Step 4: Determine the fitted mean and the fitted variance response functions by regressing y_i against the control factors X and regressing s^2_i against the control factors X using the OLS method.
Step 5: Determine the optimal setting condition $X = (x^*_{i1},\ldots,x^*_{ip})$
Step 6: Determine the estimated optimal mean response by substituting the optimal settings $X = (x^*_{i1},\ldots,x^*_{ip})$ into the obtained fitted mean and variance functions in Step 4.

PROPOSED OPTIMIZATION SCHEME FOR DUAL RESPONSE FUNCTION

In this section, a dual response surface optimization technique based on the penalty function approach is derived, specifically for our proposed PFO method. The penalty function method convert a series of constrained optimization into unconstrained optimization problem whose optimum solution are also true solution of the formulated function and the original objective function. The unconstrained objective function is formulated by adding a penalty parameter to the real objective function which includes the penalty term multiply by the measure of violation of the constraints equation (Dong 2006; Shin et al. 1990; Wan et al. 2009). To derive the objective function, we first consider the general form of the constrained optimization problem defined by

Minimize $f(x)$

$$\text{Subject to } g_j(x) \le 0, j = 1, 2, \ldots, m \qquad h_i(x) = 0, i = 1, 2, \ldots, n \tag{3}$$

By applying the method of penalty function, one can determine the solution of Equation (3) from the following objective function

$$F(x) = f(x) + \textstyle\sum_{j=1}^{m} \mu\left(g_j(x)\right) + \sum_{i=1}^{n} \mu\left(h_i(x)\right) \tag{4}$$

where $f(x)$ is the original objective function to be minimized, h_i and g_j are set of the inequality and equality constraints function, respectively. This article, specifically focuses on a quadratic penalty function defined by;

$$F(x, \mu) = f(x) + \tfrac{\mu}{2} \textstyle\sum_{i=1}^{n} \left(h_i(x)\right)^2 \tag{5}$$

where μ is called the penalty parameter that penalizes the equality constraints when the constraints relations are not satisfied. For simplicity, we substitute $h_i = [\hat{m}(x) - T]$ and $f(x) = \hat{v}(x)$ in Equation (5) and then write the following quadratic unconstrained minimization problem as;

$$\min F(x\,\mu,) = \hat{v}(x) + \tfrac{\mu}{2}[\hat{m}(x) - T]^2 \tag{6}$$

where $\hat{m}(x)$ is the estimated mean response, $\hat{v}(x)$ is the estimated variance response surface function and T is the desired target selected by the decision maker. If $\mu = \infty$ the solution of (6) is exact. For the quadratic function in Equation (6), we may use nonlinear optimization package in any programming software to determine the optimal setting condition of the estimated mean response. In this paper, a statistical software package in R programming Language (Rsolnp) introduced in Ghalanos and Theussl (2012) and Ye (1989) are used to compute the approximate optimum solution for the newly formulated and existing optimization schemes. Our goal is to find the optimum value so that the estimated mean response will be equal to or varies to the target value T, while making the variance small. The optimization scheme proposed is superior over the existing approaches. Firstly, the proposed approach takes into account the measure of violation of the constrained function, while LT optimization functions are minimized without given concern to the effect of the violation of the constrained. Secondly, the penalty term in Equation (6) pushes $\hat{m}(x) - T$ to be equal or close to zero so that it can achieve the target of the decision maker. These two properties make the proposed method more efficient and reliable to estimate the mean and the variance functions for approximation of the optimum settings conditions. In the next section, we will prove that the PFO method produces smaller variance than the LT method.

