Application of Quantum Theory to Super-parametric Density Estimation

Yeong-Shyeong Tsai
Department of Applied Mathematics, National Chung Hsing University, Taichung, Taiwan

Abstract
Since the consistency of maximum likelihood estimator has been proved, the only problem which is left is the problem of optimization. In last century, it was found that some splines were very useful. From Stone-Weirstrass theorem, we can approximate continuous functions by the polynomials and hence we can construct the estimator by using the splines. Therefore, it might not be so important to stress the difference between the parametric approach and nonparametric approach. Usually, a nonlinear optimization problem is not so easy to solve and it is assumed that the optimization problem can be solved by existent packages. From the view point of mathematics, the results of the optimization problem should be verified or reinvestigated because the nonlinear optimization problem is not simple. It seems that the nonlinear optimization play an important role in density estimation. Though nonlinear equations must be solved in most optimization problems, we will show how an optimization problem can be solved by finding the solution of systems of linear equations. Basing on this approach, the optimization problem can be solved by solving a quadratic equation finally. Some numerical examples are studied as well. From the figures, it can be found this is a good approach on density function estimation.

Introduction
The problem of density estimation is to estimate the density function $f$ by a set of observations, $x_1, x_2, \ldots, x_m$. Roughly, the function with parameters, denoted by the notation $f(x, \theta)$, is called the estimator of $f$. We assume that there is a family of functions, say

$$\mathcal{F} = \{f(x, \theta); \theta \in \mathbb{R}^n\}, \quad (1)$$

and $f \in \mathcal{F}$. The likelihood function $l$ is defined

$$l = \prod_{j=1}^m f(x_j, \theta). \quad (2)$$

From the work of the statistician, the information of $f$ can be obtained by maximizing the likelihood function of the density estimator [1]. Usually, it is not a simple work to solve the nonlinear equations. So far, we know how to solve a single linear equation, a system of linear equations and a single quadratic equation. In this paper, the optimization problem is transformed to system of linear equations first. Basing on the approach, the optimization problem is transformed to a single quadratic equation. Finally, we can solve the optimization problem effectively. The work of transformation is not so simple though the idea is simple. Besides, the undesired roughness of nonparametric estimator is a serious problem. Since our approach is expected to estimate the density
function of general cases, this serious problem must be studied in the same time. In the middle of 20th century, several splines were studied. There are many applications of these splines such as computer aid design of cars [2], curve fitting in statistics, computation of energy levels of multi-electron atoms etc [3]. These splines were introduced to diminish the oscillations of the curve which is obtained by the method of traditional polynomial curve fitting. Therefore, these splines can remove the roughness of density estimators. It is possible to solve these problems in the same time. Anyone who knows the elementary calculus [4] or second year calculus [5] is able to understand this paper.

Parzen windows
In order to avoid the difficulty of the nonlinear optimization problem, the orthogonal polynomials are used in most nonparametric methods. It seems that the orthogonal function will introduce more roughness. In order to avoid introducing the roughness, the orthonormal basis is abandoned and the Parzen window functions [6], nonnegative functions, are adopted. Let $\delta$ be the Dirac delta function. The Dirac delta function is a generalized function,

$$\delta(x) = 0$$  \hspace{1cm} (3)

when $x \neq 0$, and

$$\int_{-\infty}^{\infty} \delta(x) = 1.$$  \hspace{1cm} (4)

If it is necessary, then we shall consider the Dirac delta function as a linear functional defined on a function space [7]. Intuitively, we can start from the following identity

$$f(x) = \int \delta(x - t)f(t)dt.$$  \hspace{1cm} (5)

Here, $f$ is the probability density function which will be estimated by observations $x_1, x_2, x_3, \ldots, x_m$. Let $\tilde{f}$ be the estimator of $f$. If the integration of (5) can be approximated by summation, then the estimator is

$$\tilde{f}(x) = \sum_{i=1}^{n} c_i \varphi_i(x),$$  \hspace{1cm} (6)

$$\varphi_i(x) \geq 0.$$  \hspace{1cm} (7)

Usually, $\varphi_i$ are called window functions or kernel functions. It seems that (3)-(5) can be ignored. We can start from the estimator which is defined in (6). If we can determine value of $c_i$ properly, then the estimator is obtained. Though there are many window functions which are available [2] [3], we find that Bernstein polynomial is good a candidate. Clearly, it must be that

$$\int \tilde{f}(x)dx = 1.$$  \hspace{1cm} (8)
Let
\[ p_i = \int \phi(x) \, dx. \] (9)

Let \( l \) be defined
\[ l = \prod_{j=1}^{m} \tilde{f}(x_j). \] (10)

Here, \( l \) is the likelihood function. From the works of statisticians, the value of \( c_i \) can be determined by maximizing the likelihood function [1]. The problem is to maximize \( l \) subjected to the constraints,
\[ \sum_{i=1}^{n} p_i c_i = 1, \] (11)
and
\[ 0 \leq c_i, \quad i = 1, 2, \ldots, n. \] (12)

Mathematically, since \( c_i \) are going to be determined, if we redefine \( \tilde{f} \),
\[ \tilde{f}(x) = \sum_{i=1}^{n} \left( c_i/p_i \right) \phi_i(x), \] (13)

Then the constraints become
\[ \sum_{i=1}^{n} c_i = 1 \] (14)
and
\[ 0 \leq c_i, \quad i = 1, 2, \ldots, n. \] (15)

Generally, this problem should be solved by Kuhn-Tucker Theorem [8]. Like many mathematical theorems, both Kuhn-Tucker and Lagrange theories are not constructive and the non-constructive results can be traced back to the last axiom of real number, axiom of completeness [4]. In physics, the orthogonal functions are very useful. In order to solve the nonlinear optimization of density estimation, the orthogonal functions were adopted by nonparametric approach. Quantum mechanics was discussed in the paper of Good and Gaskins 1971 [9] [10]. Since then most, if not all, nonparametric density estimators were built on the orthogonal functions which were inferred from quantum mechanics directly or indirectly. Let \( V \) be a vector space over the field of complex numbers. Let \( v_1, v_2, \ldots, v_n \) be orthonormal basis of \( V \). Let \( z \) be a unit vector of \( V \). Roughly speaking, If \( z = \sum_{i=1}^{n} c_i v_i \), then \( |c_i|^2 \) is interpreted as the probability that \( z \) might be \( v_i \) in quantum theory. Hence \( c_i \) is called the probability amplitude. In
statistics, the real numbers work well. Therefore, the complex field is replaced by
the real field. The difference between the probability density and the probability
amplitude is clear and simple. Mathematically or symbolically, the symbol $c_i$ is
replaced by $c_i^2$. Obviously, the constraints become
\[
\sum_{i=1}^{n} c_i^2 = 1. \quad (16)
\]
Only one constraint is left. Then the Lagrange’s multiplier technique can be
applied easily. Clearly, optimization problem play an important role in density
function estimation. In order to avoid the difficulties, we will follow the approach
of quantum theory and the concept of the probability amplitude is adopted. But
we will use the result of Stone-Weirstrass theorem instead of the orthogonal
functions

**Optimization on the compact manifold**

Since the likelihood function $l$ is a $C^\infty$ function of $c_i$ defined on the compact
subset of $\mathbb{R}^n$, $l$ must has maximum value on the sphere. Let observations be $x_1,$
$x_2, x_3, \ldots, x_m$.

