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Mathematical Expressions for Estimation of Errors in the Formulas which are used to obtaining intermediate values of Biological Activity in QSAR

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ABSTRACT: Quantitative structure-activity relationships (QSAR) attempts to find consistent relationships between the variations in the values of molecular properties and the biological activity for a series of compounds. These physicochemical descriptors, which include parameters to account for hydrophobicity, topology, electronic properties, and steric effects, are determined empirically or, more recently, by computational methods. Quantitative structure-activity relationships (QSAR) generally take the form of a linear equation where the biological activity is dependent variable. Biological activity is depended on the parameters and the coefficients. Parameters are computed for each molecule in the series. Coefficients are calculated by fitting variations in the parameters. Intermediate values of the biological activity are obtained by some formulas. These formulas are worked in tabulated values of biological activity in Quantitative structure-activity relationships. These formulas are worked in the conditions and all conditions are based on the position of the point lies in the table. Derived formulas using Newton's method for interpolation are worked in conditions which are depending on the point lies. If the point lies in the upper half then used Newton's forward interpolation formula. If the point lies in the lower half then we used Newton's backward interpolation formula. And when the interval is not equally spaced then used Newton's divide difference interpolation formula. When the tabulated values of the function are not equidistant then used Lagrangian polynomial. Mathematical expressions are derived for estimation of errors using intermediate values and formulas.

KEYWORDS: Biological activity, Estimation of Errors, Intermediate values, Mathematical Expressions, QSAR.

1 INTRODUCTION

Quantitative structure-activity relationships (QSAR) represent an attempt to correlate structural or property descriptors of compounds with activities. These physicochemical descriptors, which include parameters to account for hydrophobicity, topology, electronic properties, and steric effects, are determined empirically or, more recently, by computational methods. Activities used in QSAR include chemical measurements and biological assays [1]-[5].

A QSAR generally takes the form of a linear equation

$$\textit{Biological Activity} = \textit{Constant} + (C_1 \bullet P_1) + (C_2 \bullet P_2) + (C_3 \bullet P_3) + \ldots \qquad (1)$$

Where the parameters P_1 through P_n are computed for each molecule in the series and the coefficients C_1 through C_n are calculated by fitting variations in the parameters and the biological activity [1].

If $$f(CP) = \textit{Constant} + (C_1 \bullet P_1) + (C_2 \bullet P_2) + (C_3 \bullet P_3) + \ldots\ldots$$

From equation (1), we got:

$$BA = f(CP)$$

Suppose $CP = X$ then we can write more simple form: $BA = f(X)$

Where BA is biological activity and X is variable from above function [1]. Some formulas are derived on the basis of this function using Newton's method for interpolation and Lagrangian polynomial. These formulas are used to obtaining intermediate values of the biological activity. Derived formulas using Newton's method for interpolation are worked in conditions which are depending on the point lies. If the point lies in the upper half then used Newton's forward interpolation formula. If the point lies in the lower half then we used Newton's backward interpolation formula. And when the interval is not equally spaced then used Newton's divide difference interpolation formula. When the tabulated values of the function are not equidistant then used Lagrangian polynomial [6]-[22].

2 If the Point Lies in the Upper Half

Let $BA = f(X)$ be a function defined by n points $(BA_0, X_0),(BA_1, X_1)\ldots\ldots\ldots(BA_n, X_n)$. Where BA is biological activity and X is the variable. When $X_1, X_2, X_3\ldots\ldots\ldots\ldots X_n$ are equally spaced with interval h. And If the point lies in the upper half then we used following formula [1] [7]-[9]:

$$BA(X) = BA_0 + \Delta BA_0(q) + \frac{\Delta^2 BA_0}{2!}(q)[(q-1)]\ldots\ldots + \frac{\Delta^n BA_0}{n!}[(q)(q-1)\ldots(q-n)]$$

[Where Δ is forward difference operator and $\frac{X - X_0}{h} = q$]

2.1 Estimation of Error

Let $BA = f(X)$ be a function defined by $(n+1)$ points $(BA_0, X_0),(BA_1, X_1)\ldots\ldots\ldots(BA_n, X_n)$. When $X_1, X_2, X_3\ldots\ldots\ldots\ldots X_n$ are equally spaced with interval h and this function is continuous and differentiable $(n+1)$ times.

