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An optimum single bounded inner energy level estimation using generalized Petersen graph and sampling method with imputation

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Abstract

Assume a large microscopic internal bonding chemical structure of a substance designed like a Petersen graph where electrons are the vertices and edges representing the bonding energy levels in between them. For large structures, it is difficult to find out the average level of bonding energy between any pair of electron-proton microscopic structures. For a chemical scientist, it is a difficulty and a challenge both to find out what is the average amount of energy bounded between any subsequent pair of electron-proton bi-valent bond, trivalent bond, or tetravalent bond. This paper presents a sample-based estimation methodology for estimating the bonding energy mean value. A node-sampling procedure is proposed whose bias, mean-squared errors and other properties are derived. Results are supported by empirical studies. Findings are compared with particular cases and confidence intervals are used as a basic tool of comparison for robustness purposes.

Keywords: Graph, Petersen Graph, Estimator, Bias, Mean Squared Error (MSE), Optimum Choice, Confidence intervals, Nodes (vertices), Pattern Imputation
2020 MSC: 05C90, 05C92

1 Introduction

From a reference [3] one can understand the followings: The effect of proton transfer coupling on the electron transfer triggered breaking of a O-O bond is illustrated by the comparison between the cyclic voltammetric responses of two aliphatic peroxide molecules, one of which contains aproximal carboxylic acid group while, in the other, the acid has been esterified. The stepwise pathway, electron transfer concerted with bond breaking followed by proton transfer. The first step is irreversible, the additional driving force offered by the follow-up protonation should not have any effect on the cyclic voltammetric response contrary to experiment [3]. Fig 1 and fig 2 support the above as proton-electron connected graphical structure, where Co-OEC is energy bond chemical structure.

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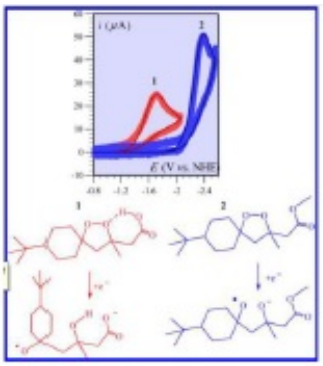

Fig 1: Breaking Bonds with Electron Proton

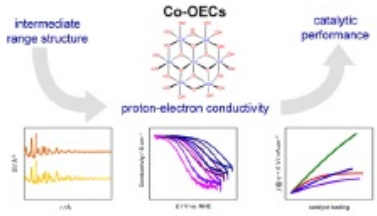

Fig 2: Proton Electron Connectivity

Note 1.1 It is well-known that electron-proton in a chemical structure of a substance remain bounded like trivalent bond, co-valent bond, tetravalent bond etc [3, 7, 9]. Their bonding energy level varies whatsoever be the micro-distances. For a chemical scientist, it is an issue and challenge to estimate the average amount of bounded energy between any subsequent pair of electron-proton of a substance. This difficulty issue and open challenge motivated to search for an estimation strategy using sampling technique.

2 Generalized Petersen Graph

The generalized Petersen graphs G(n,k) is a family of cubic graph which is a 3-regular graph. The Cubic graph is also called trivalent graph who connects the vertices of a regular polygon to corresponding vertices of a star polygon. A cubic graph is a graphical structure of vertices (nodes) and edge where all the vertices have degree three.

The generalized Petersen graph G(n,k) was introduced by Coxeter et al. [4] and named by Watkins [21] from very interesting family of trivalent graphs that can be described by only two integer parameters. They include Hamiltonian and non-Hamiltonian graph, Bipartite and non-Bipartite graphs, vertex transitive and non-vertex transitive graphs, cayley and non-cayley graphs of girth 3,4,5,6,7 or 8 according to[8].

Following notations of Watkins [21] for a given integer n and $k < \frac{n}{2}$ one can define a Petersen graph $G\ (n, k)$ as a graph of vertex set $(\mu_0, \mu_1, ..., \mu_{n-1}, \nu_0, \nu_1, ..., \nu_{n-1})$ and edge set partitioned into three equal parts $(\mu_i\mu_{i+1}, \mu_i\nu_i, \nu_i\nu_{i+k} \mid 0 \leq i \leq n$ where subscripts are to be read modulo n. The $G\ (3, 1)$ and $G\ (4, 1)$ are given below as a examples (Fig. 3 and 4).

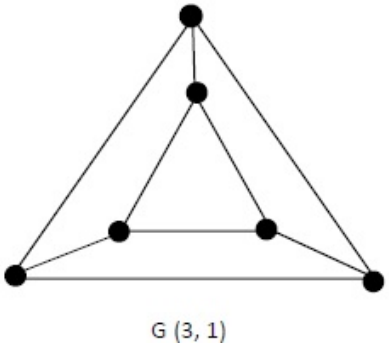

Fig 3: Petersen Graph

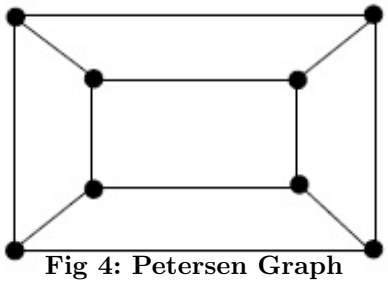

Fig 4: Petersen Graph

Let $\mu = (\mu_1, \mu_2, \mu_3, ...)$ denotes a set of vertices and $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3, ...)$ is a set of edges. The $G = (\mu, \epsilon, R)$ constitutes a graph, in general, where R is a set of relations. In the microscopic internal chemical structure of metals, there are electrons and protons bounded by the different energy levels. One can take electrons (proton-electron [3]) as vertices and edge-length (weight) as the amount of energy bounded between them (fig 5) [see [3, 7, 9]].

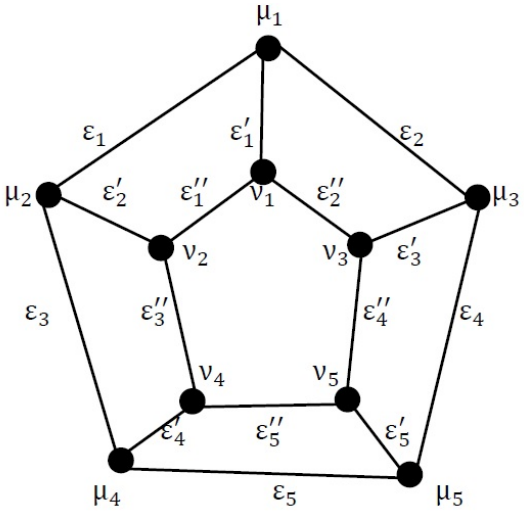

Fig 5: Petersen Graph G(5,1)

The matter of interest herein is to estimate the average energy level existing between any two consecutive pair of electrons (or proton [3]). This could be obtain by using Petersen graph as a model tool. Consider Petersen graph of fig 5 and define the outer vertices $\mu = (\mu_1, \mu_2, \mu_3, \mu_4, \mu_5)$ and inner vertices $\nu = (\nu_1, \nu_2, \nu_3, \nu_4, \nu_5)$. The edge-vertex relations are in table 1. **Note 2.1** The set of vertices $\mu = (\mu_1, \mu_2, \mu_3, \mu_4, \mu_5)$ denotes outer energy level where as set

Table 1: Relation of Vertices and edges in Petersen graph

S.No.	Set μ	Set ν
1.	$\mu_1 = (\epsilon_1, \epsilon_2, \epsilon'_1)$	$\nu_1 = (\epsilon''_1, \epsilon''_2, \epsilon'_1)$
2.	$\mu_2 = (\epsilon_1, \epsilon_3, \epsilon'_2)$	$\nu_2 = (\epsilon''_1, \epsilon''_3, \epsilon'_2)$
3.	$\mu_3 = (\epsilon_2, \epsilon_4, \epsilon'_3)$	$\nu_3 = (\epsilon''_2, \epsilon''_4, \epsilon'_3)$
4.	$\mu_1 = (\epsilon_3, \epsilon_5, \epsilon'_4)$	$\nu_4 = (\epsilon''_3, \epsilon''_5, \epsilon'_4)$
5.	$\mu_1 = (\epsilon_4, \epsilon_5, \epsilon'_5)$	$\nu_5 = (\epsilon''_4, \epsilon''_5, \epsilon'_5)$

$\nu = (\nu_1, \nu_2, \nu_3, \nu_4, \nu_5)$ denotes inner-energy level. The paired set of vertices $w = \{(\mu_i, \nu_i) : i = 1, 2, 3, 4, 5\}$ represents intermediate energy level.