Let
\[
l_j = \sum_{i=1}^{n} c_i^2 \phi_i(x_j). \quad (17)
\]

Let
\[
l = \prod_{j=1}^{m} l_j. \quad (18)
\]

Let
\[
\sum_{i=1}^{n} c_i c_i = r \quad (19)
\]
be the constraint. Now, we start to solve the optimization problem.

Let
\[
a_{ij} = \phi_i(x_j). \quad (20)
\]

Let
\[
l_L = l - \lambda (\sum_{i=1}^{n} c_i c_i - r). \quad (21)
\]

By the method of Lagrange’s multiplier, we have
\[
\frac{\partial l_L}{\partial c_k} = 0. \quad (22)
\]
From (17)- (22), we get
\[ l \sum_{j=1}^{m} \frac{a_{kj}c_k}{l_j} - \lambda c_k = 0, \quad k = 1, 2, ..., n. \quad (23) \]

Multiplying (23) by \( c_k \) and taking the summation of index \( k \), we get
\[
\sum_{k=1}^{n} \left( l \sum_{j=1}^{m} \frac{a_{kj}c_k}{l_j} - \lambda c_k \right) c_k = 0, \quad (24) \]

Interchanging the summations, we get
\[
\sum_{j=1}^{m} \left( l \sum_{k=1}^{n} a_{kj}c_k c_k c_k/l_j - \lambda c_k c_k \right) = 0. \quad (25) \]

From (17), (18), (19), (20) and (25), we get
\[
lm - \lambda r = 0. \quad (26)\]

Hence
\[ l = \lambda r/m. \quad (27) \]

Substituting (27) into (23), we get
\[
c_k \left( \sum_{j=1}^{m} \frac{a_{kj}r}{ml_j} - 1 \right) = 0, \quad k = 1, 2, ..., n. \quad (28) \]

Clearly, either
\[ c_k = 0, \quad (29) \]

or
\[
\left( \sum_{j=1}^{m} \frac{a_{kj}r}{ml_j} - 1 \right) = 0, \quad k = 1, 2, ..., n. \quad (30) \]

It should be emphasized that (29) and (30) are not mutually exclusive. In order to linearization the equations (30), we take some transformations of variables.

Let
\[ y_j = r/(ml_j). \quad (31) \]

Substituting (31) into (30), we get
\[
\sum_{j=1}^{m} a_{kj}y_j = 1 \quad (32) \]

Multiplying both side (32) by a constant \( \theta^2 \), we have
\[
\sum_{j=1}^{m} a_{kj} \theta^2 y_j = \theta^2. \quad (33)
\]

Since the solutions of (29) are not affected by any factor, the constant \( \theta \) is introduced in equations (32) to fit the constraint. It seems that the constant \( \theta \) is a redundancy because that \( \theta \) must be 1. Later, it will be found in following lemmas and theorems that \( \theta \) play an important role.

Let
\[
\theta_j = \theta^2 y_j. \quad (34)
\]

Substituting (34) into (33), we get
\[
\sum_{j=1}^{m} a_{kj} \theta_j = \theta^2, \quad k = 1, 2, ..., n \quad (35)
\]

Clearly, equations (35) is a system of linear equations of \( \theta_j \).

From (31), we have
\[
m l_j = \frac{r}{y_j}. \quad (36)
\]

From (17), (20), (34) and (36), we have
\[
\sum_{i=1}^{n} a_{ij} c_i^2 = \frac{r \theta^2}{m \theta_j}. \quad (37)
\]

And hence
\[
\sum_{i=1}^{n} a_{ij} \left( \frac{c_i}{\theta} \right)^2 = \frac{r}{m \theta_j}, \quad j = 1, 2, ..., m. \quad (38)
\]

Clearly, equations (38) are also linear equations of \( (c_i/\theta)^2 \). Equations (39) are replaced by two system of linear equations, (35) and (38). The problem seems to be very simple. Actually, there are many combinations of (29) and (30). Though, in these combinations, some of them may not yield the solutions of this optimization problem, all the feasible solutions of this problem are contained in the suitable combinations of equations (29) and equations (30).

If we solve the problem directly, then there will be the same complexities as the simplex method for solving linear programming problem. Furthermore, it is very difficulty to design the algorithm and to implement the computer program if it is not impossible. Even if the computer program is designed, then it might be a time-consuming program. However, it can be concluded that the nonlinear optimization problem is solvable theoretically. If the numbers \( m \) and \( n \) are very small, say 3, then it is a simple problem to solve the systems of linear equations. Generally, the extreme point of likelihood function is not unique. The results of computer simulation show that the extreme point of likelihood function seems
to be unique. The computer simulations are implemented when \( m \) and \( n \) are less than 10.

**Quantum theory approach**

In quantum mechanics, the wave function is linear combination of basis functions and the normalization of the wave function requires that the sum of the squares of coefficients should be unit. This gives us a clue to remodel our problem and the problem becomes easier.

Let

\[
\bar{f}(x) = \sum_{i=1}^{n} u_i v_i \varphi_i(x),
\]

where \( \varphi_i \) is the window function.

Let

\[
\bar{l} = \prod_{j=1}^{m} f(x_j)
\]

be the likelihood function. The constraints are

\[
\sum_{i=1}^{n} u_i u_i = r,
\]

and

\[
\sum_{i=1}^{n} v_i v_i = r.
\]

The problem is to maximize \( \bar{l} \) subjected to constraints (41) and (42). In order to find the connection of two models, we should define the following notations. Let

\[
\sum_{i=1}^{n} c_i c_i = r.
\]

Let

\[
l_j = \sum_{i=1}^{n} c_i^2 \varphi_i(x_j).
\]

Let

\[
l = \prod_{j=1}^{m} l_j.
\]
\[ S_n = \{(c_1, \ldots, c_n); \sum_{i=1}^{n} c_i c_i = r \}. \]  

(46)

The first model is to find the extreme point of \( l \) on \( S_n \). Let

\[ \sum_{i=1}^{n} u_i u_i = r. \]  

(47)

Let

\[ \sum_{i=1}^{n} v_i v_i = r. \]  

(48)

Let

\[ \bar{t}_j = \sum_{i=1}^{n} u_i v_i \varphi_i(x_j). \]  

(49)

Let

\[ \bar{t} = \prod_{j=1}^{m} \bar{t}_j. \]  

(50)

Let

\[ S_{2n} = \{(u_1, \ldots, u_n, v_1, \ldots, v_n); \sum_{i=1}^{n} u_i u_i = r, \sum_{i=1}^{n} v_i v_i = r \}. \]  

(51)

The second model is to find the extreme point of \( \bar{t} \) on \( S_{2n} \). It is clear that \( S_n \) and \( S_{2n} \) are compact subsets of \( \mathbb{R}^n \) and \( \mathbb{R}^{2n} \) respectively. Let \( \bar{t} \) and \( \bar{t} \) be the likelihood functions defined above. Clearly, both \( \bar{t} \) and \( \bar{t} \) have maximum. Let \( A \) be the set of all \( \bar{t} \). Let \( A \) be the set of all \( \bar{t} \). It is obvious that \( A \subseteq A \). Therefore, the maximum of \( A \) is less than or equal to that of \( A \). It will be shown, in theorem 1, that the extreme points of \( \bar{t} \) should be located at the points such that \( u_i = v_i \), \( i = 1, 2, \ldots, n \). Therefore, the problem to maximize \( \bar{t} \) subjected to the constraint (43) is equivalent to that of maximizing \( \bar{t} \) subjected to the constraints (47) and (48).

