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RESEARCH ARTICLE

BIHARMONIC FUNCTION OF PROTEIN IN MOCORIN AND ITS OPTIMIZATION

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ABSTRACT

Nutritional values of MOCORIN (Modification Of Bisi 2 Variety Yellow Corn (*Zea Mays L.*) - Rice Bran Flour) are studied based on the used mass, i.e. carbohydrate and protein. Optimal protein in MOCORIN is studied due to the observed carbohydrate and mass from 5 types of data which are mixtures of yellow corn and rice bran. There are 5 types proportion used in the observation. The proportions of rice bran are 0% (only yellow corn), 12.5%, 25%, 37.5%, 50% respectively. The purpose of the research is to determine best proportion with maximum protein leading to optimization problem. By assuming protein follows a biharmonic function, the function is possible to be convex or concave. Therefore one cannot have only maximum value of protein. Hessian matrix and convexity properties are used and the result shows that 37.5% of rice bran is the best proportion.

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INTRODUCTION

There are two objective functions required to set up optimization problem based on the given data, i.e. the first objective function is due to parameter determination and the second one is due to optimal values of the obtained objective function after the parameters are found. Before solving the second optimization problem, some basic properties must be known, i.e. convexity of the chosen objective function in a convex domain leading to minimum value of the objective function and a concave function in a concave domain leading to maximum value. However two properties may be hold locally in some sub domains. This situation is found in this paper since the given data provide these two properties, i.e. convexity and concavity of the obtained objective function. Hence to model a minimization problem one needs convexity of an objective function and only some data satisfy convexity. Five sets of data are taken from observation of nutritional values of MOCORIN (Modification Of Bisi 2 Variety Yellow Corn (*Zea Mays L.*) - Rice Bran Flour) in Chemistry Department of SWCU 2012 where some experiments were set up to study moisture content, mineral content, protein content by biuret method, fat content, carbohydrate content by anthrone method, fiber content and making of "cat's tongue" cookies.

The materials were the mixtures between yellow corn and rice bran with proportion 0%, 12.5%, 25%, 37.5%, 50% respectively (Silvia, 2012). Since there are 5 sets of data, there will be 5 objective functions to optimize. Each set has a set of parameters that relates to each objective function. We focus on this study by considering that the protein content depends on mass and carbohydrate contents. The optimal values of protein are determined due to the mass and carbohydrate in the materials and one yields best proportion. Some variables must be introduced which are all dimensionless, i.e. all variables are in the interval (0,1], these are : $M :=$ mass ; $K :=$ carbohydrate; and $P :=$ protein.

In this research, we consider firstly that protein (P), carbohydrate (K) and mass (M) are dependent variables as function of absorbance as independent variable. By interpolating each variable to the used absorbance, protein is then considered to be dependent variable and carbohydrate and mass are its independent variable. Assuming protein as a biharmonic function of carbohydrate and mass, one has 5 continuous explicit form of objective functions. Construction of biharmonic function and some underline theories are shown in the next sections. The results of its optimization are discussed in the analysis.

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DESIGN OF OBJECTIVE FUCTION AND ITS OPTIMIZATION

Construction of Biharmonic function for model of protein in MOCORIN

Biharmonic function can be considered as a solution of biharmonic operator in the form of forth order of partial differential equation. One possible solution is a linear combination of Green functions centered at each data point for one dimensional biharmonic operator. In two dimensional case, Green functions were applied to create interpolation technique (Sandwell, 1987) to produce and accurate sea surface topography maps from satellite altimeter profiles. In this paper, the biharmonic function is the solution of the forth order of partial differential equation in the form

$$\frac{\partial^4 P}{\partial K^4} + 2 \frac{\partial^4 P}{\partial M^2 \partial K^2} + \frac{\partial^4 P}{\partial M^4} = 0 \quad \dots\dots\dots (1)$$

The analytic representation of $P(K,M)$ had been known (Ugail,2006) and its representation was a combination of a searable function, i.e

$$P(K, M) = X(K) \cos(nM) + X(K) \sin(nM) \quad \dots\dots\dots (2)$$

where n is an integer number and $X(K)$ was also investigated (Ugail, 2006), that is

$$X(K) = c_1 e^{nK} + c_2 K e^{nK} + c_3 e^{-nK} + c_4 K e^{-nK} \quad \dots\dots\dots (3)$$

