$$\log P(\{\mathbf{s}_i\} \mid \{\tilde{\rho}(\mathbf{r})\}) = -\frac{1}{2} \left\| \tilde{\rho} - \sum \sigma_i \right\|^2 + \text{const} \tag{86}$$

where $\sigma_i = \sigma(\mathbf{r} - \mathbf{s}_i)$ is proportional to the canonical distribution function $\exp(-\beta U)$, where U is given by (78), if we assume that

$$\int_{\Omega} d\mathbf{r}\, \Delta(\mathbf{r} - \mathbf{r}')\, \rho(\mathbf{r}') = -\psi(\mathbf{r}) \tag{87}$$

The term (σ_i, σ_j) is obviously equal to $\beta v^{(2)}(\mathbf{s}_i - \mathbf{s}_j)$ and the self-term $\| \sigma_i \|^2$ can readily be shown to be independent of $\mathbf{s}_i$.

Now let us turn to the problem of calculating the *a posteriori* average of the microscopic number density

$$n(\mathbf{x}) = n(\mathbf{x}; \{\mathbf{s}_i\}) = \sum_{i=1}^{N} \delta(\mathbf{x} - \mathbf{s}_i) \tag{88}$$

We will use the least mean square estimation technique employing the linear estimator

$$\hat{n}(\mathbf{x}) = \hat{n}(\mathbf{x}; \{\rho(\mathbf{r})\}) = a_0(\mathbf{x}) + \int d\mathbf{r}\, a_1(\mathbf{x}, \mathbf{r})\, \rho(\mathbf{r}) \tag{89}$$

Minimizing $E(n - \hat{n})^2$ on $a_0(\mathbf{x})$ and $a_1(\mathbf{x}, \mathbf{r})$ yields the moment equations

$$E(n - \hat{n}) = 0 \tag{90}$$

$$E(n - \hat{n})\, \rho(\mathbf{r}') = 0 \tag{91}$$

Using the relations

$$E\rho(\mathbf{r}) = E\left(\sum \sigma_i + \nu\right) = 0 \tag{92}$$

$$E\rho(\mathbf{r})\, \rho(\mathbf{r}') = n_0 w(\mathbf{r} - \mathbf{r}') - \frac{1}{4\pi\beta} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \tag{93}$$

$$En(\mathbf{x})\, \rho(\mathbf{r}') = n_0 \sigma(\mathbf{r}' - \mathbf{x}) \tag{94}$$

where $n_0 = N/\Omega$ and

$$w(\mathbf{r} - \mathbf{r}') = \int_{\Omega} d\mathbf{s}\, \tau(\mathbf{r} - \mathbf{s})\, \tau(\mathbf{r}' - \mathbf{s}) \tag{95}$$

we obtain

$$a_0(\mathbf{x}) = n_0 \tag{96}$$

and

$$-\frac{1}{4\pi\beta}\nabla_r^2 a_1(\mathbf{x}, \mathbf{r}) + n_0 \int_\Omega d\mathbf{r}'\, w(\mathbf{r} - \mathbf{r}')\, a_1(\mathbf{x}, \mathbf{r}') = n_0\sigma(\mathbf{r} - \mathbf{x}) \tag{97}$$

Of particular interest is the case in which

$$\tau(\mathbf{r}) \to e\delta(\mathbf{r}) \tag{98}$$

i.e., the charge distribution approaches a point charge. In this limit we obtain

$$w(\mathbf{r}) \to e^2\delta(\mathbf{r}) \tag{99}$$

and (94) can now be written as

$$(-\nabla_r^2 + \lambda^{-2})\, a_1(\mathbf{x}, \mathbf{r}) = \lambda^{-2}e^{-1}\big(\delta(\mathbf{r} - \mathbf{x}) - \Omega^{-1}\big) \tag{100}$$

where

$$\lambda = (4\pi n_0 e^2\beta)^{-1/2} \tag{101}$$

is the well-known Debye length. Translational invariance implies that

$$a_1(\mathbf{x}, \mathbf{r}) = a_1(\mathbf{x}, -\mathbf{r}) \tag{102}$$

and hence we can rewrite (100) in the form

$$(-\nabla_x^2 + \lambda^{-2})\, a_1(\mathbf{x} - \mathbf{r}) = \lambda^{-2}e^{-1}(\delta(\mathbf{x} - \mathbf{r}) - \Omega^{-1}) \tag{103}$$

Since the exact optimal estimator $\hat{n}$ is equal to $E(n \mid \{\tilde{\rho}\})$, which in turn is the average of n in the corresponding canonical ensemble, we will write $\hat{n} = \bar{n}$, where the bar denotes the canonical average. The linear estimator (89) can now be written as

$$\bar{n}(\mathbf{x}) - n_0 = \int_\Omega d\mathbf{r}\, a_1(\mathbf{x} - \mathbf{r})\, \rho(\mathbf{r}) \tag{104}$$

Operating on this equation by $(-\Delta_x^2 + \lambda^{-2})$ and using the fact that $\int_\Omega d\mathbf{r}\rho(\mathbf{r}) = 0$, we obtain

$$(-\nabla_x^2 + \lambda^{-2})(\bar{n}(\mathbf{x}) - n_0) = \lambda^{-2}e^{-1}\rho(\mathbf{x}) \tag{105}$$

which is a well-known alternative form of the Poisson–Boltzmann equation giving the response of the average number density to a given fixed charge distribution equal to $-\rho(\mathbf{x})$. This result is known to be exact in the limit of low concentration [and small $\rho(\mathbf{x})$].

9. CONCLUSIONS

We have established a mathematical connection between the problem of the recognition of specified properties of patterns containing many targets, on one hand, and the calculation of the average value of certain observables in a canonical ensemble

of classical systems of interacting particles, on the other. This connection enabled us to transfer the least mean square estimation technique from the pattern recognition domain over to the statistical mechanics domain. Using the simplest nontrivial approximate forms of the estimators, i.e., linear forms, we obtained results pertaining to the one-dimensional Ising model and the one-component plasma that are known to be exact in certain limits.

Although considerable space was devoted in each case to defining the statistical mechanical problem and showing its connection with least mean square estimation, the essential steps involved in the actual approximation procedure were relatively straightforward and simple. These results give us hope that significantly better answers would be obtained by adroit choices of more elaborate forms of estimators. The author is currently investigating the application of these techniques to the classical statistical mechanics of liquids, liquid–solid and liquid–vapor phase transitions, dielectric phenomena, and dense plasmas.