**Theorem 1.** For each observation \( x_j \), if there is \( \varphi_i \) such that \( \varphi_i(x_j) > 0 \), then the extreme points of \( \bar{t} \) should be located at the points such that \( u_i = v_i \), \( i = 1, 2, \ldots, n \).

**Proof.** We assume that

\[ v_1 > u_1 \]  

(52)

and the maximum is \( \bar{t}_M \), that is,
\[ l_M \geq l \] (53)
for all \( l \). Let
\[ u'_i = v'_i = \theta \sqrt{u_i v_i}. \] (54)

By choosing a proper value \( \theta \), constraints
\[ \sum_{i=1}^{n} u'_i u'_i = r \] (55)
and
\[ \sum_{i=1}^{n} v'_i v'_i = r \] (56)
are satisfied simultaneously. By Cauchy-Schwartz inequality and (52), we get
\[ \theta > 1 \] (57)
and hence we have
\[ l_M < \bar{l} \] (58)
for some \( \bar{l} \). This is a contradiction.

**The iteration procedures**

Tough we have stated and proved Theorem 1, we need a constructive procedure to find the extreme point. It is not so easy to solve the nonlinear optimization problem. Usually, the sequences are constructed by iteration procedures. The well designed iteration procedures can generate monotonic sequences which are useful in theory and application. With the nested iteration procedures, the complicated problems such as mathematical formulation, designing of the computation algorithm and the computer programming can be solved in parallel. It seems that it is easier to maximize \( l \) than to maximize \( \bar{l} \). The reason why we solve the more complicated problem can be shown in the method of Lagrange’s multiplier. The strategy of solving the nonlinear optimization problem with constraints is ignoring one of the constraints, say equation (52). This can be done by choosing the initial value of \( v_i \), \( v_i = \sqrt{r/n} \). Then the optimization problem becomes simpler because only one constraint is left. In order make it more clearly and precisely, we recall and define some identities.

Let
\[ \psi_i(x) = v_i \varphi_i(x). \] (59)

Let
\[ \bar{f}(x) = \sum_{i=1}^{n} u_i \psi_i(x). \] (60)
Let
\[ l_j = f(x_j). \quad (61) \]

Let
\[ \bar{t} = \prod_{j=1}^{m} t_j. \quad (62) \]

The problem is to maximize \( \bar{t} \) subject to the constraint (47). After the values of \( u_i \) being obtained, the value of \( v_i \) is updated by \( \overline{\theta} \sqrt{u_i v_i} \). By choosing the factor \( \overline{\theta} \), the constraint (48) is satisfied. Clearly, the iteration procedures can be obtained. And the Cauchy-Schwartz inequality is able to test the termination of the iteration procedures. First, we summarize the whole procedures. Later, the associated mathematical theory of the procedure will be shown. The procedures are:

**Step (i).** Initialize the procedure by setting \( k = 1 \) and \( v^k_i = \sqrt{r/n_i} \), \( i = 1, 2, ..., n \).

**Step (ii),** maximize \( \bar{t} \) subject to the constraint (47). Then values of \( u^k_i, i = 1, 2, ..., n \), are obtained.

**Step (iii),** Check the condition \( \sum_{i=1}^{n} u^k_i v^k_i \geq r \) is satisfied or not, where \( \varepsilon \) is a small positive number to control the termination of the procedures.

If the condition is satisfied, then stop the iteration procedures and the density estimator, \( \hat{f}(x) = \sum_{i=1}^{n} u^k_i v^k_i \phi_i(x) \), is obtained. Otherwise, increase the value of \( k \) by one, set \( v^k_i = \overline{\theta}^{k} \sqrt{u^{k-1}_i v^{k-1}_i} \), here \( \overline{\theta}^{k} \) is a factor to fit the constraint (48). Then go to Step (ii) and proceed the procedures.

**Remark 1.** From Cauchy-Schwartz inequality, the values of \( \overline{\theta}^{k} \) must be greater than or equal to 1 and hence the set of the values of the likelihood function is an increasing sequence.

Since step (i) and step (iii) are so simple, the only problem which is left is how to complete the step (ii). Now, we will show how step (ii) can work well. In order to complete the step(ii), another nested iteration procedures will be designed and studied. In order to collaborate with the computer algorithm, new notations must be introduced. Let \( u^k_i \) and \( v^k_i \) be obtained in the \( k^{th} \) iteration. Let

\[ \hat{f}(x) = \sum_{i=1}^{n} u^k_i (u^k_i \phi_i(x)). \quad (63) \]

Let
\[ \psi_i(x) = v^k_i \phi_i(x). \quad (64) \]

The simple notation,
\[ \hat{f}(x) = \sum_{i=1}^{n} u_i \psi_i(x) \]  

(65)

shall be used hereafter.

The constructive proof and the procedures of optimization

**Lemma 1.** Let \( \hat{f}(x) = \sum_{i=1}^{n} u_i \psi_i(x) \), where \( \psi_i \) are nonnegative functions. Let \( \hat{l}_j \) be \( \hat{f}(x_j) \). Let \( \hat{\ell} = \prod_{j=1}^{m} \hat{l}_j \) be the likelihood function. For each \( x_j \), there is a \( \psi_i \) such that \( \psi_i(x_j) > 0 \). Then there are constructive procedures to maximize \( \hat{\ell} \) subject to the constraint. We recall the constraint \( \sum_{i=1}^{n} u_i u_i = r \).

**Remark 2:** Since \( \psi_i \) are nonnegative functions and the constraint is invariant under the transformation, \( u_i = -u_i \), the solution of this optimization problem, \( u_i \), must be nonnegative.

**Proof.** Let

\[ b_{ij} = \psi_i(x_j). \]

(66)

Let

\[ \hat{\ell}_L = \hat{\ell} - \lambda \left( \sum_{i=1}^{n} u_i u_i - r \right). \]

(67)

By the method of Lagrange’s multiplier, we have

\[ \frac{\partial \hat{\ell}_L}{\partial u_k} = 0. \]

(68)

By simple symbolic computation of derivatives, we get

\[ \hat{l} \sum_{j=1}^{m} \frac{b_{kj}}{\hat{l}_j} - 2\lambda u_k = 0, \quad k = 1, 2, ..., n. \]

(69)

Multiplying (69) by \( u_k \) and taking the summation of index \( k \), we get

\[ \sum_{k=1}^{n} \hat{l} \left( \sum_{j=1}^{n} \frac{b_{kj}}{\hat{l}_j} \right) - 2\lambda u_k u_k = 0, \quad k = 1, 2, ..., n. \]

(70)

Interchanging the summations, we get

\[ \sum_{j=1}^{m} \hat{l} \left( \sum_{k=1}^{n} \frac{b_{kj} u_k}{\hat{l}_j} \right) - 2\lambda u_k u_k = 0. \]

(71)
From (47), (65), (66), (71) and definition of \( \hat{l}_j \), we get

\[
\hat{l} m - 2\lambda r = 0,
\]

(72)

and hence

\[
\hat{l} = (2\lambda r) / m.
\]

(73)

Substituting (73) into (69), we get

\[
\sum_{j=1}^{m} r b_{kj} - u_k = 0, \quad k = 1, 2, \ldots, n.
\]

(74)