The parameters are c_1, c_2, c_3, c_4 and n were analytically completely defined. However in order to simplify the procedure, we use least square method to find the best c_1, c_2, c_3, c_4 . As soon as these parameters are found, minimize

$$R = \sum_{i=1}^N (P_{i,data} - P_{i,model})^2 \quad \dots\dots\dots (4)$$

where $P_{i,model}$ given by Eq. (2)-(3) . Denoting \vec{y} to be the vector in R with each component is

$$y_i = P_{i,data} - P_{i,model}, \forall i,$$

then Eq.(4) in vector form is $R = \vec{y}^T \vec{y}$ and the best parameters c_1, c_2, c_3, c_4 must satisfy $\nabla R = \vec{0}$. Solving this nonlinear system leads to find critical solution of R .

Optimization of biharmonic function with Karush Kuhn Tucker theorem

Karush Kuhn-Tucker theorem (Peressini,et.al.1987) guarantees the existence of solution in the convex domain (D) due to the minimization Lagrangian

$$L(K, M, \lambda) = f(K, M) + \sum_{i=1}^n \lambda_i g_i(K, M) \text{ as a convex program, i.e.:}$$

$$\text{minimize } f(K, M) \quad \dots\dots\dots (5)$$

subject to the constraints

$$g_i(K, M) \leq 0 \quad \dots\dots\dots (6)$$

where $\vec{x} = [K, M]^T \in D$.

The optimizer $\vec{x}^* = [K^*, M^*]^T$ exists if only if there is a $\lambda^* \in R^n$ such that

- i. $\vec{\lambda}^* \geq \vec{0}$
- ii. $L(\vec{x}^*, \vec{\lambda}) \leq L(\vec{x}^*, \vec{\lambda}^*) \leq L(\vec{x}^*, \vec{\lambda})$ for all $\vec{x} = [K, M]^T$ and for all $\vec{\lambda} \geq \vec{0}$
- iii. $\lambda_i^* g_i(\vec{x}^*) = 0$ for $i=1,2,\dots,m$.

The proof has been shown rigorously (Peressini,et.al,1987) and the fmincon.m function provided by MATLAB will be implemented to find the optimizers automatically without solving the gradient of L . The sufficient conditions for the local optimal $\vec{x}^* = [K^*, M^*]^T$ are

- i. $\vec{\lambda}^* \geq \vec{0}$
- ii. $\mu_i^* g_i(\vec{x}^*) = 0 \forall i \in I$.
- iii. $\nabla f(\vec{x}^*) + \sum_{i=1}^m \lambda_i^* \nabla g_i(\vec{x}^*) = 0$.

The optimization result will be analyzed based on this theorem. Defining the problem into standard problem in Eq.(4) and Eq.(5) in fmincon.m, one yields the optimizers. Additionally, the convexity of the objective function is also required where we assume that the given domain is a convex subset D of R^n . By assuming $f(K, M)$ has continuous first partial derivatives on D , then the function $f(\vec{x}) = f(K, M)$ is convex if and only if

$$f(\vec{x}) + \nabla f \circ (\vec{y} - \vec{x}) \leq f(\vec{y}) \text{ for all } \vec{x}, \vec{y} \text{ in } D \dots\dots\dots (6)$$

One may recall the complete proof in the literature (Peressini,et.al,1987,pp.52-53). There exists another definition of convexity which depends on a parameter and ∇f is not required. For simplicity, we will use the definition given by Eq.(6). However the objective function needs to be maximized, and hence instead of convexity, one needs the objective function must be concave, which means that the inequality sign in Eq.(6) must be defined reversely. Unfortunately, each variable depends on the used absorbance. To reduce this difficulty, all necessary variables are interpolated as functions of absorbance

Interpolation of Protein, Carbohydrate and Mass into functions of absorbance

Linear interpolation is one of the most widely used interpolation techniques where the usual least square leads to a

problem of solving the linear system $\bar{a} = (J^T J)^{-1} J^T \bar{y}$ and hence the approximation will be $\tilde{y} = J \bar{a}$ where J is a matrix with its i -th row contains $\{1 \ z_i \ z_i^2 \ z_i^3 \dots z_i^M\}$ (Yang *et al.*, 2005). This type of interpolation is not good enough for high oscillation data and small number of samples. Higher order polynomial frequently leads to singular matrix of $J^T J$ for such data. We prefer to use spline interpolation for our data set. Exercises data are presented in Table 1. Table 1 gives us two sets of values of z which are given in the first column and the third column. Spline interpolation relies on piecewise cubic polynomial interpolation on each two pairs consecutive data where the derivatives of each polynomial on each subinterval are taken into account. One of examples in our research was that this method had been used to interpolate spectrum of β charoten through acetone (Parhusip *et al.* 2005).