Let $BA = f(X)$ be approximated by a polynomial $P_n(X)$ of degree not exceeding a such that

$$P_n(X_i) = BA_i \qquad \text{[Where } i = 1,2,3\ldots\ldots\ldots\ldots n\text{]} \tag{2}$$

Since the expression $f(X) - P_n(X)$ vanishes for $X_1, X_2, X_3\ldots\ldots\ldots\ldots X_n$,

We put $f(X) - P_n(X) = K\phi(X)$ (3)

Where $\phi(X) = (X - X_0)(X - X_1)\ldots\ldots\ldots\ldots(X - X_n)$ (4)

And K is to be determined in such a way that equation (3) holds for any intermediate values of X, say $X - X'$ [where $X_0 \le X' \le X_n$].

Therefore from (3): $K = \frac{f(X') - P(X')}{\varphi(X')}$ (5)

Now we construct a function $f(X)$ such that: $f(X_0) = f(X_1) - P_n(X) - K\varphi(X)$

Where K is given by equation (5).

It is clear that: $f(X_0) = f(X_1) = f(X_2) = f(X_3) = \ldots\ldots\ldots\ldots f(X_n) = f(X') = 0$ (6)

Let $f(X)$ vanishes $(n+2)$ times in the interval $X_0 \le X \le X_n$; consequently, by the repeated application of Rolle's Theorem [23] [24], $f'(X)$ must vanish $(n+1)$ times, $f''(X)$ must vanish n times etc in the interval $X_0 \le X \le X_n$.

Particularly, $f^{(n+1)}(X)$ must vanish once in the interval $X_0 \le X \le X_n$. Let this point be $X = U,\ X_0 < W < X_n$.

Now differentiating equation (6) $(n+1)$ times with respect to X and putting $X = U$, we got:

$$f^{(n+1)}(U) - K(n+1)! = 0$$

Or $$K = \frac{f^{(n+1)}(U)}{(n+1)!} \tag{7}$$

Putting this value of K in equation (5), we got: $\frac{f^{(n+1)}(U)}{(n+1)!} = \frac{f(X') - P_n(X')}{\varphi(X')}$

Or $$f(X') - P_n(X') = \frac{f^{(n+1)}(U)}{(n+1)!}\varphi(X'), \qquad X_0 < U < X_n$$

Since X' is arbitrary therefore on dropping the prime on X' we got:

$$f(X) - P_n(X) = \frac{f^{(n+1)}(U)}{(n+1)!}\varphi(X), \quad X_0 < U < X_n \tag{8}$$

Now we use Taylor's theorem [25] [26]: $f(X+h) = f(U) + hf'(U) + \frac{h^2}{2!}f''(U) + \dots\dots\dots + \frac{h^n}{n!}f^n(U) + \dots\dots$ (9)

Neglecting the terms containing second and higher powers of h in equation (9), we got:

$$f(U+h) = f(U) + hf'(U)$$

Or $$f'(U) = \frac{f(U+h) - f(U)}{h} \tag{10}$$

Or $$f'(U) = \frac{1}{h}\Delta f(U) \qquad [\therefore \Delta f(X+h) f(X)]$$

$$Df(U) = \frac{1}{h}\Delta f(U) \qquad [\therefore D = \frac{d}{dU}]$$

$$D = \frac{1}{h}\Delta \qquad \text{[Because } f(U) \text{ is arbitrary]}$$

$$\therefore D^{n+1} = \frac{1}{h^{n+1}}\Delta^{n+1}$$

From equation (10), we got: $f^{(n+1)}(U) = \frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(U)$

Putting the values of $f^{(n+1)}(U)$ in equation (8), we got:

$$f(X) - P_n(X) = \left[\frac{\varphi(X)}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(U)\right]$$

$$f(X) - P_n(X) = \left[\frac{(X-X_0)(X-X_1)(X-X_2)\dots\dots\dots\dots\dots\dots(X-X_0)}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(U)\right] \tag{11}$$