Let \( \mathbf{u} \) and \( \mathbf{b}_j \) be \( n \) components vectors, where \( \mathbf{u} = [u_1, u_2, \ldots, u_n]^t \) and \( \mathbf{b}_j = [b_{1j}, b_{2j}, \ldots, b_{nj}]^t \). By the constraint (47) and the assumption of this lemma, \( \mathbf{u} \) and \( \mathbf{b}_j \) are not zero vectors. Rewrite equations (74)

\[
\frac{r}{m} \sum_{j=1}^{m} \frac{b_j}{r \mathbf{b}_j} - \mathbf{u} = 0.
\]

(75)

Let

\[
\alpha_k = \frac{1}{u \cdot \mathbf{b}_k}, \quad k = 1, 2, \ldots, m.
\]

(76)

Substituting (76) into (75), we get

\[
\mathbf{u} = \frac{r}{m} \sum_{j=1}^{m} \alpha_j \mathbf{b}_j.
\]

(77)

Substituting (77) into (76), we obtain

\[
\alpha_k = \frac{1}{\frac{r}{m} \sum_{j=1}^{m} \alpha_j (\mathbf{b}_j \cdot \mathbf{b}_k)}, \quad k = 1, 2, \ldots, m.
\]

(78)

Let

\[
D_{ij} = \frac{r}{m} (\mathbf{b}_i \cdot \mathbf{b}_j), \quad i, j = 1, 2, \ldots, m.
\]

(79)

Substituting (79) into (78), we obtain

\[
\sum_{j=1}^{m} D_{kj} \alpha_k \alpha_j = 1, \quad k = 1, 2, \ldots, m.
\]

(80)

It should noticed that the major differences between (74) and (80) are the range of the indices since \( m \) and \( n \) are different. If \( m = 1 \), then the solution of equation (80) can be obtained. From (77), the lemma is proved. Fortunately, if \( m > 1 \), then we can solve equations (80) one by one. It is very simple to show
that the existence and the uniqueness of the solution of (80), we will complete
the details of works in the following lemmas and theorems. Now, we assume
that the solution of (80) can be obtained effectively and the solution is unique.
Therefore, the lemma is proved and it seems that step (i), (ii) and (iii) can work
well.

In deriving the equations, the systematic notations are adopted. Therefore,
the variables, $\alpha_k$ and $\alpha_j$ in the equations (80) are interchangeable. In order
to simplify the problem, these equations will be solved one by one in iteration
procedures. The symmetry shall be destroyed because only one variable, $\alpha_k$,
will be focused. Usually, there are at least two sets of variables in iteration
procedures, one set is associated with the old value and the other set is associated
with the updated new value. Therefore, we use the symbols with prime for new
value. In order to analyze the details of algorithm, the delta notation shall
be used, for example, $\alpha_k' = \alpha_k + \Delta \alpha_k$. Therefore, there are different forms
of equations (80) in different notations. The functions of different forms of
equations (80) are obvious because each form is associated with a meaning.
The error of each equation is denoted by $E_j$, $j = 1, 2, ..., m$, and $\Delta E_j$ is the
variation of $E_j$ in iteration procedure. The total sum of the absolute value of
$E_j$ is denoted by $E$, and $\Delta E$ is the variation of $E$. $E^{(j)}$ is the value of $E$ in $j^{th}$
iteration. These notations and their meanings shall be defined in the context.

**Remark 3:** From identity (76) and remark 2, $\alpha_k$ must be nonnegative.
Clearly, the solution of (77), u, shall satisfy the constraint, $u \cdot u = r$. It is not
necessary to worry about that the quantity $u \cdot b_k$ in (76) might be zero. The
identity (76) and (78) are adopted for the convention of symbolic computations.
These will be shown later.

Though the likelihood function is highly nonlinear, equations in (80) are a
system of quadratic equations. Intuitively, the solution of a single quadratic
equation can be obtained easily. In order to solve the equations (80) one by
one, the nested iteration procedures are constructed. We write one of them, say
$k^{th}$ equation, the quadratic equation of $\alpha_k$,

$$D_{kk} \alpha_k^2 + \left( \sum_{i \neq k} D_{ik} \alpha_i \right) \alpha_k - 1 = 0. \quad (81)$$

Clearly, the only positive solution of (81) is $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$,
where $s = \sum_{i \neq k} D_{ik} \alpha_i$. If the equations in (80) can be solved one by one, then
the problem becomes simpler. Indeed, the equations in (80) can be solved one
by one and the sum of all errors is reduced in each time. Basing on this fact,
we are able to design another set of iteration procedures step (a), (b) and (c)
to solve the problem. Now, we start to design the procedures.

Let

$$E_i = \sum_{j=1}^{m} D_{ij} \alpha_i \alpha_j - 1. \quad (82)$$

Let
\[ E = \sum_{i=1}^{m} |E_i|. \]  

(83)

In the iteration procedures, the values of \( E_i \) and \( E \) shall be changed. Let \( \Delta E_i \) be variation of \( E_i \). Let \( \Delta E \) be variation of \( E \). In order to collaborate with the algorithm, the nested iteration procedures are designed in the step (ii). Clearly, the problem is to minimize the value of \( E \). And it must be proved that the minimum of \( E \) is zero. Therefore, the solution of (80) and the solution of (77) are obtained. Now, we construct the iteration procedures to complete step(ii). The associated mathematical lemmas and theorems of algorithm will emerge.

First, initialize the procedure by setting \( \alpha_k = \sqrt{1/(Dm)} \), \( k = 1, 2, ..., m \), where \( D \) is the maximum of \( D_{ij} \). Then the iteration procedures are:

**Step (a).** Compute \( E_i = \sum_{j=1}^{m} D_{ij} \alpha_i \alpha_j - 1, i = 1, 2, ..., m, \) and \( E = \sum_{i=1}^{m} |E_i| \). Go to step (b).

**Step (b).** Test the condition whether \( E \leq \delta \) is satisfied or not, where \( \delta \) is a small positive number to control the termination of the procedures. If \( E \leq \delta \), then the desired results are obtained. Compute \( u_k \) by the identity (77), \( k = 1, 2, ..., n \), and terminate the iteration. Otherwise, go to step (c).

**Step (c).** Find the largest element of the set of all \(|E_i|\). Suppose that the largest element is \(|E_k|\) for some \( k \). Eliminate \( E_k \) by updating the value of \( \alpha_k \) by \( \alpha'_k = \left(-s + \sqrt{s^2 + 4D_{kk}}\right)/(2D_{kk}) \), where \( s = \sum_{i \neq k} D_{ik} \alpha_i \). Go to Step (a).

Now, there will be no difficulty to implement steps (a), (b) and (c). Intuitively, steps (a), (b) and (c) shall be terminated in finite steps if the values of \( E \) is strictly decreasing sequence which converges to zero. In lemma 3, it will be proved that the values of \( E \) is a decreasing sequence. Lemma 2 will support lemma 3. In lemma 5, it will be proved that the values of \( E \) is a strictly decreasing sequence which converges to zero. Lemma 4 will support lemma 5.

**Lemma 2.** All iterations, steps (a), (b) and (c), the set of all \( \alpha_k, k = 1, 2, ..., m \), are bounded above and the set of all \( \alpha_k, k = 1, 2, ..., m \), are bounded below by a positive number, say \( B, B > 0 \). That is, \( \alpha_k > B, k = 1, 2, ..., m \).