Table 2. Variation error due to stepsize of absorbance

Size of stepsize	Error of biharmonic function (%)
0.01	20.9628
0.02	21.0393
0.03	11.1217
0.04	31.5323
0.05	10.5954
0.06	33.0270

Protein as a Biharmonic function of carbohydrate and mass

In this case protein is assumed to be the dependent variable where mass and carbohydrate are the independent variables. To guarantee that the objective function is good enough, we observe for several step sizes and study the resulting errors as shown in Table 2. For the given data Table 1, we have the error may decrease for a bigger step size and hence we will vary the step size for the whole given data in the research which is shown in Results and Discussion.

Table 1. Some lists of data obtained by observation (dimensionless) of absorbance, protein and carbohydrate with no addition of rice bran (in the proportion 100% of yellow corn)

Absorbance used for protein	Protein	Absorbance used for carbohydrate and mass	Carbohydrate	Mass
0.9899	0.2296	0.9792	0.8689	0.6882
0.9975	0.2437	0.9431	0.8359	0.6882
1.0000	0.2484	0.8793	0.7775	0.6882
0.4605	0.1855	1.0000	0.8880	0.6882
0.4782	0.2516	0.8849	0.7825	0.6882
0.4731	0.2327	0.9293	0.8232	0.6882
0.4924	0.2579	0.5298	0.8733	0.7207
0.4992	0.2830	0.5132	0.8442	0.7207
0.7286	0.1871	0.5381	0.8879	0.7207
0.2798	0.2201	0.5146	0.8223	0.7420
0.2832	0.2327	0.5451	0.8742	0.7420
0.2899	0.2579	0.5423	0.8695	0.7420
0.3706	0.2579	0.4951	0.8334	0.7028
0.3513	0.1855	0.5160	0.8707	0.7028
0.3563	0.2044	0.5687	0.9653	0.7028

Advantages of this method are that we do not need to choose any smooth function explicitly and additional data can be generated to fit with original data. The function is available in MATLAB 6.5 (or higher version) that can be used easily. Suppose some of the given data absorbance and the related carbohydrates are given in Table 1. The Spline method leads to generate additional data that depend on the used step size in the spline function provided by MATLAB. For instance, the number of original data is 15, the number of data becomes 721 by using step size 0.001 on absorbance. If the used step size too small (e.g. :0.001), the error of harmonic function is too big (> 30%) and hence we choose bigger step size. Using 0.01 step size of absorbance, the error harmonic function is 20.9628 %. The comparison of each data and the approximation is shown in Figure 4 and Figure 5. The error function becomes 21.0393% if we use step size 0.02. Numerical examples are shown in Figure 1-3. The spline curves present the protein and carbohydrate as functions of absorbance. Data are generated by spline will be used in Eq (2)-(3) to define the objective function.

Each set of data indicated by observation set of each proportion has some multiples values which lead to technical errors. The error is shown by comment MATLAB's spline() function complains that "the data sites should be distinct". Referring to some comments of programmers in webs, one may replace the function spline with parametric representation of data and using interp1() function provided in MATLAB. Thus two kinds of interpolation functions are employed here to present protein, carbohydrate and mass as functions of absorbance.

RESULTS AND DISCUSSION

Convexity and concavity of biharmonic function

The convexity and concavity are required conditions for the existences of optimal of objective functions. Therefore here the convexity and concavity are studied for each set of data based on Eq.(6). Some observation are shown in the Figure 6.a-6.e. For 5 data sets, we have the biharmonic functions are possible

to be convex and concave. Figure 6.a-6.c illustrate that the biharmonic functions for the first three data sets are convex. The fourth data set is concave and the last one is nearly undetected. The practical application based on this result is that if the proportion of yellow corn and rice bran in the type of 87.5%:12.5% and 50%:50% then maximum protein will not be obtained. This research suggests that one may use 62.5%:37.5% for gaining maximum protein where mass and carbohydrate contents have been taken into account.