2.1 Pattern Imputation

In light of fig 5 and table 2, for large number of outer vertices N and large number of inner vertices N, the general relationship R

Table 2: Node-edge matrix of Petersen graph [as per [15, 16]]

	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_1'	ϵ_2'	ϵ_3'	ϵ_4'	ϵ_5'	ϵ_1''	ϵ_2''	ϵ_3''	ϵ_4''	ϵ_5''	row total
μ_1	1	1	0	0	0	1	0	0	0	0	1	0	0	0	0	3
μ_2	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	3
μ_3	0	1	0	1	0	0	0	1	0	0	0	0	0	0	0	3
μ_4	0	0	1	0	1	0	0	0	1	0	0	0	0	0	0	3
μ_5	0	0	0	1	1	0	0	0	0	1	0	0	0	0	0	3
ν_1	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	3
ν_2	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	3
ν_3	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	3
ν_4	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	3
ν_5	0	0	0	0	0	0	0	0	0	1	0	0	0	1	1	3

At i=1 $\mu_1 \rightarrow (\epsilon_1, \epsilon_2, \epsilon_1'); \nu_1 \rightarrow (\epsilon_1'', \epsilon_2'', \epsilon_1')$, $\mu_i \rightarrow (\epsilon_{i-1}, \epsilon_{i+1}, \epsilon_i'); \nu_i \rightarrow (\epsilon_{i-1}'', \epsilon_{i+1}'', \epsilon_i'), i = 2, 3...n-1$ At i=N, $\mu_N \rightarrow (\epsilon_{N-1}, \epsilon_{N+1}, \epsilon_N'); \nu_N \rightarrow (\epsilon_{N-1}'', \epsilon_N'', \epsilon_N')$.
Under large N, for outer set of vertices μ, inner set of vertices ν and intermediate set ω, the pattern imputation is proposed as:

Step I At i=2 take $\mu_i \rightarrow (\epsilon_{i-1}, \epsilon_{i+1}, \epsilon_i'); \nu_i \rightarrow (\epsilon_{i-1}'', \epsilon_{i+1}'', \epsilon_i'), i = 2, 3...N-1$

Step II At i=1 impute in step I, ϵ_0 by ϵ_1, ϵ_0'' by ϵ_1'' and take $\mu_1 \rightarrow (\epsilon_1, \epsilon_2, \epsilon_1'); \nu_1 \rightarrow (\epsilon_1'', \epsilon_2'', \epsilon_1')$

Step III At i=N impute in step I, ϵ_{N+1} by ϵ_N and ϵ_{N+1}'' by ϵ_N'' and take $\mu_N \rightarrow (\epsilon_{N-1}, \epsilon_N, \epsilon_N'); \nu_N \rightarrow (\epsilon_{N-1}'', \epsilon_N'', \epsilon_N')$.

To note that imputation of [ϵ_0 *by* ϵ_1 ϵ_{N+1} *by* ϵ_N] and [ϵ_0'' by ϵ_1'', ϵ_{N+1}'' by ϵ_N''] is like a specific imputation just to maintain a pattern so it is called pattern imputation. In general, it may random imputation also like ϵ_0 to replace by any ϵ_i, ϵ_{N+1} by any ϵ_i, ϵ_0'' by any ϵ_i'' ϵ_{N+1}'' by any ϵ_i'' randomly chosen. The Pattern Imputation is closed to the nearest neighbour imputation, but earlier maintains a pattern later do not do so.

2.2 Energy Bond Structure

Looking at fig 5 and assuming large N, the generalised Petersen graph G(N,k) can be expressed having edge weights as different energy levels bounded between vertices.

(a)**Single Pair Energy Bonding:** The bonding is between any pair (μ_i, μ_{i+1}) at outer level any pair (ν_i, ν_{i+1}) at inner level and any pair (μ_i, ν_i) at intermediate level. The symbols δ_i, δ_i', δ_i'' represent value of corresponding bonding as shown in Fig 6.

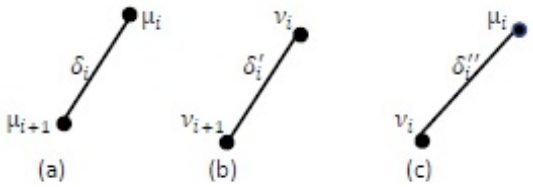

Fig 6: Single Pair Energy Bonding

(b)**Double Pair Energy Bonding:** This bonding is between one outer pair of vertices and one intermediate pair or one inner pair with one intermediate pair. The α_i and α_i' are edge-weights revealing in Fig 7.

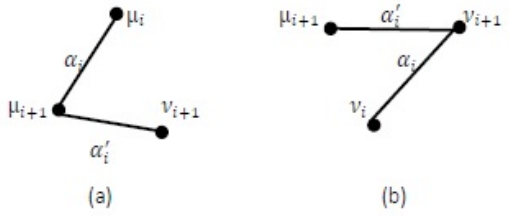

Fig 7: Double Pair Energy Bonding

(c)**Triple Pair Energy Bonding:** This consitutes bonding among two vertex pairs at outer and inner level and one at intermediate level. The β_i, β_i', β_i'' are edge weights as energy levels as shown in fig 8.

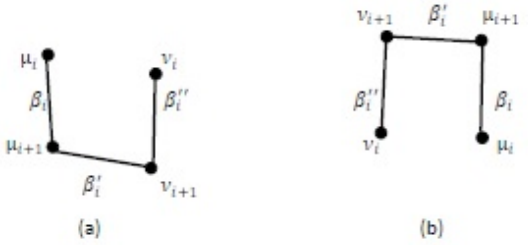

Fig 8: Triple Pair Energy Bonding

3 Estimation

Note 3.1 The aggregate vertices (population) count is N and size of random sample is n (N¿n).
Consider the case of single pair energy bond estimation only in the content of this paper assuming large N. Define $U_i = \epsilon_i$ as outer edges and $Z_i = \epsilon_i''$ as inner edges. Some symbols are as under:

$\bar{U} = \frac{\sum_{i=1}^{N} U_i}{N} = \frac{\sum_{i=1}^{N} \epsilon_i}{N}$; $\bar{Z} = \frac{\sum_{i=1}^{N} Z_i}{N} = \frac{\sum_{i=1}^{N} \epsilon_i''}{N}$ (Population means)
$S_U^2 = \frac{\sum_{i=1}^{N} (U_i - \bar{U})^2}{N-1}$; $S_Z^2 = \frac{\sum_{i=1}^{N} (Z_i - \bar{Z})^2}{N-1}$ (Population mean square)
$C_U = (\frac{S_U}{\bar{U}})$; $C_Z = (\frac{S_Z}{\bar{Z}})$(Population coefficient of variation)
$S_{UZ} = \frac{\sum_{i=1}^{N} (U_i - \bar{U})(Z_i - \bar{Z})}{N-1}$; $\rho_{UZ} = \rho_{ZU} = \frac{S_{UZ}}{S_U . S_Z}$ (Population correlation coefficient)

Let a simple random sample of large size n ($n < N$) vertices like (μ_j, ν_j), j=1,2,3...n is drawn from N vertices using without replacement procedure.