**Remark 4.** What we mean all \( \alpha_k \) is including all \( \alpha_k \) and all \( \alpha'_k \).

 Proof. The value of \( \alpha_k \) is either the initial value \( \sqrt{1/(Dm)} \) or the updated value \( (-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk}) \). It is very easy to verify the following inequalities

\[ \frac{-s + \sqrt{s^2 + 4D_{kk}}}{2D_{kk}} < \frac{-s + \sqrt{s^2 + 2sD_{kk} + D_{kk}^2}}{2D_{kk}} = \frac{1}{2}, \]  

(84)
when \( s \geq 2 \).

\[ \frac{-s + \sqrt{s^2 + 4D_{kk}}}{2D_{kk}} < \frac{\sqrt{4 + 4D_{kk}}}{2D_{kk}}, \]  

(85)
when \( s < 2 \).
It is obvious that $\alpha_k$ are bounded above. Since $s = \sum_{i \neq k} D_{ik} \alpha_i$, $s$ is bounded above. Next, we are going to prove that there is a positive number $B$ such that $\alpha_k > B$, $k = 1, 2, ..., m$, in all iterations. Clearly, $\alpha_k$ are either the initial value or updated by $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$. The derivative of $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$ is $(-1 + s/\sqrt{s^2 + 4D_{kk}})/(2D_{kk})$, which is negative for all $s \geq 0$. Therefore, $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$ is a decreasing function of $s$. It is obvious that

$$\lim_{s \to \infty} (-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk}) = 0. \quad (86)$$

Since $s$ is bounded above, $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$ has a positive lower bound. Therefore, $\alpha_k$ is bounded below by a positive lower bound, say $B$.

**Remark 5.** Lemma 2 does not imply $u_k$ are bounded below by a positive number, some $u_k$ might tend to zero.

**Lemma 3.** The values of $E$ in iteration procedures, step (a), (b) and (c), is a decreasing sequence.

**Proof.** From (82) and (83), we find that equations (80) can be solved one by one. One of equations (80) with one variable, say $\alpha'_k$, will be solved. The error of the equation with index $k$, $E_k$, is removed completely in step (c). Therefore,

$$|\Delta E_k| = |E_k| \quad (87)$$

for the particular index $k$ and it might be that

$$|\Delta E_j| \neq |E_j| \quad (88)$$

when $j \neq k$. Though there are two roots of a quadratic equation, only one of them is positive. From equation (81), it must be $(-s + \sqrt{s^2 + 4D_{kk}})/(2D_{kk})$.

Let

$$\Delta \alpha_k = \alpha'_k - \alpha_k. \quad (89)$$

The value of $\Delta \alpha_k$ is the difference of two positive numbers which are bounded above. Clearly,

$$|\Delta \alpha_k| \leq \alpha_k \quad (90)$$

when $\Delta \alpha_k \leq 0$. In the step (c), the value of $E$ is reduced by $\Delta E$. In order to update the value of $\alpha_k$, we rewrite the equation (81)

$$\alpha'_k \sum_{i \neq k} D_{ki} \alpha_i + D_{kk} \alpha'_k \alpha'_k - 1 = 0. \quad (91)$$

Some times, it is more convenient to use the delta notation. Therefore, equation (91) becomes

$$(\alpha_k + \Delta \alpha_k) \sum_{i \neq k} D_{ki} \alpha_i + D_{kk} (\alpha_k + \Delta \alpha_k)^2 - 1 = 0, \quad (92)$$

15
\[
\Delta \alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i + \Delta \alpha_k D_{kk} \alpha_k + D_{kk}(\Delta \alpha_k)^2 + \alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i - 1 = 0. \quad (93)
\]

From (82), we get

\[
\Delta E_k = \alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i - 1, \quad (94)
\]

for this particular index \(k\).

Rewrite (93)

\[
\Delta \alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i + \Delta \alpha_k D_{kk} \alpha_k + D_{kk}(\Delta \alpha_k)^2 = -(\alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i - 1). \quad (95)
\]

Clearly,

\[
\left| \Delta \alpha_k \sum_{i=1}^{m} D_{ki} \alpha_i + \Delta \alpha_k D_{kk} \alpha_k + D_{kk}(\Delta \alpha_k)^2 \right| = |\Delta E_k|, \quad (96)
\]

\[
|\Delta \alpha_k| \left( \sum_{i \neq k}^{m} D_{ki} \alpha_i + D_{kk} 2 \alpha_k + D_{kk} \Delta \alpha_k \right) = |\Delta E_k|. \quad (97)
\]

All quantities in \(\sum_{i \neq k}^{m} D_{ki} \alpha_i + D_{kk} 2 \alpha_k + D_{kk} \Delta \alpha_k\), except \(\Delta \alpha_k\), are positive.

From (90), for any case,

\[
\left| \sum_{i \neq k}^{m} D_{ki} \alpha_i + D_{kk} \alpha_k \right| \leq \left| \sum_{i \neq k}^{m} D_{ki} \alpha_i + D_{kk} 2 \alpha_k + D_{kk} \Delta \alpha_k \right|. \quad (98)
\]

Therefore,

\[
|\Delta \alpha_k| \left( \sum_{i \neq k}^{m} D_{ki} \alpha_i + D_{kk} \alpha_k \right) \leq |\Delta E_k|. \quad (99)
\]

If we write whole system of equations (80), then the upper bound of all \(|\Delta E_i|, i \neq k\), can be figured out. From (82), we get

\[
\Delta E_i = (\alpha_i + \Delta \alpha_i) \sum_{j=1}^{m} D_{ij} (\alpha_j + \Delta \alpha_j) - 1 - E_i. \quad (100)
\]

for all \(i\). But

\[
\Delta \alpha_i = 0, \quad i \neq k. \quad (101)
\]
From (100) and (101), we get
\[ \Delta E_i = \Delta \alpha_k D_{ik} \alpha_i, \quad i \neq k. \] (102)

Since
\[ D_{ik} = D_{ki}, \] (103)

\[ \Delta \alpha_k D_{ik} \alpha_i = \Delta \alpha_k D_{ki} \alpha_i. \] (104)

From the inequality (99) and (102), we get
\[ \sum_{i \neq k} |\Delta E_i| + |\Delta \alpha_k| D_{kk} \alpha_k < |\Delta E_k|. \] (105)

From (105),
\[ |\Delta \alpha_k| D_{kk} \alpha_k < |\Delta E_k| - \sum_{i \neq k} |\Delta E_i|. \] (106)

From (83), we get
\[ \Delta E = \sum_{i=1}^{m} \Delta |E_i|. \] (107)

Since
\[ |a + b| \geq |a| - |b| \] (108)
for any \( a \) and \( b \),

\[ |\Delta E| \geq |\Delta E_k| - \sum_{i \neq k} |\Delta E_i|. \] (109)

Clearly, \( \Delta E \) is negative and dominated by \( |\Delta E_k| \),

\[ |\Delta E| > |\Delta \alpha_k| D_{kk} \alpha_k. \] (110)

An hence the set of the values of \( E \) generated by iterations is a decreasing sequence. We have proved the lemma.

For each iteration, the value of \( E \) is denoted by a symbol, say \( E^{(i)} \) in the \( i^{th} \) iteration. The notations \( E_i \) and \( E^{(i)} \) are associated with different meanings.

Let \( \lim_{i \to \infty} E^{(i)} = E^\infty \). Clearly, the lower bound of \( |\Delta \alpha_k| D_{kk} \alpha_k \) will serve for two purposes, one is to prove that the sequence \( E^{(i)} \) is a strictly decreasing sequence and the other is to prove that \( E^\infty = 0 \).