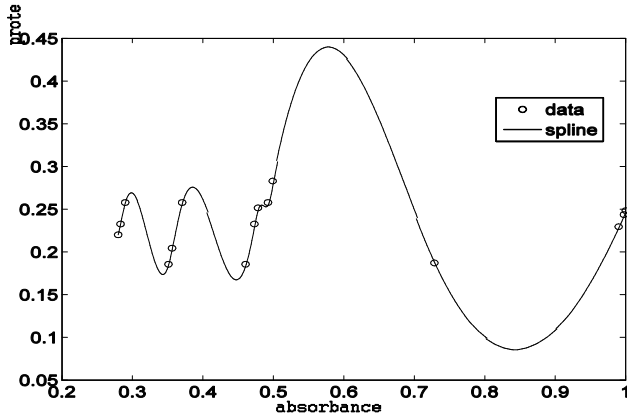


Figure 1. Protein is fitted as a function of absorbance.

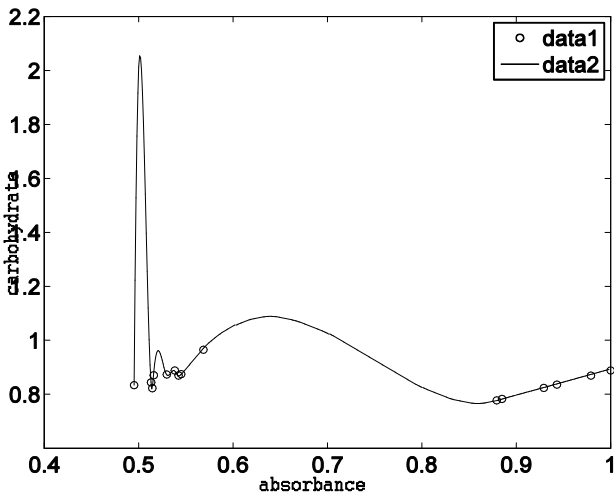


Figure 2. Carbohydrate is fitted as a function of absorbance

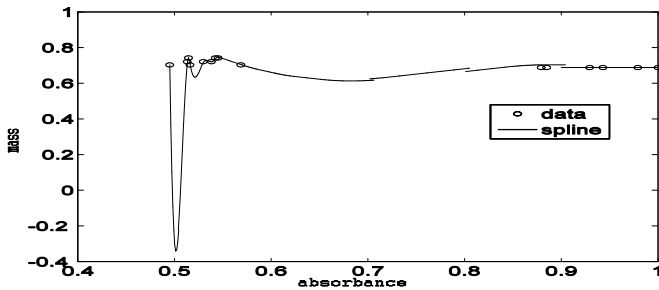


Figure 3. Spline interpolation of mass as a function of absorbance

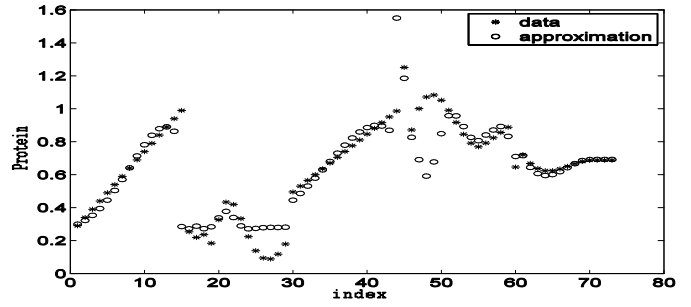


Figure 4. Protein is a harmonic function of carbohydrate and mass compared to data obtained by spline.

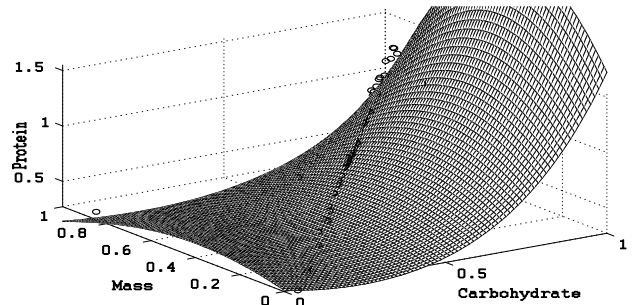


Figure 5. Protein is a harmonic surface of carbohydrate and mass with error 20.9628%.