If $\frac{X - X_0}{h} = q$ Then: $X - X_0 = hq$

$X - X_1 = X - (X_0 + h) = (X - X_0) - h = (hq - h) = h(q-1)$

Similarly $X - X_2 = h(q-2)$

:

:

:

Similarly $X - X_n = h(q-n)$

Putting these values in equation (11), we got:

$$f(X)-P_n(X)=\left[\frac{(hq)\{h(q-1)\}\{h(q-2)\}\{h(q-3)\}.............\{(q-n)\}}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(U)\right]$$

$$f(X)-P_n(X)=\left[\frac{q(q-1)(q-2)(q-3).........(q-n)}{(n+1)!}\right]\left[\Delta^{(n+1)}f(U)\right]$$

This is mathematical expression for estimation of error, if the point lies in the upper half.

3 IF THE POINT LIES IN THE LOWER HALF

Let $BA=f(X)$ be a function defined by n points $(BA_0,X_0),(BA_1,X_1).........(BA_n,X_n)$. Where BA is biological activity and X is the variable. When $X_1,X_2,X_3.............X_n$ are equally spaced with interval h. And If the point lies in the lower half then we used following formula [1] [7]-[9]

$$\mathrm{BA(X)}=\mathrm{BA_n}=\nabla.\mathrm{BA_n(r)}+\frac{\nabla^2\mathrm{BA_n}}{2!}[\mathrm{r(r+1)}]+.....+\frac{\nabla^n\mathrm{BA_n}}{n!}[(\mathrm{r})\{(\mathrm{r}+1)\}..\{\mathrm{r}+(\mathrm{n}\text{-}1)\}]$$

[Where ∇ is backward difference operator and $\frac{X-X_n}{h}=r$]

3.1 ESTIMATION OF ERROR

Let $BA=f(X)$ be a function defined by $(n+1)$ points $(BA_0,X_0),(BA_1,X_1).........(BA_n,X_n)$. When $X_1,X_2,X_3.............X_n$ are equally spaced with interval h and this function is continuous and differentiable $(n+1)$ times.

Let $BA=f(X)$ be approximated by a polynomial $P_n(X)$ of degree not exceeding a such that

$P_n(X_i)=BA_i$ [Where $i=1,2,3..........n$] (12)

Since the expression $f(X)-P_n(X)$ vanishes for $X_1,X_2,X_3.............X_n$,

We put we put $f(X)-P_n(X)=K\varphi(X)$ (13)

Where $\varphi(X)=(X-X_n)(X-X_{n-1}).............(X-X_0)$ (14)

And K is to be determined in such a way that equation (13) holds for any intermediate values of X, say $X-X'$ [where $X_0\le X'\le X_n$].

Therefore from equation (13),

$$K=\frac{f(X')-P(X')}{\varphi_1(X')} \quad (15)$$

Now we construct a function $f(X)$ such that: $f(X_0)=f(X_1)-P_n(X)-K\varphi_1(X)$

Where K is given by equation (15).

It is clear that: $f(X_0)=f(X_1)=f(X_2)=f(X_3)=...........f(X_n)=f(X')=0$ (16)

Let $f(X)$ vanishes $(n+2)$ times in the interval $X_0\le X\le X_n$; consequently, by the repeated application of Rolle's Theorem [23] [24], $f'(X)$ must vanish $(n+1)$ times, $f''(X)$ must vanish n times etc in the interval $X_0\le X\le X_n$.