THE WEIGHTED LEAST SQUARES AND OPTIMIZATION PROCEDURES

In the presence of heteroscedasticity in the response observations, the usual assumption of constant variance in linear regression model may not hold in many real life problems. The OLS regression assumed that the observed response Y come from a normal distribution function with mean $X\beta$ and variance $\sigma^2 I$ where X is a data matrix of containing the predictor variables, β is a vector of estimated coefficients, and I is an identity matrix. The summary of the OLS assumption can be express as:

$$y \sim N(X\beta, \sigma^2 I)$$

Suppose that the distribution of the errors have non constant variance whose constant of proportionality k_i are known, then the variance of regression errors $\varepsilon_1, \ldots, \varepsilon_n$ is given as:

Var(ε) = $k_i\,\sigma^2$, for i = 1,..., n, in matrix form is given as; $y \sim N(X\beta,\sigma^2 V)$ where V = diag[c_1, ...c_n]. Therefore we can express

$$\varepsilon = y\text{-}\ X\beta \sim N\,(0, \sigma^2\ V) \tag{7}$$

Applying the symmetric diagonal matrix, $W^{\frac{1}{2}} =$ daig$\left[1/\sqrt{c_1},\ldots,\ 1/\sqrt{c_n}\right]$, note that $W = W^{\frac{1}{2}}W^{\frac{1}{2}} = V^{-1}$, multiplying both side of equation (7) by $W^{\frac{1}{2}}$ we have

$$W^{\frac{1}{2}}\varepsilon = W^{\frac{1}{2}}(y - X\beta) \sim N(0,\sigma^2 V) \tag{8}$$

For convenience, we rewrite equation (8) as:

$$W^{\frac{1}{2}}y = W^{\frac{1}{2}}X\beta + W^{\frac{1}{2}}\varepsilon$$

This can be express as:

$$y_{wsl} = X_{wsl}\,\beta_{wsl} + \varepsilon_{wsl} \tag{9}$$

Equation (8) is equivalent to the standard regression model $y = X\beta + \varepsilon$. Applying the ordinary least squares (OLS) method, the transformed model in Equation (8) becomes:
$\beta_{wsl} = (X'_{wls}X_{wsl})^{-1}X_{wsl}y_{wsl}$, where $y_{wsl} = W^{\frac{1}{2}}, X_{wsl} = W^{\frac{1}{2}}X$,

$$\hat{\beta}_{wls} = \left[(W^{\frac{1}{2}}X)'W^{\frac{1}{2}}X\right]^{-1}(W^{\frac{1}{2}}X)'W^{\frac{1}{2}}y$$

$$= \left(X'W^{\frac{1}{2}}W^{\frac{1}{2}}X\right)^{-1}X'W^{\frac{1}{2}}W^{\frac{1}{2}}y \tag{10}$$

$$= (X'WX)^{-1}X'Wy$$

Incorporating the WLS in Equation (9) into robust design approach, we developed the fitted response functions for the process mean and variance as:

$$\widehat{m}(x) = X\hat{\beta}_\mu \tag{11}$$

$$\hat{V}(x) = X\hat{\beta}_\sigma\,, \tag{12}$$

where $\hat{\beta}_\mu = (X'WX)^{-1}X'W\bar{y}_i$

and $\hat{\beta}_\sigma = (X'WX)^{-1}X'Ws_i^2$

Furthermore, this approach work effectively when the number of replications is complete for each design value, but it may not be suitable for unbalanced data when the sample sizes are not equal. Hence, an alternative technique which choose weight based on the sample sizes at each design point were suggested by Goethals and Cho (2011) and Cho and Park (2005). They defined weights for mean and variance as W_m = diag[m_1, ..., m_n], W_v = diag[m_1-1, ..., m_n-1] where (m_1, ..., m_n) is the number of observation at each design point. More so, applying the formulated models for the mean and variance, the MSE objective function used in the LT optimization scheme is defined as:

$$\text{MSE} = \left\{[m(x_n) - T]^2 + v(x_n)\right\} \tag{13}$$

such that $x_i \in [L_j, U_j]$ for $j = 1,\ldots,k,$

where T is the specified target value, usually selected according to the quality characteristic of interest of the experimenter and x_j is the experimental region of the factorial designs with k levels. However, the mean squared error model introduced some bias and it does not take into account how large the estimated mean response should deviate from the actual specify target output (Copeland & Nelson 1996). This shortcoming often results to large difference between the estimated mean response and the target output that may lead to misleading conclusion. Therefore, we employ the weighted least squares (WLS) combined with the newly proposed PFO optimization scheme to obtain the optimal setting of the estimated mean response. For convenient, we re-write the newly propose optimization scheme (PFO) as follows:

$$\min\left\{\tfrac{\mu}{2}[m(x_n) - T]^2 + v(x_n)\right\} \tag{14}$$

Equations (13) and (14) can be used to find the optimal setting condition that optimizes the fitted mean and variance functions while achieving the target output. The PFO optimization scheme is based on the following fact:

Let $x_n \to x_0$ as $n \to \infty$.
If $m(x_n) \to T, v(x_n) \to v_0$ as $n \to \infty$
where v_0 is the minimum of $v(x_n)$
Then, clearly $\left\{[m(x_n) - T]^2 + v(x_n)\right\} \to v_0$ as $x_n \to \infty$.

Also, $\left\{\tfrac{\mu}{2}[m(x_n) - T]^2 + v(x_n)\right\} \to v_0$ as $x_n \to \infty$ since the first term approaches zero, where μ is any positive number. The parameter μ plays a key role to manage the convergence rate of limit. Therefore, we consider the function (14) instead of (13) because it will tend to produce less bias and less variability.

SIMULATION STUDY

In this section, we consider two simulation studies. The first objective of the simulation study is to show that our proposed PFO method is more efficient than some existing methods in this study. As per Midi and Aziz (2019), Lee et al. (2007) and Park and Cho (2003) simulation studies, at each control factor setting $\mathbf{x}_{\boldsymbol{i}} = (x_{i1}, x_{i2}, x_{i3})$, $i = 1, \ldots, 27$, five responses (y_{i1}, y_{i2}, y_{i5}) are randomly generated from a normal distribution with mean, $m(x_i) = 500 + (x_1 + x_2 + x_3)^2 + x_1 + x_2 + x_3$ and variance, $v(x_i) = 100 + (x_1 + x_2 + x_3)^2 + x_1 + x_2 + x_3$ where the target value, T equals 500. The VM, LT, WMSE, and PFO were then applied to the data and we considered 1000 simulation runs. The estimated mean of the optimal mean response, computed over m iterations are given by $\bar{\hat{\mu}} = \sum_{i=1}^{m}(\hat{\mu}/m)$, Bias $= \bar{\hat{\mu}} - 500$, and $var(\hat{\mu}) = \sum_{i=1}^{m}(\hat{\mu} - \bar{\hat{\mu}})^2/m$. The mean squared error (MSE) is written as MSE $(\mu) = (\text{Bias})^2 + \text{var}(\mu)$. The results are exhibited in Table 2. It is interesting to observe that the proposed PFO is the most efficient method as it has the smallest bias, SE, and RMSE, followed by the LT, WMSE and VM methods. Hence, we will consider the PFO and the LT in the next objective.

TABLE 2. Bias, standard error (SE) and RMSE of the optimal mean response

Method	Bias	SE	RMSE
VM	1.30	4.41	4.52
LT	1.46	3.73	4.01
WMSE	1.47	3.78	4.06
PFO	0.07	0.23	0.24

The second objective of the simulation study is to show that the PFO combined with the WLS methods is more efficient than the LT combined with the WLS methods for unbalanced data. The VM and the WMSE were not considered in this study because both methods do not perform very well based on the results of the first objective. Moreover, as already mentioned in the introduction section, these methods have some drawbacks. Following the simulation technique developed by Cho and Park (2005) and Park and Cho (2003), 3^2 factorial design with two factors and 3 levels represented by the digits (-1, 0, +1) were considered. The responses $(y_{i1}, y_{i2}, \ldots, y_{im})$ are generated from a normal distribution with mean $m(x_i) = 50 + 10(x_1^2 + x_2^2)$ and variance $v(x_i) = 100 + 25(x_1^2 + x_2^2)$. For each factor settings $x_i = (x_{i1}, x_{i2})$ for $i = 1,2,\ldots,9$, the response variables are replicated for a specific number represented in a circle as shown in the simulation scheme given in Figure 1. The customer target value is assumed to be 50, i.e. T = 50 and a total of 1000 iteration were considered.