Sample statistic estimates based on n observations are:
$\bar{u} = \frac{\sum_{j=1}^{n} u_j}{n}$(sample mean of outer vertices)
$\bar{z} = \frac{\sum_{j=1}^{n} z_j}{n}$ (sample mean of inner vertices)
$s_u^2 = \frac{\sum_{j=1}^{n} (u_j - \bar{u})^2}{n-1}$; $s_z^2 = \frac{\sum_{j=1}^{n} (z_j - \bar{z})^2}{n-1}$ (sample mean square)
$c_u = (\frac{s_u}{\bar{u}})$; $c_z = (\frac{s_z}{\bar{z}})$ (sample coefficient of variation)
$s_{uz} = \frac{\sum_{j=1}^{n} (u_j - \bar{u})(z_j - \bar{z})}{n-1}$; $\rho_{uz} = \frac{s_{uz}}{s_u . s_z}$ (sample correlation)

Objective of this paper is to estimate, using sampling, the average amount of energy bond existing between any two consecutive pair of electrons (or electron-proton [3, 7, 9]) in a substance whose microscopic chemical structure is like a Petersen graph with N vertices. The out mean $\bar{U}$ is known but inner mean $\bar{Z}$ is unknown and the aim is focused to estimate unknown $\bar{Z}$, using ($\bar{u}$,$\bar{z}$, $\bar{U}$) with the help of an appropriate efficient estimation strategy.

3.1 Proposed Estimation Strategy

To estimate unknown $\bar{Z}$ in the inner structure of single energy bond between any pair of consecutive electrons (vertices), the proposed estimation strategy $[using\ \bar{z}, \bar{U}, \bar{u}]$ is:

$$E = (\bar{z})[\phi_1(\bar{u}, \bar{U})][\phi_2(\bar{u}, \bar{U})]^{-1}$$

where,

$$\phi_1(\bar{u}, \bar{U}) = [(A + C + D)\bar{U} + gB\bar{u}]$$

$$\phi_2(\bar{u}, \bar{U}) = [(A + gB + D)\bar{U} + C\bar{u}]$$

$A = (q-1)(q-2); B = (q-1)(q-4); C = (q-2)(q-3)(q-4); D = (q-1)(q-2)(q-3)(q-4)(q-5), g = \frac{n}{N},\ 0 < q < \infty$

The proposed is in accordance with shukla et al.[17] but as a part of new structure, a term is added which is in of power five in q . At q=4, as a special case, the proposed strategy converts to the inner single mean based energy bond value estimation through a sample.

4 Setting Approximations

For two real numbers $h_1\ and\ h_2$, $|h_1| < 1\ and\ |h_2| < 1$, assuming N, n large, one can express approximations as per [19], [10], [11].

$$\bar{z} = \bar{Z}(1 + h_1) \tag{4.1}$$

$$\bar{u} = \bar{U}(1 + h_2) \tag{4.2}$$

Let $E^*(.)$ denotes expected value of random variables $\bar{z}$ and $\bar{u}$, then one can get following using [5], [13],[15], [16], [18], [10], [6], [11].

$$E^*(h_1) = E^*(h_2) = 0 \tag{4.3}$$

$$E^*({h_1}^2) = \frac{(N-n)}{Nn} C_Z^2 \tag{4.4}$$

$$E^*({h_2}^2) = \frac{(N-n)}{Nn} C_U^2 \tag{4.5}$$

$$E^*(h_1 h_2) = \left(\frac{(N-n)}{Nn}\right)(\rho_{ZU}.C_Z.C_U) \tag{4.6}$$

Theorem 4.1. Under large sample approximations, the proposed E could be expressed as:

$$E = \bar{Z}\left[(1 + h_1) + \Delta^*\left\{(h_1 + h_1 h_2) - \frac{C h_2^2}{\Delta}\right\}\right]$$

where $\Delta = (A + gB + C + D),\ \Delta^* = [\frac{(gB-C)}{\Delta}]$.

Proof . We have

$$E = (\bar{z})[\phi_1(\bar{u}, \bar{U})][\phi_2(\bar{u}, \bar{U})]^{-1}$$

where,

$$\phi_1(\bar{u}, \bar{U}) = [(A + C + D)\bar{U} + gB\bar{u}]$$
$$\phi_2(\bar{u}, \bar{U}) = [(A + gB + D)\bar{U} + C\bar{u}].$$

Using (4.1) and (4.2) $|h_1| < 1$, $|h_2| < 1$

$$\phi_1(\bar{u}, \bar{U}) = \left[(A + C + D)\bar{U} + gB\left\{\bar{U}(1 + h_2)\right\}\right] \tag{4.7}$$
$$\phi_2(\bar{u}, \bar{U}) = \left[(A + gB + D)\bar{U} + C\left\{\bar{U}(1 + h_2)\right\}\right]. \tag{4.8}$$

Then $\phi_1(\bar{u}, \bar{U})$ could be expressed as:

$$\phi_1(\bar{u}, \bar{U}) = [\bar{U}(A + gB + C + D)]\left[1 + \frac{(gBh_2)}{(A + gB + C + D)}\right]. \tag{4.9}$$

Since $|h_2| < 1$, $|\frac{gBh_2}{(A+fB+C+D)}| < 1$, for all $g > 0, q > 0$. Moreover, for $\phi_2(\bar{u}, \bar{U})$ using expansion of $(1 + x)^{-1}$, one gets

$$\begin{aligned}
\left[\phi_2(\bar{u}, \bar{U})\right]^{-1} &= \left[(A + gB + C + D)\bar{U} + \bar{U}Ch_2\right]^{-1} \\
&= (\bar{U})^{-1}[A + gB + C + D]^{-1}\left[1 + \frac{Ch_2}{(A + gB + C + D)}\right]^{-1} \\
&= (\bar{U})^{-1}[A + gB + C + D]^{-1}\left[1 - \frac{Ch_2}{(A + gB + C + D)} + \frac{C^2h_2^2}{(A + gB + C + D)}\cdots\right].
\end{aligned}$$

Define $\Delta = (A + gB + C + D)$, then one can express E as $E = (\bar{z})[\phi_1(\bar{u}, \bar{U})][\phi_2(\bar{u}, \bar{U})]^{-1}$. This implies that

$$\begin{aligned}
E &= \bar{Z}(1 + h_1)\left[1 + \frac{gBh_2}{\Delta}\right]\left[1 - \frac{Ch_2}{\Delta} + \frac{C^2h_2^2}{\Delta^2}\cdots\right] \\
&= \bar{Z}(1 + h_1)\left[1 - \frac{Ch_2}{\Delta} + \frac{C^2h_2^2}{\Delta^2} + \left\{\frac{gBh_2}{\Delta} - \frac{gBCh_2^2}{\Delta^2} + \frac{gBC^2h_2^3}{\Delta^3}\cdots\right\}\right] \\
&= \bar{Z}\left[(1 + h_1) + \frac{(gB - C)}{\Delta}\left\{(h_2 + h_1h_2) - \frac{Ch_2^2}{\Delta}\right\}\right],
\end{aligned}$$

which is expressed after ignoring terms $(h_1^s.\ h_2^t), (s + t) > 2$, $s, t = 0, 1, 2, 3, 4, \ldots$, because of having high power on h_1 and h_2. The denominator Δ is high for $g > 0$, therefore, one can narrate that contribution of these terms in estimation will be low (negligible). Define $\Delta^* = \frac{(gB-C)}{\Delta}$.Then

$$E = \bar{Z}\left[(1 + h_1) + \Delta^*\left\{(h_1 + h_1h_2) - \frac{Ch_2^2}{\Delta}\right\}\right].$$

□

Theorem 4.2. The bias of estimator E under (4.1), (4.2) using Theorem 4.1 is

$$B[E] = Bias[E] = \bar{Z}\left[\Delta^*\left\{\frac{N - n}{Nn}\right\}\left\{\rho_{ZU}.C_Z.C_U) - \frac{C}{\Delta}C_U^2\right\}\right],$$

where $\rho_{UZ} = rho_{ZU}$ is correlation coefficient between inner and outer energy bond levels in Petersen graph.