Particularly, $f^{(n+1)}(X)$ must vanish once in the interval $X_0\le X\le X_n$. Let this point be $X=Z,\ X_0<Z<X_n$.

$$f^{(n+1)}(Z)-K(n+1)!=0$$

Or: $$K = \frac{f^{(n+1)}(Z)}{(n+1)!} \quad (17)$$

Putting this value of K in equation (15), we got: $\frac{f^{(n+1)}(Z)}{(n+1)!} = \frac{f(X') - P_n(X')}{\varphi_1(X')}$

Or $$f(X') - P_n(X') = \frac{f^{(n+1)}(Z)}{(n+1)!}\varphi_1(X'), \qquad X_0 < Z < X_n$$

Since X' is arbitrary therefore on dropping the prime on X' we got:

$$f(X) - P_n(X) = \frac{f^{(n+1)}(Z)}{(n+1)!}\varphi_1(X), \quad X_0 < Z < X_n \quad (18)$$

Now we use Taylor's theorem [25] [26]:

$$f(X+h) = f(Z) + hf'(Z) + \frac{h^2}{2!}f''(Z) + ... + \frac{h^n}{n!}f^n(Z) + ... \quad (19)$$

Neglecting the terms containing second and higher powers of h in equation (19), we got:

$$f(Z+h) = f(Z) + hf'(Z)$$

Or: $$f'(Z) = \frac{f(Z+h) - f(Z)}{h} \quad (20)$$

Or: $$f'(Z) = \frac{1}{h}\Delta f(Z) \qquad [\therefore \Delta f(X+h) f(X)]$$

$$Df(Z) = \frac{1}{h}\Delta f(Z) \qquad [\therefore D = \frac{d}{dZ}]$$

$$D = \frac{1}{h}\Delta \qquad \text{[Because } f(Z) \text{ is arbitrary]}$$

$$\therefore D^{n+1} = \frac{1}{h^{n+1}}\Delta^{n+1}$$

From equation (20), we got: $f^{(n+1)}(Z) = \frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(Z)$

Putting the values of $f^{(n+1)}(W)$ in equation (18), we got:

$$f(X) - P_n(X) = \left[\frac{\varphi_1(X)}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(Z)\right]$$

$$f(X) - P_n(X) = \left[\frac{(X-X_0)(X-X_1)(X-X_2)................(X-X_0)}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)} f(Z)\right] \quad (21)$$

If $\frac{X - X_0}{h} = r$ Then

$$X - X_0 = hr$$
$$X - X_1 = X - (X_0 + h) = (X - X_0) - h = (hr - h) = h(r-1)$$

Similarly $X - X_2 = h(r-2)$

:

:

:

Similarly $X - X_n = h(r-n)$

Putting these values in equation (21), we got:

$$f(T)-P_n(T)=\left[\frac{(hr)\{h(r-1)\}\{h(r-2)\}\{h(r-3)\}.............\{(r-n)\}}{(n+1)!}\right]\left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(Z)\right]$$

$$f(X)-P_n(X)=\left[\frac{r(r-1)(r-2)(r-3).........(r-n)}{(n+1)!}\right]\left[\Delta^{(n+1)}f(Z)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

4 IF INTERVALS ARE NOT BE EQUALLY SPACED

Let $BA = f(X)$ be a function defined by n points $(BA_0, X_0), (BA_1, X_1).........(BA_n, X_n)$. Where BA is biological activity and X is the variable. When $X_1, X_2, X_3..............X_n$ are equally spaced with interval h. And If Intervals are not be equally spaced then we used following formula we used following formula [1] [7]-[9]:

$$\mathrm{BA(X)}= \mathrm{BA}_1 + \Delta_d \mathrm{BA}_1(\mathrm{X}-X_1) + \Delta_d^2 \mathrm{BA}_1(\mathrm{X}-X_1)(\mathrm{X}-X_2) + ...+ \Delta_d^n \mathrm{BA}_1[(\mathrm{X}-X_1)(\mathrm{X}-X_2)...(\mathrm{X}-X_n)]$$

[Where Δ_d is divide difference operator]

4.1 ESTIMATION OF ERROR

Let $f(X)$ be a real-valued function define n interval and $(n+1)$ times differentiable on (a,b). If $P_n(X)$ is the polynomial. Which interpolates $f(X)$ at the $(n+1)$ distinct points $X_0, X_1.....X_n \in (a,b)$, then for all $\overline{X} \in [a,b]$,there exists $\xi = \xi(\overline{X}) \in (a,b)$

$$e_n(\overline{X}) = f(\overline{X}) - P_n(\overline{X})$$

$$= \frac{f^{(n+1)}(\xi)}{(n+1)} \prod_{j=0}^{n} (\overline{X} - X_j) \tag{22}$$

This is mathematical expression for estimation of error, if intervals are not be equally spaced.