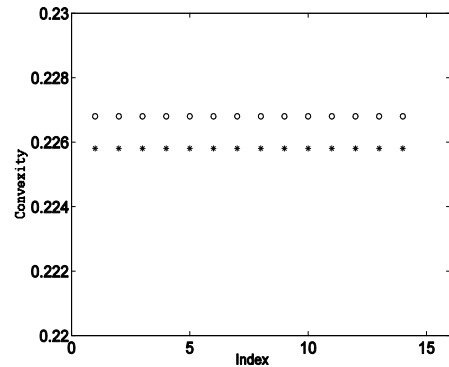


Figure 6.a. Convexity of biharmonic function from the set of data with proportion of yellow corn and rice bran is 100%:0%; o: denotes the right hand side of Eq.(6), *: denotes the left hand side of Eq.(6).

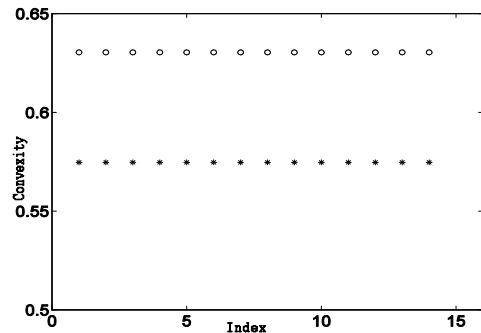


Figure 6.b. Convexity of biharmonic function from the set of data with proportion of yellow corn and rice bran is 87.5%:12.5%; o: denotes the right hand side of Eq.(6), *: denotes the left hand side of Eq.(6)

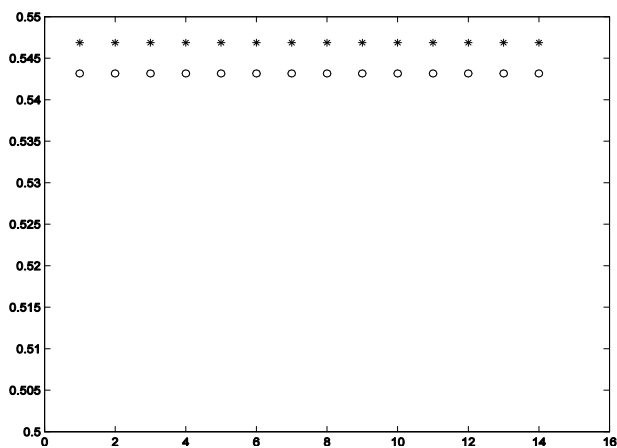


Figure 6.c. Convexity of biharmonic function from the set of data with proportion of yellow corn and rice bran is 75%:25%; o: denotes the right hand side of Eq.(6),*: denotes the left hand side of Eq.(6).

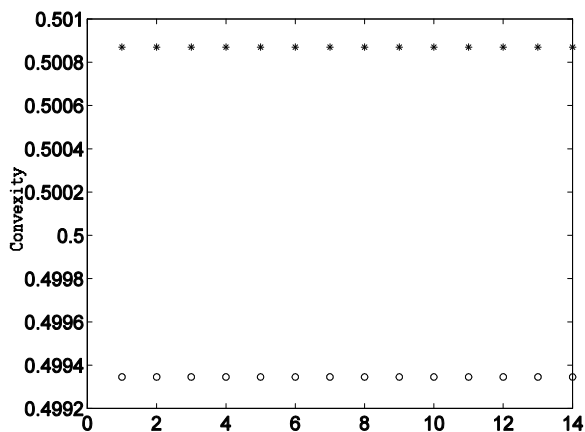


Figure 6.d. Convexity of biharmonic function from the set of data with proportion of yellow corn and rice bran is 62.5%:37.5%; o: denotes the right hand side of Eq.(6),*: denotes the left hand side of Eq.(6).