Proof . Let $E^*(.)$ denotes expected value of the proposed estimator E and $B[E] = \left[E^*(E) - \bar{Z}\right]$. Now, we have

$$\begin{aligned}
E^*(E) &= E^*\left[\bar{Z}(1 + h_1) + \bar{Z}\Delta^*\left\{h_1 + h_1h_2 - \frac{Ch_2^2}{\Delta}\right\}\right] \\
&= \left[\bar{Z} + \bar{Z}E^*(h_1) + \bar{Z}\Delta^*\left\{E^*(h_1) + E^*(h_1h_2) - \frac{CE^*(h_2^2)}{\Delta}\right\}\right] \\
&= \left[\bar{Z} + \bar{Z}\Delta^*\left\{E^*(h_1h_2) - \frac{C}{\Delta}E^*(h_2^2)\right\}\right].
\end{aligned}$$

Using (4.1) and (4.2) and Theorem 4.1

$$\begin{aligned} B[E] &= \left[E^*(E) - \bar{Z}\right] \\ &= \bar{Z}\left[\Delta^*\left\{E^*(h_1h_2) - \frac{C}{\Delta}E^*(h_2^2)\right\}\right] \\ &= \bar{Z}\left[\Delta^*\left(\frac{N-n}{Nn}\right)\left\{(\rho_{ZU}C_ZC_U) - (\frac{C}{\Delta})C_U^2\right\}\right]. \end{aligned}$$

□

Corollary 4.3. The estimator E is unbiased under condition $(\rho_{ZU}C_ZC_U) = (\frac{C}{\Delta})C_U^2$ implies that

$$M(A + gB + C + D) + C(M - 1) + MD = 0. \tag{4.10}$$

Note 4.1: The above equation 4.10 is having highest power five in terms of q. Therefore, it may has maximum of five roots satisfying the equation. Best root will be that having lowest mean square error (MSE).
Note 4.2 If the t_n is biased estimator of unknown parameter θ then mean squared error is defined as

$$MSE(t_n) = E[t_n - \theta]^2$$

In finite sampling theory, the MSE(t_n) is used as a tool of measuring precision. Since this paper considers a finite setup of vertices only, therefore, it is recommended to use MSE(t_n) instead of any other kind of loss function [see [2]].

Theorem 4.4. The mean squared error (MSE) of the proposed strategy E is

$$MSE[E] = \bar{Z}^2\left[(\frac{N-n}{Nn})\left\{C_Z^2 + (\Delta^*)^2C_U^2 + 2\Delta^*\rho_{UZ}C_UC_Z\right\}\right].$$

Proof . We have

$$\begin{aligned} MSE[E] &= E^*[E - \bar{Z}]^2 \\ &= E^*\left[\bar{Z}(1 + h_1) + \Delta^*\left\{h_1 + h_1h_2 - \frac{Ch_2^2}{\Delta} + ...\right\} - \bar{Z}\right]^2 \\ &= E^*\left[\bar{Z}(h_1 + \Delta^*h_2)\right]^2. \end{aligned}$$

Ignoring terms $(h^sh^t), (s + t) > 2, s, t = 1, 2, 3, 4, 5$, implies that

$$MSE[E] = \bar{Z}^2\left[E^*(h_1^2) + (\Delta^*)^2E^*(h_2^2) + 2\Delta^*E^*(h_1h_2)\right].$$

Thus,

$$MSE[E] = \bar{Z}^2\left[(\frac{N-n}{Nn})\left\{C_Z^2 + (\Delta^*)^2C_U^2 + 2\Delta^*\rho_{UZ}C_UC_Z\right\}\right]. \tag{4.11}$$

□

Theorem 4.5. The minimum (optimum) mean squared error is attained when
$\Delta^* = -M$ *where* $M = \rho_{ZU}(\frac{C_Z}{C_U})$.

Proof . Differentiating MSE[E] with respect to the term Δ^* and equating to zero, one gets

$$\frac{MSE[E]}{\Delta^*} = 0 \implies \Delta^* = -\rho_{ZU}(\frac{C_Z}{C_U}) = -M. \tag{4.12}$$

□

Corollary 4.6. The optimuum MSE expression (4.12) could be expressed as $\frac{(gB-C)}{(A+gB+C+D)} = -M$. Then

$$AM + gB(M+1) + C(M-1) + DM = 0. \tag{4.13}$$

Note 4.3 The equation (4.13) of optimum MSE is having highest power five on terms q, therefore, there will be maximum of five roots of equation (4.13). The best q will be that containing lowest bias value. The proposed strategy attains the optimum level of MSE and also reduces the bias. This is a novel feature of proposed estimation procedure E.

5 Numerical Illustration

Define F=Inner Level Energy Bonds $\epsilon_i^{''} = Z_i$; G=Outer Level Energy Bonds $\epsilon_i = U_i$; H=Intermediate Level Energy Bonds ϵ_i'. Consider the generalized Petersen structure with N=150 electrons (or protons) as vertices in a molecular structure of a substance. The energy bonds are given below: To note that efficiency depends on choice of constant

Table 3: Energy bond data of N=150 electrons as population

S.No.	$F=\epsilon_i^{''}=Z_i$	$G=\epsilon_i=U_i$	$H=\epsilon_i'$	S.No.	$F=\epsilon_i^{''}=Z_i$	$G=\epsilon_i=U_i$	$H=\epsilon_i'$
1.	25 units	43units	86units	76.	41 units	87units	34units
2.	53 units	81units	64units	77.	75 units	32units	66units
3.	34 units	14units	86units	78.	48 units	32units	71units
4.	43 units	61units	74units	79.	87 units	92units	56units
5.	37 units	28units	69units	80.	49 units	22units	76units
6.	91 units	23units	41units	81.	65 units	86units	56units
7.	34 units	48units	72units	82.	45 units	33units	31units
8.	92 units	43units	21units	83.	49 units	64units	88units
9.	35 units	63units	71units	84.	93 units	21units	65units
10.	27 units	83units	34units	85.	75 units	83units	89units
11.	51 units	63units	86units	86.	46 units	26units	18units
12.	63 units	72units	65units	87.	68 units	37units	28units
13.	39 units	84units	42units	88.	88 units	63units	29units
14.	52 units	26units	75units	89.	28 units	44units	75units
15.	84 units	35units	42units	90.	39 units	42units	56units
16.	28 units	39units	67units	91.	37units	47units	76units
17.	56 units	42units	63units	92.	82 units	56units	96units
18.	81 units	33units	26units	93.	17 units	47units	89units
19.	29 units	57units	76units	94.	76 units	44units	28units
20.	85 units	38units	43units	95.	45 units	63units	60units
21.	91 units	34units	78units	96.	77 units	42units	63units
22.	38 units	49units	65units	97.	29 units	51units	36units
23.	57 units	63units	84units	98.	39 units	53units	56units
24.	19 units	43units	96units	99.	78 units	88units	40units
25.	65 units	36units	73units	100.	20 units	75units	64units
26.	48 units	96units	21units	101.	73units	37units	58units
27.	43 units	65units	92units	102.	84 units	73units	36units
28.	45 units	39units	17units	103.	95 units	43units	21units
29.	83 units	91units	26units	104.	58 units	68units	28units
30.	57units	48units	21units	105.	71 units	39units	50units
31.	23 units	58units	61units	106.	47 units	40units	19units
32.	47 units	82units	53units	107.	85 units	73units	26units
33.	27 units	63units	73units	108.	60 units	53units	44units
34.	98 units	34units	61units	109.	28 units	49units	81units
35.	45 units	23units	54units	110.	35 units	63units	66units
36.	81 units	53units	66units	111.	48 units	28units	39 units
37.	22 units	93units	81units	112.	56 units	54units	87 units
38.	55 units	42units	76units	113.	41 units	40 units	81 units
39.	29 units	63units	66units	114.	45 units	63 units	21 units
40.	68 units	41units	96units	115.	35 units	71 units	66 units
41.	25 units	93units	46units	116.	88 units	23 units	86 units
42.	63 units	71units	32units	117.	35 units	43 units	88 units
43.	73 units	61units	24units	118.	69 units	40 units	66 units
44.	58 units	83units	46units	119.	38 units	33units	96units
45.	48 units	43units	22units	120.	68 units	43units	56units
46.	31 units	48units	69units	121.	21 units	84 units	26 units
47.	47 units	33units	26units	122.	25 units	49units	77units
48.	35 units	87units	76units	123.	48 units	64 units	92 units
49.	63 units	71units	36units	124.	20 units	63units	29 units
50.	85 units	53units	46units	125.	28 units	33 units	83 units
51.	76 units	29units	36units	126.	77 units	62 units	55 units
52.	32 units	61units	59units	127.	60 units	43 units	56 units
53.	47 units	93units	73units	128.	65 units	74 units	78 units
54.	93 units	84units	64units	129.	48 units	66 units	58 units
55.	55 units	84units	29units	130.	94 units	47units	76units
56.	48 units	19units	36units	131.	59 units	31 units	63 units
57.	71 units	94units	68units	132.	76 units	93 units	84 units
58.	92units	83units	57units	133.	95 units	73 units	66units
59.	28 units	59units	28units	134.	70 units	83 units	56 units
60.	38 units	47units	71units	135.	46 units	29 units	46units
61.	93 units	72units	65units	136.	79 units	92 units	36units
62.	35 units	83units	57units	137.	54 units	54 units	47 units
63.	45 units	84units	91units	138.	80 units	43units	98 units
64.	46 units	52units	29units	139.	95 units	46units	19 units
65.	15 units	73units	82units	140.	39 units	63 units	93 units
66.	37 units	87units	62units	141.	97 units	76 units	34 units
67.	93 units	13units	96units	142.	85 units	94 units	33 units
68.	75 units	84units	56units	143.	76 units	33 units	57 units
69.	39 units	83units	92units	144.	79 units	65 units	88 units
70.	72units	65units	86units	145.	83 units	60 units	59 units
71.	47 units	41units	68units	146.	90 units	22 units	86units
72.	85 units	38units	21units	147.	79 units	39 units	88 units
73.	68 units	91units	26units	148.	46 units	55 units	39 units
74.	45 units	38units	56units	149.	98 units	68 units	88 units
75.	30 units	43units	82units	150.	29 units	85 units	89 units