**Lemma 4.** If \( E^\infty > 0 \) and \( k \) is the index such that \( |E_k| \geq |E_i| \quad i = 1, 2, ..., m \), then the set of all \( |\Delta \alpha_k| D_{kk} \alpha_k \), in all iterations of step (a), (b) and (c) has a nonzero lower bound.

**Proof.** It is obvious that
\[ |E_k| \geq E^\infty / m. \] \hspace{1cm} (111)

In each iteration procedure, only one equation is solved. From (97) and (111), we get
\[ |\Delta \alpha_k| \left( \sum_{i \neq k} D_{ki} \alpha_i + D_{kk} 2 \alpha_k + D_{kk} \Delta \alpha_k \right) \geq \frac{E^\infty}{m}. \hspace{1cm} (112) \]

The first term absorbing \( D_{kk} \alpha_k \) from the second term, we get
\[ |\Delta \alpha_k| \left( \sum_{i=1}^{m} D_{ki} \alpha_i + D_{kk} \alpha_k + D_{kk} \Delta \alpha_k \right) \geq \frac{E^\infty}{m}. \hspace{1cm} (113) \]

Since \( |\Delta \alpha_k| \) and \( \alpha_i \) are bounded above, \( \left| \sum_{i=1}^{m} D_{ki} \alpha_i + D_{kk} \alpha_k + D_{kk} \Delta \alpha_k \right| \) is also bounded above, say
\[ \left| \sum_{i=1}^{m} D_{ki} \alpha_i + D_{kk} \alpha_k + D_{kk} \Delta \alpha_k \right| < M. \hspace{1cm} (114) \]

From (113) and (114), we get
\[ |\Delta \alpha_k| > E^\infty / (Mm). \hspace{1cm} (115) \]

Therefore, \( |\Delta \alpha_k| \) is bounded below by a positive number and hence \( |\Delta \alpha_k| D_{kk} \alpha_k \) is bounded below by a positive number in all iterations. Therefore, we have proved the lemma.

**Lemma 5.** \( \lim_{k \to \infty} E^k = 0 \), that is, \( E^\infty = 0 \).

**Proof.** For any \( \varepsilon, \varepsilon > 0 \), there is an positive integer \( N \) such that
\[ E^{(j)} - \varepsilon < E^\infty, \] \hspace{1cm} (116)

whenever \( j \geq N \). Since \( |E_k| \) is the largest one in the \( j^{th} \) iteration,
\[ |E_k| \geq E^\infty / m. \] \hspace{1cm} (117)

From inequality (110),
\[ E^{(j+1)} + |\Delta \alpha_k| D_{kk} \alpha_k < E^{(j)}. \] \hspace{1cm} (118)

Therefore,
\[ E^{(j+1)} + |\Delta \alpha_k| D_{kk} \alpha_k - \varepsilon < E^{(j)} - \varepsilon. \] \hspace{1cm} (119)

If we assume that
\[ E^\infty > 0. \] \hspace{1cm} (120)
By lemma 4, the set of all $|\Delta \alpha_k| D_{kk} \alpha_k$ has a nonzero lower bound. We choose $\varepsilon$ such that $\varepsilon$ is less than the lower bound of $|\Delta \alpha_k| D_{kk} \alpha_k$. That is,

$$|\Delta \alpha_k| D_{kk} \alpha_k - \varepsilon > 0.$$  \hspace{1cm} (121)

Then

$$E^{(j+1)} < E^{(j)} - \varepsilon.$$  \hspace{1cm} (122)

From (116), we get

$$E^{(j+1)} < E^\infty.$$  \hspace{1cm} (123)

It is a contradiction because $E^{(j)} \geq E^\infty$ for all $j$. Therefore, we have proved the lemma and hence $E^\infty = 0$.

Since $E^\infty = 0$, the iteration procedures, step (a), step (b) and step (c), should terminate in finite steps of iterations and step (ii) can be executed completely. Therefore, lemma 1 is proved completely. In lemma 7, it will be proved that the iteration procedures, step (i), step(ii) and step (iii), shall be terminated in finite steps. Lemma 6 will support lemma 7.

**Lemma 6.** Let $\theta^k$ be obtained in the iteration procedures, step (i), step(ii) and step (iii). Then $\lim_{k \to \infty} \theta^k = 1$.

**Proof.** It is obvious that

$$\theta^k \geq 1.$$  \hspace{1cm} (124)

and hence $\hat{l}^k$ is an increasing sequence.

Let

$$\lim_{k \to \infty} \hat{l}^k = \hat{l}^\infty.$$  \hspace{1cm} (125)

For any $\varepsilon > 0$, there is $\hat{l}^k$ such that

$$\hat{l}^k + \varepsilon > \hat{l}^\infty.$$  \hspace{1cm} (126)

If $\lim_{k \to \infty} \theta^k$ does not exist, then there exist $\varepsilon > 0$, for any $K$, there is $k > K$ such that

$$\hat{l}^k > 1 + \varepsilon.$$  \hspace{1cm} (127)

From (64), (65) and the definition $\hat{l}$, we get

$$\hat{l}^{k+1} > (\theta^k)^m \hat{l}^k,$$  \hspace{1cm} (128)

where $m$ is the sample size. Since

$$(1 + \varepsilon)^m > 1 + m\varepsilon,$$  \hspace{1cm} (129)
\[ \hat{l}^{k+1} > (1 + m\varepsilon)\hat{l}^k. \]  

(130)

Therefore,

\[ \hat{l}^{k+1} > \hat{l}^k + m\varepsilon\hat{l}^1. \]  

(131)

Choosing \( e = m\varepsilon\hat{l}^1 \), we have

\[ \hat{l}^{k+1} > \hat{l}^k + e. \]  

(132)

From (126), we get

\[ \hat{l}^{k+1} > \hat{l}^\infty. \]  

(133)

It is a contradiction. Therefore,

\[ \lim_{k \to \infty} \hat{l}^k = 1. \]  

(134)

**Lemma 7.** Let \( P^k = \sum_{i=1}^{n} u_i^k v_i^k \). Then \( \lim_{k \to \infty} P^k = r \) and the iteration procedures, step (i), step(ii) and step (iii), shall be terminated in finite steps.

**Proof.** From the definition of \( \hat{l}^k \) in step (iii), we get

\[ \hat{l}^k \hat{l}^{k-1} \sum_{i=1}^{n} u_i^{k-1} v_i^{k-1} = r. \]  

(135)

From (134) and (135), we get

\[ \lim_{k \to \infty} P^k = r. \]  

(136)

Therefore, the iteration procedures, step (i), step(ii) and step (iii), shall be terminated in finite steps.

Lemma 8 will show the result of theorem 1 can be obtained by constructive method.

**Lemma 8.** Let \( w_i^k = |u_i^k - v_i^k|, i = 1, 2, ..., n, k = 1, 2, ..., \) be a set sequences generated by the iteration procedures, step (i), step(ii) and step (iii). Then \( \lim_{k \to \infty} w_i^k = 0, i = 1, 2, ..., n. \)

**Remark 6.** By Cauchy-Schwartz inequality, \( (\sum_{i=1}^{n} u_i^k v_i^k)^2 \leq \sum_{i=1}^{n} (u_i^k)^2 \sum_{i=1}^{n} (v_i^k)^2, \) the equal sign hold only if \( u_i^k = v_i^k, i = 1, 2, ..., n. \) Intuitively, it is obvious that the condition in step (iii) must be satisfied. Otherwise, \( \hat{l} \) does not have maximum.