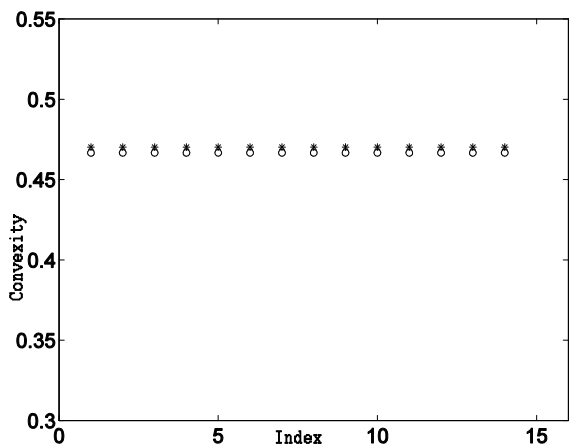


Figure 6.e. Convexity of biharmonic function from the set of data with proportion of yellow corn and rice bran is 50%:50%; o: denotes the right hand side of Eq.(6),*: denotes the left hand side of Eq.(6).

Construction of biharmonic function and its maximum

All observation data are used, i.e. each proportion contains observation of protein content, carbohydrate and mass contents. We have 5 sets of these type of data. Thus we have 5 sets of parameters in Eq.(2)-(3). Using lsqnonlin.m function provided by MATLAB, one obtains the parameters listed in

Table 3. These parameters are then implemented to the objective functions subject to the given constraints, i.e. the minimum of each independent variable. The objective function becomes : maximize protein subject to the constraints : $M \geq M_{min}$ and $K \geq K_{min}$.

Table 3. Parameter values in biharmonic function of each set of data and its error

Type of Mocaroin (Proportion) Yellow corn: rice bran	Biharmonic parameters $\vec{c} = [c_1 \ c_2 \ c_3 \ c_4 \ c_5]^T$					Error function (%)
0%	-0.2724	0.4762	0.3118	1.7113	2	11.8218
12.5%	-0.7571	0.8962	0.0454	6.4448	2	4.9585
25%	-0.7528	0.8845	0.0575	6.4954	2	5.8468
37.5%	-0.5355	0.7127	0.2671	4.0530	2	4.1528
50%	-0.4049	0.5908	0.2061	3.1654	2	4.6074

Without these bounds, negative values may occur which are not realistic in practical application. The fmincon.m function is implemented to obtain minimum value of protein. Since the maximum value of protein of each set is 1, then the maximum will be 1 minus the obtained minimum and the result shown in Table 4. Table 4 shows the maximum protein with optimal carbohydrate and mass of each proportion. Mathematically, each surface has its own local maximum and local optimizer. Of course, we may consider 37.5 % addition of rice bran is the best proportion to produce maximum protein. Its harmonic surface is shown in Figure 7. Each item of data and its approximation is depicted in Figure 8. Though 0% has no significant different result compared to 37.5% of rice bran, we cannot rely on 0% result since it means no rice bran is added. Statistical result (Silvia, 2012) has shown that the proportion of 50% of rice bran give the maximal protein where protein here was not considered as a function of mass and carbohydrate.

As we expected, that the optimal carbohydrate and mass satisfy the given constraints. Additionally, the forth data set have shown the maximum protein and the biharmonic function is concave. Therefore this result satisfies the underline theory shown in Section 2.

Table 4. Optimizers (Carbohydrate and Mass) and the corresponding maximal protein (P*)

Proportion	(K*, M*)	Maximal protein (P*)	Minimal K	Minimal M
0%	(0.1855; 0.7420)	0.8187	0.1855	0.6882
12.5%	(0.5610, 0.7188)	0.5380	0.5610	0.6822
25%	(0.5454, 0.9714)	0.7702	0.5454	0.6742
37.5%	(0.5066, 1)	0.8215	0.5066	0.6636
50%	(0.4663, 0.7487)	0.6439	0.4663	0.6755

Analysis of optimality of parameters

Note that two optimization problems appear in this research, i.e. optimization due to parameter determination of biharmonic function and optimization due to maximization of protein. In the first case, one needs to solve the critical condition to determine best parameters of biharmonic function. Thus, $\nabla R = \vec{0}$. Suppose that R can be written in vector form :