q. There are multiple best and optimum choices available. The best is that who reduces bias and MSE both.

$$\text{Percentage Relative Efficiency (PRE)} = \left[\frac{MSE(E)_q - MSE(E)q_{opt}}{MSE(E)_q}\right] X100, \text{ where } q = 1,2,3,4,5.$$

The proposed E is best efficient at q_{opt} while comparing with some specific q values (see table 10). The 43% and 50% efficiency observed with respect to q=1 and q=2.

Table 4: Petersen graph population parameters

S.No.	Parameters	Value	Description/Equation no.
1.	N	150	Population Size
2.	n	40	Sample Size
3.	$\bar{Z}$	56.7266	Population Mean
4.	$\bar{U}$	57.7666	Population Mean
5.	S_Z	22.8684	Populatin Variance
6.	S_U	21.8792	Population Varance
7.	C_Z	0.4031	Population Coefficient of Variation
8.	C_U	0.3787	Population Coefficient of Variation
9.	ρ_{UZ}	0.0726	Population Correlation Coefficient
10.	M	0.0773	Using Corollary 4.1

Table 5: Almost unbiased choice of q for given (M, g) [from eq. (4.10)]

S.No.	M	g	Choice of q	Bias	MSE
1.	0.0773	0.2666	$q_1 = 1.0182$	0.1585	17.8592
2.	0.0773	0.2666	$q_2 = 1.9950$	0.0087	19.5375
3.	0.0773	0.2666	$q_3 = 2.9742$	-0.0037	10.6090
4.	0.0773	0.2666	$q_4 = --$	–	–
5.	0.0773	0.2666	$q_5 = --$	–	–

Note 5.1 In [7] the graphical structure spanning tree is used while in [8] the planar graph structure is used. Moreover, in [10] the binary tree is used whereas in [12,15,17] the stratified sampling procedure is applied for parameter estimation. Likewise in [18] , the Hamiltonian Circuit is selected for application purpose and in [20] the Bipartite graph is used. No researcher has yet used Petersen graph as a population who is considered in this paper. Therefore, comparison with above mentioned references cannot be performed because they are linked with other different graphical structures.

6 Simulation of Confidence Interval for Robustness

Consider the 10 random samples $A_1, A_2, A_3, ..., A_{10}$ each of size n=40 from population N=150. Description of samples are in table 11 given below:

6.1 Confidence Interval

Let P[H] denotes the probability of an event H. The 95% optimum confidence interval (if sample from normal population) is defined as:
$P[estimated \;\; mean - 1.96\sqrt{est[MSE(E)]q_{opt}}] < \bar{Z} < P[estimated \;\; mean + 1.96\sqrt{est[MSE(E)]q_{opt}}] = 0.95$, where q_{opt} is obtained by eq. (4.13) along with sample estimate of MSE using (g, M). The g, M are treated known. It is evident from table 13 that average confidence intervals are independent of different q_{opt} values.

7 Discussion

The proposed estimation strategy has constants A, B, C, D who are linked with another single constant $q > 0$. For data in table 5.1 and population parameters in table 5.2, the most suitable choices of q are in table 5.3 and table 5.4. For given population (M = 0.0773, g = 0.2666), the proposed estimation strategy is almost unbiased when $q_1 = 1.0182, q_2 = 1.9950$ and $q_3 = 2.9742$. The best is $q = q_3 = 2.9742$ because it reduces MSE also as shown in table 5.3. Likewise, in table 5.4 the choices of q are $q_1 = 1.8187, q_2 = 3.2377, q_3 = 4.2569$ on which the MSE is optimum (minimum). Best option is $q = q_3 = 4.2569$ having the least bias. Overall, for given data in table 5.1, the most suitable range for q is $q \in (1.8, 2.99)$ producing optimum MSE with least bias.

The general Ready-Reckoner table 5.6 and table 5.7 reveal for any given data where M ranging $M \in (0.05, 0.95)$, g ranging $g \in (0.3, 0.9)$, the best q ranging $q \in (1.9, 4.45)$ for which MSE and bias both are at the lowest level, whatever

Table 6: Choice of q for optimum MSE for given (M, g) [from eq. (4.13)]

S.No.	M	g	Choice of q	MSE	Bias
1.	0.0773	0.2666	$q_{1(opt)} = 1.8187$	9.5372	-0.0412
2.	0.0773	0.2666	$q_{2(opt)} = 3.2377$	9.5370	-0.0017
3.	0.0773	0.2666	$q_{3(opt)} = 4.2569$	9.5370	0.0003
4.	0.0773	0.2666	$q_{4(opt)} = --$	–	–
5.	0.0773	0.2666	$q_{5(opt)} = --$	–	–

Table 7: At some special cases of q = 1,2,3,4,5 for (g= 0.2666, M= 0.0773)

S.No.	q	A	B	C	D	Bias (theorem 4.2)	MSE (theorem 4.3)
1.	1	0	0	-6	0	0.1376	16.7410
2.	2	0	-2	0	0	0.0115	19.3604
3.	3	2	-2	0	0	-0.0042	10.2305
4.	4	6	0	0	0	0.0000	9.5876
5.	5	12	4	6	0	0.0091	9.8154

be positive $0 < M < 1$ and $0 < g < 1$ using the proposed estimation strategy. The simulation results of confidence interval (CI) over 10 samples, each of size n = 40, are in table 6.1 who estimate sample statistic of the proposed over 10 samples as in table 6.2. The calculation of 95% confidence intervals are in table 6.3. All the CI are catching the true mean value of inner energy variable Z = 56.7. The length of confidence intervals have extremely minor variations among them. The efficiency comparision of proposed is in table 5.8 over different q. The 43% and 50% efficiency found with respect to q=1 and q=2. The confidence intervals are robust over different q_{opt} values.

Note 7.1 The main findings are:

(a) thought to estimate energy bonding through sampling procedure,

(b) application of Petersen graph as a model tool for such estimator which is found well proved effective for energy bonds,

(c) introduction of a new imputation procedure named after "Pattern Imputation" against a sample based missing value in sample data in Petersen Graph which is found useful,

(d) proposal of a new sample based estimation strategy E which is proved efficient enough for estimating the energy levels at the optimum choice of constant $q = q_{opt}$,

(e) use of confidence intervals as a tool to check the robustness of predicted value of energy bonds,

(f) generation of ready-reckoner tables for quick and best selection of constant value q whatever be characterization of population in terms of M and g.