**Proof.** By simple computation, we get

\[ \sum_{i=1}^{n} (u_i^k - v_i^k)^2 = \sum_{i=1}^{n} u_i^k u_i^k + \sum_{i=1}^{n} v_i^k v_i^k - 2 \sum_{i=1}^{n} u_i^k v_i^k. \]  

(137)
In all iteration procedures, the constraints (47) and (48) must be satisfied. Therefore

\[ \sum_{i=1}^{n} (u_k^i - v_k^i)^2 = 2r - 2\sum_{i=1}^{n} u_k^i v_k^i. \]  

(138)

From (136) and (138), we get

\[ \lim_{k \to \infty} w_k^i = 0, \quad i = 1, 2, ..., n. \]  

(139)

Combining the results theorem 1 and lemma 8, the problem of optimization is solved almost.

**The unique theorem**

**Theorem 2.** The solution of equations (80) is unique.

**Proof:** Of course, only the positive solutions make sense. Let \( e_i = \alpha_i b_i \), where \( \alpha_i \) is a solution that we have obtained by the iteration procedures step(a), step(b) and step (c) . Let

\[ e_{ij} = e_i \cdot e_j. \]  

(140)

From (80) and (140), we get

\[ \sum_{j=1}^{m} e_{ij} = 1, \quad i = 1, 2, ..., m. \]  

(141)

Consider the following equations,

\[ \sum_{j=1}^{m} e_{ij} \beta_i \beta_j = 1, \quad i = 1, 2, ..., m. \]  

(142)

Here \( \beta_i, i = 1, 2, ..., m \), are unknowns. Then

\[ \beta_i = 1, \quad i = 1, 2, ..., m, \]  

(143)

is a solution of (141). If there is another solution set, say

\[ \beta_1 \geq \beta_2 \geq \ldots \geq \beta_m. \]  

(144)

From (141), we know that the equal sign cannot hold all times. From (142), we have

\[ \beta_1 \sum_{j=1}^{m} e_{1j} \beta_j = 1, \]  

(145)

and

\[ \beta_m \sum_{j=1}^{m} e_{mj} \beta_j = 1. \]  

(146)
It is obvious that
\[ e_{ii} > 0, \]  
for all \( i \). Therefore,
\[ \beta_1 \sum_{j=1}^{m} e_{1j} \beta_j > \beta_1 \sum_{j=1}^{m} e_{1j} \beta_m \beta \sum_{j=1}^{m} e_{mj} \beta_j. \]  
(148)

We have used the identities (141) at least two times. From (142), (146) and (148), we find that it is a contradiction. We have completed the proof of the theorem.

**Theorem 3.** The solution of (74) is unique and hence the maximum value obtained by step (ii) is the global maximum on the sphere \( \sum_{i=1}^{n} u_i u_i = r \).

Proof. For simplicity, we use (75), the vector notations, instead of (74). If there are two solutions say \( u \) and \( u' \). Therefore,
\[ \frac{r}{m} \sum_{j=1}^{m} \frac{b_j}{u \cdot b_j} - u = 0, \]  
(149)

And
\[ \frac{r}{m} \sum_{j=1}^{m} \frac{b_j}{u' \cdot b_j} - u' = 0. \]  
(150)

Let
\[ \alpha_k = \frac{1}{u \cdot b_k}, \quad k = 1, 2, ..., m. \]  
(151)

Let
\[ \alpha'_k = \frac{1}{u' \cdot b_k}, k = 1, 2, ..., m. \]  
(152)

Substituting (151) into (149), we get
\[ u = \frac{r}{m} \sum_{j=1}^{m} \alpha_j b_j, \]  
(153)

Substituting (152) into (150), we get
\[ u' = \frac{r}{m} \sum_{j=1}^{m} \alpha'_j b_j. \]  
(154)

Substituting (153) into (151), we get
\[ \alpha_k = \frac{1}{\frac{1}{m} \sum_{j=1}^{m} \alpha_j (b_j \cdot b_k) \sum_{j=1}^{m} \alpha_j (b_j \cdot b_k)}, \quad k = 1, 2, \ldots, m, \]  

(155)

Substituting (154) into (152), we get

\[ \alpha'_k = \frac{1}{\frac{1}{m} \sum_{j=1}^{m} \alpha'_j (b_j \cdot b_k) \sum_{j=1}^{m} \alpha'_j (b_j \cdot b_k)}, \quad k = 1, 2, \ldots, m. \]  

(156)

From (79), (155) and (156), we get two systems of equations

\[ \sum_{j=1}^{m} D_{kj} \alpha_k \alpha_j = 1, \quad k = 1, 2, \ldots, m, \]  

(157)

and

\[ \sum_{j=1}^{m} D_{kj} \alpha'_k \alpha'_j = 1, \quad k = 1, 2, \ldots, m. \]  

(158)

By theorem 2,

\[ \alpha'_k = \alpha_k, \]  

(159)

for \( k = 1, 2, \ldots, m \). From (158), (154) and (159), we get

\[ u' = u. \]  

(160)

And hence the maximum which is obtained in this algorithm is the global maximum on the manifold, the sphere \( \sum_{i} u_i u_i = r \).

**Numerical examples**

No matter how good might the paper be, the final result must be verified by numerical examples. There are three examples. The results are shown in Figure 1, Figure 2 and Figure 3. The estimator is obtained by Bernstein polynomials [2], [3].

Let

\[ \varphi_i(x) = N_i (n!/(i!(n-i)!)) x^i (1-x)^{n-i}, \quad 0 \leq x \leq 1. \]  

(161)

Here, \( N_i \) is a factor to make

\[ \int_{0}^{1} \varphi_i(x) dx = 1. \]  

(162)

Let

\[ \tilde{f}(x) = \sum_{i=1}^{n} c_i \varphi_i(x). \]  

(163)
We use the density estimator which is defined in the very beginning identity \( (6) \) though it is computed by \( (39) \). All the observations, \( x_1, x_2, \ldots, x_m \), must be contained in an interval \([a, b]\). It is a simple work to transform the interval \([a, b]\) to the interval \([0, 1]\).

Example 1.
The density function is defined on \([0, \infty)\),

\[
f(x) = \exp(-x).
\]

Example 2.
The density function is defined on \([0, 4]\),

\[
f(x) = \begin{cases} 2/3, & \text{when } 1 \leq x \leq 2; \\ 1/3, & \text{when } 3 \leq x \leq 4; \\ 0, & \text{otherwise.} \end{cases}
\]

Example 3.
The density function is defined on \([0, 4]\),

\[
f(x) = \begin{cases} 1, & \text{when } 0 \leq x \leq 1/2; \\ 1/2, & \text{when } 1 \leq x \leq 3/2; \\ 1/2, & \text{when } 3 \leq x \leq 7/2; \\ 0, & \text{otherwise.} \end{cases}
\]

The density function of Example 2 and Example 3 are not continuous and hence it is inappropriate to apply Bernstein polynomial to these examples. If the piecewise spline is used, then the result shall be better actually. We will not discuss the piecewise Bernstein polynomial in this paper. Comparing with the existent method [11],[12] etc., the spline kernel or spline window is a new method with potential because there will be new useful splines that might be designed in near future. At least, there are three useful splines, B-spline, Cubic
spline and Bezier spline. The works of source program designing, debugging and maintaining are more difficult than the mathematical proofs because they are tedious works. More than four kernel functions or window functions are tested, including B-spline, overlap B-spline, Bezier spline and piecewise Bezier spline. Though we do not show the result of B-spline approach, most programs are tested by B-spline method first. We will not list the definition of B-spline because it is available to find the definition of the splines in the books of numerical analysis. It seems that B-spline method can be taken as the priori in Bayesian approach and hence piecewise Bezier spline method can be taken as posterior in Bayesian approach. Unlike the Bezier spline, the B-spline need the extra control points, the knot points [2], and these knot points make the programs more complicated and difficult. In the testing program, there are about 300 window functions are used in B-spline method. It is a good experiment to solve about 300 nonlinear equations. The whole work is accomplished by using the oldest fashion and the most modern language, visual fortran. If it is necessary, then the fortran source programs will be appended.