$R = \vec{y}^T \vec{y}$ with \vec{y} denotes the coloum vector which its component $y_i = P_{i,data} - P_{i,model}$ Therefore the

components ∇R are : $\frac{\partial R}{\partial c_j}$ for $j=1, \dots, 4$. One yields

$$\frac{\partial R}{\partial c_1} = 2\vec{y} \cdot \nabla_{c_1} \vec{y} \text{ with } \{\nabla_{c_1} \vec{y}\} = -(e^{nK_i}) (\cos nM_i + \sin nM_i) \dots \quad (7.1)$$

denotes the i -th component of $\nabla_{c_1} \vec{y}$ Similarly one has

$$\frac{\partial R}{\partial c_2} = 2\vec{y} \cdot \nabla_{c_2} \vec{y}; \frac{\partial R}{\partial c_3} = 2\vec{y} \cdot \nabla_{c_3} \vec{y}; \frac{\partial R}{\partial c_4} = 2\vec{y} \cdot \nabla_{c_4} \vec{y} \dots \dots \dots \quad (7.2)$$

where

$$\begin{aligned} \{\nabla_{c_2} \vec{y}\}_i &= -(K_i e^{nK_i}) (\cos nM_i + \sin nM_i); \\ \{\nabla_{c_3} \vec{y}\}_i &= -(e^{-nK_i}) (\cos nM_i + \sin nM_i); \\ \{\nabla_{c_4} \vec{y}\}_i &= -(K_i e^{-nK_i}) (\cos nM_i + \sin nM_i) \dots \dots \dots \quad (7.3) \end{aligned}$$

Solving $\nabla R = \vec{0}$ given by Eq.(7.1)-(7.3), we obtain the critical solution which some possible answers shown in Table 3. Since results in Table 3 are obtained through lsqnonlin.m, we will analyze the result by substituting these values in Table 3 in Eq.(7.1)-(7.3). The computation shows that the condition $\nabla R = \vec{0}$ is violated though the given error less than 20% for each data set. We leave this situation for further study.

Hessian matrix

The properties of symmetrical Hessian matrix of objective function can also be used as identifiers of optimality. This idea has been applied to select data before presenting further optimization based on the underline theory (Parhusip, 2009). We know that

$$\begin{aligned} \frac{\partial R}{\partial c_1} &= 2\vec{y} \cdot \nabla_{c_1} \vec{y} \text{ with} \\ \{\nabla_{c_1} \vec{y}\} &= -(e^{nK_i}) (\cos nM_i + \sin nM_i) \dots \dots \dots \quad (8) \end{aligned}$$

The first component of Hessian matrix is

$$\frac{\partial^2 R}{\partial c_1^2} = 2(\nabla_{c_1} \vec{y} \cdot \nabla_{c_1} \vec{y} + \vec{y} \cdot \nabla_{c_1} (\nabla_{c_1} \vec{y})).$$

Notice that $\nabla_{c_1} (\nabla_{c_1} \vec{y}) = 0$, therefore $\frac{\partial^2 R}{\partial c_1^2} = 2\nabla_{c_1} \vec{y} \cdot \nabla_{c_1} \vec{y}$.

The other components are derived similarly, we get

$$\begin{aligned} \frac{\partial^2 R}{\partial c_1 c_2} &= 2(\nabla_{c_2} \vec{y} \cdot \nabla_{c_1} \vec{y} + \vec{y} \cdot \nabla_{c_2} (\nabla_{c_1} \vec{y})) = 2\nabla_{c_2} \vec{y} \cdot \nabla_{c_1} \vec{y} \\ \frac{\partial^2 R}{\partial c_1 c_3} &= 2(\nabla_{c_3} \vec{y} \cdot \nabla_{c_1} \vec{y} + \vec{y} \cdot \nabla_{c_3} (\nabla_{c_1} \vec{y})) = 2\nabla_{c_3} \vec{y} \cdot \nabla_{c_1} \vec{y} \\ \frac{\partial^2 R}{\partial c_1 c_4} &= 2(\nabla_{c_4} \vec{y} \cdot \nabla_{c_1} \vec{y} + \vec{y} \cdot \nabla_{c_4} (\nabla_{c_1} \vec{y})) = 2\nabla_{c_4} \vec{y} \cdot \nabla_{c_1} \vec{y}. \end{aligned}$$