8 Conclusion

On recapitulation, the problem opted in this paper is to estimate the average optimum bounded inner energy level between any two inner vertices of a chemical bond structure like the generalised Petersen graph, with the use of sampling and imputation technique. As a matter of simplicity, the single pair energy bonding was taken into consideration among inner and outer chemical structure. A method of imputation, named after "Pattern Imputation" is proposed in the content to maintain the completeness in the symmetry in view to sampling strategy implementation. Pattern imputation was found efficient and useful for filling the missing data. An estimation strategy is proposed whose expressions of bias and mean squared error are derived. It has four constants A, B, C and D who are linked with another single constant q having expression in terms of power five. This has led to the best selection of q for making the proposed estimation strategy optimum with least bias. The most plausible selection of q is $q \in (1.8, 2.99)$ for given M = 0.0773, g = 0.2666. Two Ready-Reckoner tables provide general range of most suitable q as $q \in (1.9, 4.45)$ whatsoever be the positive most frequent M (0¡M¡1) and g (0¡g¡1) values characterizing the population. As a part of secondary verification of performance of proposed estimation strategy, which is sample based with pattern imputation, the method of simulation of 95% confidence interval (CI) is used as a tool. It is found that all the estimated confidence intervals are catching the true mean value of main inner energy bond of interest which is major strength of the proposed. There is minor insignificant variations in the lengths of C.I. (Confidence Interval) which support to the robustness of efficiency. Future prospects of the work undertaken herein are to extend the same to the case of Double

Table 8: Ready reckoner for choice of q providing almost unbiasedness for given (M,g) (using corollary 4.1, eq. (4.10)) [*Range* $0.05 \leq M \leq 0.95$; *Range* $0.3 \leq g \leq 0.9$]

S.No.	M	g	Choice of q	Bias	MSE	S.No.	M	g	Choice of q	Bias	MSE
1.	0.05	0.3	$q_1 = 1.0120$	0.1508	17.4464	31.	0.65	0.3	$q_1 = 1.1049$	0.3519	28.1439
2.	0.05	0.3	$q_2 = 1.9949$	0.0089	19.5205	32.	0.65	0.3	$q_2 = 1.9538$	-0.0241	21.3308
3.	0.05	0.3	$q_3 = 2.9840$	-0.0046	10.8929	33.	0.65	0.3	$q_3 = 2.8847$	0.0136	17.8414
4.	0.05	0.3	$q_4 = --$	–	–	34.	0.65	0.3	$q_4 = --$	–	–
5.	0.05	0.3	$q_5 = --$	–	–	35.	0.65	0.3	$q_5 = --$	–	–
6.	0.05	0.6	$q_1 = 1.0120$	0.1500	17.3825	36.	0.65	0.6	$q_1 = 1.1070$	0.3320	26.6866
7.	0.05	0.6	$q_2 = 1.9903$	0.0090	19.5127	37.	0.65	0.6	$q_2 = 1.9124$	-0.0251	21.1868
8.	0.05	0.6	$q_3 = 2.9898$	-0.0157	30.7244	38.	0.65	0.6	$q_3 = 2.9365$	0.0426	99.8734
9.	0.05	0.6	$q_4 = --$	–	–	39.	0.65	0.6	$q_4 = --$	–	–
10.	0.05	0.6	$q_5 = --$	–	–	40.	0.65	0.6	$q_5 = --$	–	–
11.	0.05	0.9	$q_1 = 1.0121$	0.1492	17.3242	41.	0.65	0.9	$q_1 = 1.1091$	0.3121	25.2619
12.	0.05	0.9	$q_2 = 1.9856$	0.0091	19.5114	42.	0.65	0.9	$q_2 = 1.8745$	-0.0260	21.0199
13.	0.05	0.9	$q_3 = 2.9976$	-0.0943	815.5990	43.	0.65	0.9	$q_3 = 2.9840$	0.3035	34.74.6470
14.	0.05	0.9	$q_4 = --$	–	–	44.	0.65	0.9	$q_4 = --$	–	–
15.	0.05	0.9	$q_5 = --$	–	–	45.	0.65	0.9	$q_5 = --$	–	–
16.	0.35	0.3	$q_1 = 1.0674$	0.2416	22.2782	46.	0.95	0.3	$q_1 = 1.1321$	0.4816	35.0244
17.	0.35	0.3	$q_2 = 1.9714$	-0.0065	20.4181	47.	0.95	0.3	$q_2 = 1.9404$	-0.0434	22.2394
18.	0.35	0.3	$q_3 = 2.9201$	0.0011	13.6369	48.	0.95	0.3	$q_3 = 2.8622$	0.0327	23.4848
19.	0.35	0.3	$q_4 = --$	–	–	49.	0.95	0.3	$q_4 = --$	–	–
20.	0.35	0.3	$q_5 = --$	–	–	50.	0.95	0.3	$q_5 = --$	–	–
21.	0.35	0.6	$q_1 = 1.0682$	0.2333	21.6708	51.	0.95	0.6	$q_1 = 1.1356$	0.4452	32.3878
22.	0.35	0.6	$q_2 = 1.9446$	-0.0069	20.3828	52.	0.95	0.6	$q_2 = 1.8883$	-0.0450	21.9297
23.	0.35	0.6	$q_3 = 2.9553$	0.0038	59.1187	53.	0.95	0.6	$q_3 = 2.9246$	0.1016	153.7084
24.	0.35	0.6	$q_4 = --$	–	–	54.	0.95	0.6	$q_4 = --$	–	–
25.	0.35	0.6	$q_5 = --$	–	–	55.	0.95	0.6	$q_5 = --$	–	–
26.	0.35	0.9	$q_1 = 1.0690$	0.2251	21.0742	56.	0.95	0.9	$q_1 = 1.1393$	0.4094	29.8488
27.	0.35	0.9	$q_2 = 1.9195$	-0.00072	20.3381	57.	0.95	0.9	$q_2 = 1.8413$	-0.0466	21.5656
28.	0.35	0.0.9	$q_3 = 2.9890$	0.0242	1805.3500	58.	095	0.9	$q_3 = 2.9810$	0.7690	5860.4860
29.	0.35	0.9	$q_4 = --$	–	–	59.	0.95	0.9	$q_4 = --$	–	–
30.	0.35	0.9	$q_5 = --$	–	–	60.	0.95	0.9	$q_5 = --$	–	–

pair and Triple pair of energy bonding using other different types of sampling strategies. This scientific contribution helps to the chemical scientists to evaluate the bonding energy among electron-proton and to utilize it for well-being of mankind in terms of anticipation in an active chemical process.

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Table 9: Ready reckoner for choice of q providing optimum MSE for given (M,g) (using corollary 4.2, eq. (4.13)) [*Range* $0.05 \leq M \leq 0.95$; *Range* $0.3 \leq g \leq 0.9$]