Discussion and conclusion.

The algorithm is so attractive that it is not necessary to prove that these sequences \( u_i^k, v_i^k \) and \( u_i^k v_i^k \), \( i = 1, 2, \ldots, n \) converge. The results of computer output show that these sequences \( u_i^k, v_i^k, u_i^k v_i^k \) converge. Moreover, \( \sum_{i=1}^{n} u_i^k v_i^k \) is an increasing sequence and \( \bar{\theta}^k \) is a decreasing sequence. The algorithm is to maximize likelihood function \( l \) and to terminate the procedures by the condition \( \sum_{i=1}^{n} u_i v_i > r - \varepsilon \). The constraints, \( (47) \) and \( (48) \), are satisfied in every step. Since it has been proved that \( \lim_{k \to \infty} u_i^k = 0 \), all \( |u_i - v_i| \) are very small when the iteration procedures are terminated. In this paper, we do not prove the convergence of the sequences \( u_i^k, v_i^k \) and \( u_i^k v_i^k \), \( i = 1, 2, \ldots, n \). It should be reminded that the problem is to maximize the likelihood function subjected to the conditions \( \sum_{i=1}^{n} u_i u_i = r \) and \( v_i = u_i, i = 1, 2, \ldots, n \). We think that the problem is solved almost. It is still an open problem whether the iterations procedures, step (i), (ii) and (iii), will serve the purpose or not, for finding the global maximum of \( A \)? Of course, step (i) play important role for searching for the global maximum of \( A \), it seems to be so. We think that only if the initial value of \( v_i \) in step (i) is set \( v_i \neq 0 \) for all \( i \), then the procedures will find the global maximum. But the proof is not completed yet. It is the unique theorems, theorem 2 and theorem 3, that simplify the complicated problem and gives us the motivation to prove the global property. Since the consistency of parametric estimator has been proved statistician [1], the only problem left is finding the point which will yield the global maximum of likelihood function. To the best knowledge of the authors, there is no definite answer for finding the global maximum of nonlinear optimization problems. Though the problem do not be solved completely in theory, the work and its related algorithm are very useful in practical problem.

The proof of the lemma 8 is short and simple because this is the final version.
The first version is abandoned because it is lengthy and complicated. In the first version of the proof, we use the method of variation. The technique of the first proof in lemma 8 is almost the same as that of quantum physics, especially in quantum field theory and string theory [13].

To follow the approach of most nonparametric approaches, we use the advantage the probability amplitude which is introduced in the quantum theory. Though the orthogonal polynomials are also used in both nonparametric approaches and quantum theory, we use the Bernstein polynomial. It is the Bernstein polynomials that unify and simplify fundamental problems such as parametric approach and nonparametric approach, consistency of the estimator and the most difficult problem of density estimation, the nonlinear optimization problem. The probability amplitude is stressed most books of quantum physics [14].

It should be clarified that the research work is initiated and completed finally by Yeong-Shyeong Tsai. Without the consultation with Lu-Hsing Tsai, Hung-Ming Tsai and Po-Yu Tsai in quantum physics and personal computing system, and the consultation with Yin-Lin Hsu in statistics, the paper can not be completed.

Allow us to discuss more mathematics. Since quantum theory is built on the Hilbert space, the physicists use the complete sets of the space. Therefore, the statisticians working on nonparametric approach use the same tool as physicists. In order to avoid the roughness introduced by the complete sets, we use the result of Stone-Weirstrass theorem. If it is necessary, then we will treat the space of continuous functions or measurable functions as metric space or topological space. Therefore, we use countable dense subset of the space, the set of Bernstein polynomials.

References

[1]. A. Wald, (1949),” Note on the Consistency of the Maximum Likelihood Estimate,” The Annal of Mathematical Statistics, Vol. 20, No. 4 pp. 595-601.
[2]. W. M. Newman and R. F. Sproull, “Principle of Interactive Computer Graphics”, McGraw-Hill, New York, (1979), pp. 309-331.
[3]. A. Quarteroni, R. Sacco and F. Saleri, ”Numerical Mathematics”, Springer, (2000), pp 361-375.
[4]. Tom M. Apostol, “ Calculus ”, Vol. 1 John Wiley & Sons, (1967), pp.374-443.
[5]. Tom M. Apostol, “ Mathematical Analysis”, Addison-Wesely, (1974), pp.183-247, pp.322.
[6]. R. O. Duda and P. E. Hart, “Pattern Classification and Scene Analysis ”. John Wiley, (1973), pp. 85-91.
[7]. S. Lang, “linear Algebra”, Springer: 3rd ed., (1976), pp.125-131.
[8]. D. G. Luenberger, “Optimization By Vector Space Methods,” Wiley (1969), pp.239-265.
[9]. I. J. Good and R. A. Gaskins, Biometrika, Vol. 58, No. 2, (1971), pp. 255-277
[10]. I. J. Good and R. A. Gaskins, Journal of the America Statistical Association, Vol. 75, No. 369, (1980), pp.42-73.
[11]. M. X. Dong and R. J-B. Wetes, “Estimating Density Functions: a Constrained Maximum Likelihood Approach,” Journal of Nonparametric statistics, Vol. 12, (2000), pp. 549-595.
[12]. I. A. Ahmad and I. S. Ran, “Kernel Contrast: A Data-Based Method Of Choosing Parameters In Nonparametric Density Estimation,” Journal of Nonparametric Statistics, Vol. 16(5), (2004), pp. 671-707.
[13]. B. Hatfield, “Quantum Field Theory of Particles and Strings,” (1992), pp.20, pp. 698.
[14]. J. S. Townsend, “A Modern Approach to Quantum Mechanics”, McGraw-Hill, (1992), pp.1-24.

Figure 1: The density function is exp(-x). The sample size is 80. There are 11 windows of Bezier spline, n=10.
Figure 2: The density function is bimodal. The domain is \([0,4]\). \(f(x)=\frac{2}{3}\) when \(x\) is in \([1,2]\); \(f(x)=\frac{1}{3}\) when \(x\) is in \([3,4]\); \(f(x)=0\), otherwise. The sample size is 180. There are 35 windows of Bezier spline.
Figure 3: The density function is trimodal. The domain is $[0,4]$. $f(x)=1$ when $x$ is in $[0,1/2]$; $f(x)=1/2$ when $x$ is in $[1,3/2]$; $f(x)=1/2$ when $x$ is in $[3,7/2]$; $f(x)=0$, otherwise. The sample size is 180. There are 35 windows of Bezier spline.