5 WHEN THE TABULATED VALUES OF THE FUNCTION ARE NOT EQUIDISTANT

Let $BA = f(X)$ be a function defined by n points $(BA_0, X_0), (BA_1, X_1).........(BA_n, X_n)$. Where BA is biological activity and X is the variable. When the tabulated values of the function are not equidistant then we used following formula [1] [7]-[9]:

$$\mathrm{BA}(X) = \sum_{i=1}^{n} \mathrm{BA}_i \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{(\mathrm{X}-X_j)}{(X_i - X_j)}$$

5.1 ESTIMATION OF ERROR

Since the approximating polynomial $f(X)$ given by Lagrangian formula has the same values $f(X_0)$ $f(X_1)$ $f(X_2)$ $f(X_3)$ $f(X_4)$ .... $f(X_n)$ as does $BA = f(X)$ for the arguments X_0 , X_1 , X_2 , X_3 , X_4 ...., X_n the error term must have zeros at these $(n+1)$ points.

Therefore $(X-X_0)$ $(X-X_1)$ $(X-X_2)$ $(X-X_3)$ .... $(X-X_n)$ must be factors of the error and we can write:

$$F(X) = f(X) + \frac{(X-X_0)(X-X_1)(X-X_2)(X-X_3)..................(X-X_n)}{(n+1)!}K(X) \tag{23}$$

Let X to be fixed in value and consider the function

$$W(x) = F(x) - f(x)\frac{(x - X_0)(x - X_1)(x - X_2)(x - X_3)...............(x - X_n)}{(n+1)!}K(X) \tag{24}$$

Then $W(x)$ has zero $x = X_0, X_1, X_2, X_3..............X_n$ and X.

Since the $(n+1)^{th}$ derivative of the n^{th} degree polynomial $f(X)$ is zero.

$$W^{(n+1)}(x) = F^{(n+1)}(x) - K(X) \tag{25}$$

As a consequence of Rolle's Theorem [23] [24], the $(n+1)^{th}$ derivative of $W(x)$ has at least one real zero $x = \xi$ in the range $X_0 < \xi < X_n$

Therefore substituting $x = \xi$ in equation (25)

$$W^{(n+1)}(\xi) = F^{(n+1)}(\xi) - K(X)$$

Or

$$K(X) = F^{(n+1)}(\xi) - W^{(n+1)}(\xi)$$

$$= F^{(n+1)}(\xi)$$

Using this expression for $K(X)$ and writing out $f(X)$

$$f(X) = \frac{(X - X_1)(X - X_2).............(X - X_n)}{(X_0 - X_1)(X_0 - X_2).............(X_0 - X_n)}f(X_0) + \frac{(X - X_0)(X - X_2).............(X - X_n)}{(X_1 - X_0)(X_1 - X_2).............(X_1 - X_n)}f(X_1) + ...$$

$$....... + \frac{(X - X_0)(X - X_1).............(X - X_{n-1})}{(X_n - X_0)(X_n - X_1).............(X_n - X_{n-1})}f(X_n) + \frac{(X - X_0)(X - X_1).............(X - X_n)}{(n+1)!}f^{(n+1)}(\xi)$$

Where $T_0 < \xi < T_n$

This is mathematical expression for estimation of error, if the tabulated values of the function are not equidistant.

6 CONCLUSION

Derived mathematical expressions are useful to estimation of the errors in the formulas for obtaining intermediate values of the biological activity in Quantitative structure-activity relationships (QSAR). All expressions are worked in n limit which is the last value in the table. When we obtain the intermediate values of the biological activity in Quantitative structure-activity relationships then these mathematical expressions are useful to estimate the errors in interpolated values of the biological activity.

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