S.No.	M	g	Choice of q	Bias	MSE	S.No.	M	g	Choice of q	Bias	MSE
1.	0.05	0.3	$q_1 = 1.8017$	-0.0301	9.5438	31.	0.65	0.3	$q_1 = 0.8539$	0.0543	12.3104
2.	0.05	0.3	$q_2 = 3.3300$	-0.0012	9.5433	32.	0.65	0.3	$q_2 = 1.8143$	-0.5697	12.3186
3.	0.05	0.3	$q_3 = 4.1927$	-0.0001	9.5433	33.	0.65	0.3	$q_3 = 2.9416$	-0.0020	12.3162
4.	0.05	0.3	$q_4 = --$	–	–	34.	0.65	0.3	$q_4 = --$	–	–
5.	0.05	0.3	$q_5 = --$	–	–	35.	0.65	0.3	$q_5 = --$	–	–
6.	0.05	0.6	$q_1 = 1.6868$	-0.1267	9.5487	36.	0.65	0.6	$q_1 = 0.8417$	0.0532	12.3115
7.	0.05	0.6	$q_2 = 3.6081$	-0.0012	9.5433	37.	0.65	0.6	$q_2 = 1.6905$	-2.7679	12.3089
8.	0.05	0.6	$q_3 = 4.3270$	0.0004	9.5433	38.	0.65	0.6	$q_3 = 3.1127$	-0.0144	12.3152
9.	0.05	0.6	$q_4 = --$	–	–	39.	0.65	0.6	$q_4 = --$	–	–
10.	0.05	0.6	$q_5 = --$	–	–	40.	0.65	0.6	$q_5 = --$	–	–
11.	0.05	0.9	$q_1 = 1.6062$	0.0634	9.5430	41.	0.65	0.9	$q_1 = 0.8279$	0.0519	12.3113
12.	0.05	0.9	$q_2 = 3.7734$	-0.0010	9.5433	42.	0.65	0.9	$q_2 = 1.5949$	1.0628	12.3181
13.	0.05	0.9	$q_3 = 4.5800$	0.0012	9.5433	43.	0.65	0.9	$q_3 = 3.2493$	-0.0189	12.3153
14.	0.05	0.9	$q_4 = --$	–	–	44.	0.65	0.9	$q_4 = --$	–	–
15.	0.05	0.9	$q_5 = --$	–	–	45.	0.65	0.9	$q_5 = --$	–	–
16.	0.35	0.3	$q_1 = 0.5383$	0.0135	10.1659	46.	0.95	0.3	$q_1 = 0.9851$	0.1233	15.9780
17.	0.35	0.3	$q_2 = 1.8094$	-0.2597	10.1632	47.	0.95	0.3	$q_2 = 1.8177$	-0.9634	15.9724
18.	0.35	0.3	$q_3 = 3.0311$	-0.0050	10.1670	48.	0.95	0.3	$q_3 = 2.8968$	0.0078	15.9752
19.	0.35	0.3	$q_4 = --$	–	–	49.	0.95	0.3	$q_4 = --$	–	–
20.	0.35	0.3	$q_5 = --$	–	–	50.	0.95	0.3	$q_5 = --$	–	–
21.	0.35	0.6	$q_1 = 0.5059$	0.0128	10.1661	51.	0.95	0.6	$q_1 = 0.9838$	0.1230	15.9810
22.	0.35	0.6	$q_2 = 1.6889$	-1.2336	10.1061	52.	0.95	0.6	$q_2 = 1.6916$	-4.4928	15.9530
23.	0.35	0.6	$q_3 = 3.2271$	-0.0088	10.1662	53.	0.95	0.6	$q_3 = 3.0551$	-0.0176	15.9906
24.	0.35	0.6	$q_4 = --$	–	–	54.	0.95	0.6	$q_4 = --$	–	–
25.	0.35	0.6	$q_5 = --$	–	–	55.	0.95	0.6	$q_5 = --$	–	–
26.	0.35	0.9	$q_1 = 0.4719$	0.0122	10.1658	56.	0.95	0.9	$q_1 = 0.9821$	0.2125	15.9781
27.	0.35	0.9	$q_2 = 1.5999$	0.50855	10.1681	57.	0.95	0.9	$q_2 = 1.5907$	1.7384	15.9981
28.	0.35	0.0.9	$q_3 = 3.3784$	-0.0099	10.1667	58.	095	0.9	$q_3 = 3.1832$	-0.0276	15.9772
29.	0.35	0.9	$q_4 = --$	–	–	59.	0.95	0.9	$q_4 = --$	–	–
30.	0.35	0.9	$q_5 = --$	–	–	60.	0.95	0.9	$q_5 = --$	–	–

Table 10: Efficiency Comparison for Proposed Estimator E

S.No.	q	PRE(%)
1	q=1	43.0308%
2	q=2	50.7386%
3	q=3	6.7787%
4	q=4	00.5277%
5	q=5	2.8300%

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Table 11: Ten random ssample selection

Sample No.	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}
(z_1, u_1)	(53,81)	(25,43)	(46,55)	(34,14)	(98,68)	(53,81)	(25,43)	(29,85)	(91,23)	(90,22)
(z_2, u_2)	(34,14)	(34,14)	(79,39)	(91,23)	(46,55)	(37,28)	(53,81)	(95,46)	(92,43)	(98,68)
(z_3, u_3)	(91,23)	(91,23)	(80,43)	(35,63)	(76,33)	(34,48)	(37,28)	(79,92)	(27,83)	(80,43)
(z_4, u_4)	(35,63)	(35,63)	(79,92)	(63,72)	(39,63)	(39,84)	(91,23)	(59,31)	(51,63)	(95,73)
(z_5, u_5)	(63,72)	(27,83)	(70,83)	(84,35)	(80,43)	(56,42)	(35,63)	(48,66)	(88,23)	(59,31)
(z_6, u_6)	(51,63)	(63,72)	(95,73)	(56,42)	(59,31)	(81,33)	(51,63)	(60,43)	(38,49)	(28,33)
(z_7, u_7)	(57,48)	(52,26)	(59,31)	(85,38)	(94,47)	(19,43)	(39,84)	(69,40)	(19,43)	(21,84)
(z_8, u_8)	(47,82)	(84,35)	(48,66)	(57,63)	(77,62)	(43,65)	(84,35)	(88,23)	(43,65)	(69,40)
(z_9, u_9)	(98,34)	(29,57)	(77,62)	(48,96)	(28,33)	(57,48)	(56,42)	(41,40)	(23,58)	(35,71)
(z_{10}, u_{10})	(55,42)	(91,34)	(28,33)	(83,91)	(20,63)	(47,82)	(91,34)	(48,28)	(98,34)	(41,40)
(z_{11}, u_{11})	(63,71)	(38,49)	(48,64)	(47,82)	(25,49)	(98,34)	(57,63)	(28,49)	(45,23)	(48,28)
(z_{12}, u_{12})	(58,83)	(19,43)	(21,84)	(45,23)	(38,33)	(55,42)	(65,36)	(60,53)	(31,48)	(29,51)
(z_{13}, u_{13})	(31,48)	(43,65)	(38,33)	(55,42)	(41,40)	(25,93)	(45,39)	(77,42)	(32,61)	(17,47)
(z_{14}, u_{14})	(35,87)	(45,39)	(69,40)	(25,93)	(60,53)	(31,48)	(57,48)	(82,56)	(48,19)	(39,42)
(z_{15}, u_{15})	(85,53)	(57,48)	(88,23)	(58,83)	(58,68)	(76,29)	(27,63)	(45,33)	(28,59)	(93,21)
(z_{16}, u_{16})	(32,61)	(47,82)	(35,71)	(47,33)	(73,37)	(93,84)	(68,41)	(49,22)	(15,73)	(65,86)
(z_{17}, u_{17})	(93,84)	(98,34)	(56,54)	(85,53)	(39,53)	(92,83)	(73,61)	(41,87)	(93,13)	(49,22)
(z_{18}, u_{18})	(48,19)	(22,93)	(28,49)	(47,93)	(77,42)	(45,84)	(31,48)	(68,91)	(68,91)	(30,43)
(z_{19}, u_{19})	(92,59)	(55,42)	(85,73)	(48,19)	(76,44)	(47,41)	(47,33)	(37,87)	(30,43)	(68,91)
(z_{20}, u_{20})	(38,47)	(29,63)	(78,88)	(28,59)	(37,47)	(68,91)	(76,29)	(48,19)	(48,32)	(72,65)
(z_{21}, u_{21})	(45,38)	(63,71)	(76,44)	(35,83)	(46,26)	(49,22)	(32,61)	(47,93)	(65,86)	(93,13)
(z_{22}, u_{22})	(30,43)	(47,93)	(37,47)	(46,52)	(75,83)	(93,21)	(55,84)	(76,29)	(68,37)	(45,84)
(z_{23}, u_{23})	(29,85)	(55,84)	(28,44)	(93,13)	(93,21)	(46,26)	(38,47)	(35,87)	(77,42)	(28,59)
(z_{24}, u_{24})	(46,55)	(75,84)	(93,21)	(72,65)	(49,64)	(28,44)	(75,83)	(25,93)	(39,53)	(55,84)
(z_{25}, u_{25})	(90, 22)	(47,41)	(87,92)	(68,91)	(87,92)	(39,42)	(54,54)	(29,63)	(73,37)	(85,53)
(z_{26}, u_{26})	(79,39)	(49,22)	(75,32)	(41,87)	(41,87)	(17,47)	(88,63)	(55,42)	(71,39)	(63,71)
(z_{27}, u_{27})	(83,60)	(45,33)	(30,43)	(87,92)	(68,91)	(60,53)	(35,71)	(81,53)	(47,40)	(48,43)
(z_{28}, u_{28})	(79,65)	(75,83)	(45,38)	(75,83)	(72,65)	(45,63)	(76,44)	(98,34)	(69,40)	(58,83)
(z_{29}, u_{29})	(85,94)	(68,37)	(85,38)	(88,63)	(39,83)	(35,71)	(20,75)	(47,82)	(20,63)	(25,93)
(z_{30}, u_{30})	(39,63)	(28,44)	(72,65)	(37,47)	(15,73)	(88,23)	(58,68)	(45,39)	(95,46)	(55,42)
(z_{31}, u_{31})	(80,43)	(39,42)	(93,13)	(76,44)	(28,59)	(69,40)	(28,49)	(65,36)	(97,76)	(22,93)
(z_{32}, u_{32})	(79,92)	(37,47)	(15,73)	(29,51)	(71,94)	(21,84)	(38,33)	(81,33)	(76,33)	(27,63)
(z_{33}, u_{33})	(70,83)	(17,47)	(46,52)	(20,75)	(55,84)	(25,49)	(65,75)	(28,39)	(90,22)	(83,91)
(z_{34}, u_{34})	(95,73)	(78,88)	(38,47)	(95,43)	(47,93)	(28,33)	(70,83)	(63,72)	(46,55)	(43,65)
(z_{35}, u_{35})	(48,66)	(84,73)	(92,83)	(47,40)	(63,71)	(65,74)	(85,94)	(27,83)	(29,85)	(65,36)
(z_{36}, u_{36})	(60,43)	(71,39)	(71,94)	(28,49)	(25,93)	(94,47)	(90,22)	(91,23)	(70,83)	(91,34)
(z_{37}, u_{37})	(28,33)	(60,53)	(55,84)	(56,54)	(45,23)	(70,83)	(46,55)	(34,14)	(48,64)	(29,57)
(z_{38}, u_{38})	(68,37)	(29,85)	(81,53)	(77,62)	(48,96)	(95,46)	(98,68)	(53,81)	(41,40)	(52,26)
(z_{39}, u_{39})	(46,26)	(90,22)	(19,43)	(79,92)	(29,57)	(85,94)	(29,85)	(29,57)	(73,37)	(39,84)
(z_{40}, u_{40})	(41,87)	(97,76)	(34,48)	(54,54)	(51,63)	(46,55)	(79,92)	(68,37)	(82,56)	(43,61)