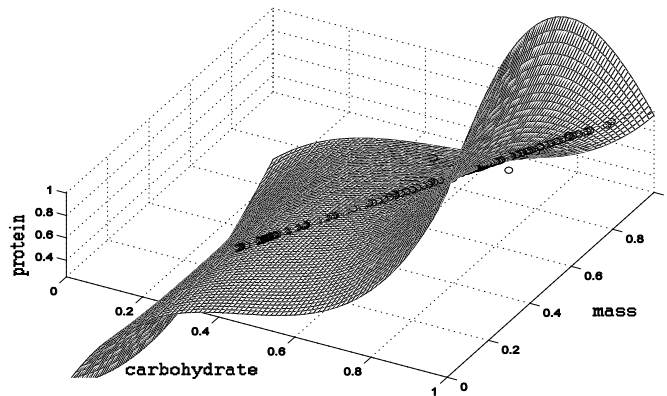


Figure 7. Biharmonic surface of protein from 37.5 % of rice bran into MOCORIN

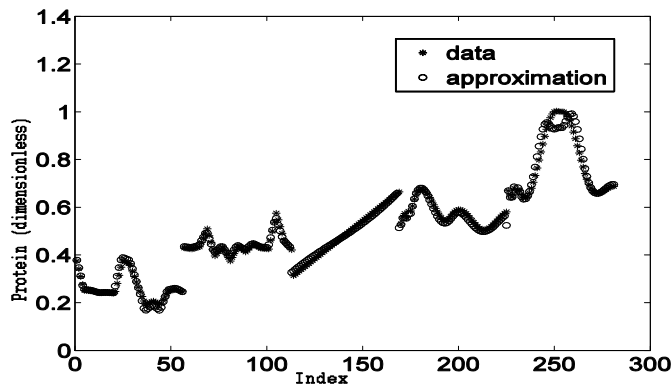


Figure 8. Comparison protein as a biharmonic function and the given data with proportion 37.5% of rice bran

One yields the general form of the component of Hessian of R in the form

$$\frac{\partial^2 R}{\partial c_j^2} = 2\nabla_{c_j} \bar{y} \cdot \nabla_{c_j} \bar{y} ; \frac{\partial^2 R}{\partial c_j \partial c_k} = 2\nabla_{c_k} \bar{y} \cdot \nabla_{c_j} \bar{y}, i,j=1,\dots,4.$$

The eigen values of Hessian matrix of R have been computed and all eigen values have nonnegative values which indicate that R has been minimized for the obtained parameters. Thus, though $\nabla R = \vec{0}$ is violated for each data set, one still has a sufficient condition for existence of the obtained optimal parameters. The computation result shown in Table 5 (third coloum).

Analysis of optimal values of the objective function

As stated above, we have used `fmincon.m` function in MATLAB to solve the optimization problem. However the convexity of the harmonic function has not been yet validated. Therefore Eq.(6) is used and implemented into MATLAB program. Obviously, the objective function is infinitely continuous differentiable function in the given domain D (where has been transformed into $(0,1] \times (0,1]$) since its form is a combination of exponential and sinus,cosinus functions.

Therefore it is guaranteed the existent of ∇f , i.e.

$$\nabla f = \left[\frac{\partial f}{\partial K} \quad \frac{\partial f}{\partial M} \right]^T \text{ where}$$

$$\frac{\partial f}{\partial K} = \frac{\partial X(K)}{\partial K} \cos(nM) + \frac{\partial X(K)}{\partial K} \sin(nM)$$

and

$$\frac{\partial f}{\partial M} = nX(K) \sin(nM) + nX(K) \cos(nM)$$

Separation variables of f leads to simpler derivation of ∇f . According to the given data, we have 5 sets of data and hence we will analyze of each data set. The obtained parameters are substituted and we expect ∇f is zero in the sense of norm. One may observe that only the third type set of data does. Future observation is suggested to improve the algorithm for better achievement of optimality.

Conclusion

Biharmonic function has been constructed for the given data of protein, carbohydrate and mass of MOCORIN (Modification Of Bisi 2 Variety Yellow Corn (*Zea Mays* L.) - Rice Bran Flour). Each variable is an interpolation of absorbance. There are 5 types of proportion of yellow corn and rice bran. This research determines the best proportion of yellow corn and rice bran. i.e. the proportion with maximum protein. One yields that 37.5% of rice bran is the best proportion for maximizing the obtained protein.

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