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Table 12: Sample statistics of 10 samples

Sample No.	Mean ($\bar{z}$)	Mean($\bar{u}$)	s_z	s_u	c_z	c_u	ρ_{zu}
A_1	59.4750	57.0250	22.0953	22.2682	0.3715	0.3905	0.0316
A_2	53.4500	54.3000	23.4728	22.5687	0.4391	0.4156	0.0910
A_3	59.4750	55.2500	24.4036	21.5737	0.4103	0.3904	0.0417
A_4	57.8500	58.9250	22.0995	24.4712	0.3820	0.4152	0.1005
A_5	54.7000	59.5500	21.9676	17.3144	0.4016	0.2907	0.0827
A_6	54.8500	55.0000	24.3548	25.2428	0.4440	0.4589	0.0493
A_7	56.6750	55.8250	21.9678	19.4786	0.3876	0.3489	0.0524
A_8	55.7000	53.0750	21.1238	23.8249	0.3792	0.4488	0.3351
A_9	57.1000	49.5000	25.4365	22.6441	0.4454	0.4574	0.3132
A_{10}	54.3750	55.9000	24.0413	22.0023	0.4421	0.3936	0.2333

Table 13: Estimated confidence intervals over 10 samples at the q_{opt} values

Sample No.	q_{opt}	E	est(MSE)	C.I.	Length
A_1	$q_{1(opt)} = 1.8187$	59.5277	8.9592	[53.66,65.39]	11.7333
A_2	$q_{1(opt)} = 1.8187$	53.6398	10.0225	[47.43,59.84]	12.4100
A_3	$q_{1(opt)} = 1.8187$	59.6364	10.9072	[53.16,66.10]	12.9462
A_4	$q_{1(opt)} = 1.8187$	57.7591	8.8675	[51.92,63.59]	11.6731
A_5	$q_{1(opt)} = 1.8187$	54.5616	8.7947	[48.74,60.37]	11.6251
A_6	$q_{1(opt)} = 1.8187$	55.0114	10.8551	[48.55,61.46]	12.9152
A_7	$q_{1(opt)} = 1.8187$	56.7976	8.8245	[50.97,62.62]	11.6447
A_8	$q_{1(opt)} = 1.8187$	5.9514	7.7704	[50.48,61.41]	10.9272
A_9	$q_{1(opt)} = 1.8187$	57.4857	11.3746	[50.87,64.09]	13.2207
A_{10}	$q_{1(opt)} = 1.8187$	54.4885	10.3214	[48.19,60.78]	12.5931
			Average	[50.32,62.66]	12.1688
A_1	$q_{2(opt)} = 3.2377$	59.5340	8.9636	[53.66,65.40]	11.7362
A_2	$q_{2(opt)} = 3.2377$	53.6975	10.0205	[47.49,59.90]	12.4088
A_3	$q_{2(opt)} = 3.2377$	59.6752	10.9103	[53.20,66.14]	12.9480
A_4	$q_{2(opt)} = 3.2377$	57.7599	8.8656	[51.92,63.59]	11.6719
A_5	$q_{2(opt)} = 3.2377$	54.5687	8.7929	[48.75,60.38]	11.6239
A_6	$q_{2(opt)} = 3.2377$	55.0529	10.8583	[48.59,61.51]	12.9170
A_7	$q_{2(opt)} = 3.2377$	56.8222	8.8257	[50.99,62.64]	11.6455
A_8	$q_{2(opt)} = 3.2377$	56.0485	7.7463	[50.59,61.50]	10.9102
A_9	$q_{2(opt)} = 3.2377$	57.7266	11.3455	[51.12,64.32]	13.2037
A_{10}	$q_{2(opt)} = 3.2377$	54.5108	10.3055	[48.21,60.80]	12.5844
			Average	[55.81,62.61]	12.1649
A_1	$q_{3(opt)} = 4.2569$	59.5341	8.9635	[53.66,65.40]	11.7361
A_2	$q_{3(opt)} = 4.2569$	53.6997	10.0206	[47.49,59.90]	12.4089
A_3	$q_{3(opt)} = 4.2569$	59.6763	10.9102	[53.20,66.15]	12.9480
A_4	$q_{3(opt)} = 4.2569$	57.7604	8.8657	[51.92,63.59]	11.6719
A_5	$q_{3(opt)} = 4.2569$	54.5698	8.7929	[48.75,60.38]	11.6239
A_6	$q_{3(opt)} = 4.2569$	55.0542	10.8582	[48.59,65.51]	12.9171
A_7	$q_{3(opt)} = 4.2569$	56.8228	8.8256	[51.00,62.64]	11.6455
A_8	$q_{3(opt)} = 4.2569$	56.0530	7.7472	[50.59,61.50]	10.9108
A_9	$q_{3(opt)} = 4.2569$	57.7421	11.3466	[51.13,64.34]	13.2044
A_{10}	$q_{3(opt)} = 4.2569$	54.5113	10.3061	[48.21,60.80]	12.5844
			Average	[50.45,69.56]	12.1651