For each of the four simulation scheme in Figure 1, we can compute the bias, variance and mean squares error (MSE) of the optimum mean response in order to evaluate the performance of the OLS and WLS based on LT optimization function and compared the results based on our proposed PFO optimization scheme given in Equation (14). Tables 3 and 4 reported the estimated bias, variance and MSE of the optimum mean response, based on LT and PFO optimization function, respectively. The results of Tables 3 and 4 show that the WLS method is superior to the OLS method irrespective of the optimization scheme used; LT or PFO. However, it is interesting to see that by comparing the results of Tables 3 and 4, the WLS based on our proposed (PFO) method is better than the WLS based on the LT method evident by having smaller values of bias, SE, and RMSE. Due to space constrained, in this paper we only consider 3^3 (first simulation) and 3^2 (second simulation) factorial designs. It is important to note that factorial design with different factors and levels may be considered. However, the results are consistent.

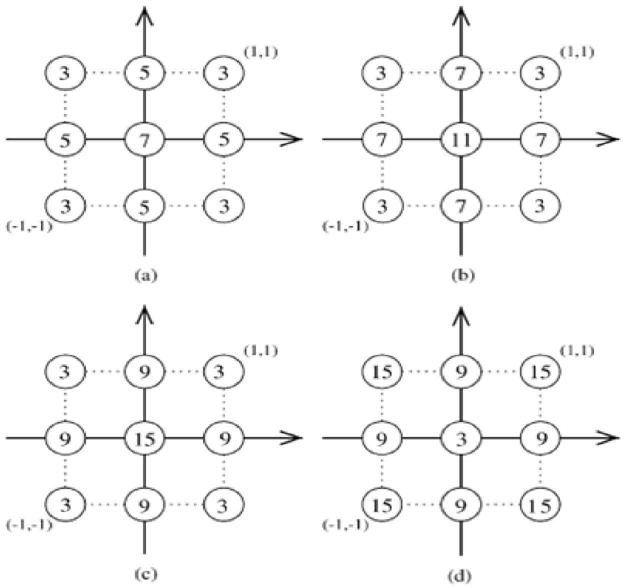

FIGURE 1. Simulation Scheme of Cho and Park (2005)

TABLE 3. Estimated bias, variance and MSE of the optimal mean response for the various simulation scheme with LT

Scheme	OLS			WLS		
	Bias	SE	RMSE	Bias	SE	RMSE
(a)	3.24	5.55	16.94	3.20	4.86	15.13
(b)	3.01	4.02	13.14	2.97	3.80	12.59
(c)	2.17	3.35	11.62	2.53	2.76	9.18
(d)	2.39	5.92	11.61	2.36	4.97	10.55

TABLE 4. Estimated bias, variance and MSE of the optimal mean response for the various simulation scheme with PFO

Scheme	OLS			WLS		
	Bias	SE	RMSE	Bias	SE	RMSE
(a)	1.19	2.85	4.26	1.17	2.63	4.01
(b)	1.08	2.41	3.58	0.96	1.76	2.70
(c)	0.94	1.70	2.58	0.86	1.43	2.16
(d)	1.55	4.35	6.77	1.20	1.20	4.89

NUMERICAL EXAMPLE

Considering the case study data reported in Cho and Park (2005), suppose that an injection modeling company is given the responsibility of producing silicon wafers for Motor Corporation. Tables 5 reported the experimental data obtained from the development of silicon wafers, where $\boldsymbol{x_1}$ and $\boldsymbol{x_2}$ are factors variable representing the mold temperature and injection flow rate and the response $\boldsymbol{y_{ij}}$ represent the coating thickness of the wafers with target value of T = 50, respectively. The weight for the mean and variance function obtained from the data based on $\boldsymbol{m_i}$ and $\boldsymbol{m_i}$**-1** is given by $\boldsymbol{W_m}$ = diag[3, 5, 3, 5 7, 5, 3, 5, 3] and $\boldsymbol{W_v}$ = diag[2, 4, 2, 4, 6, 2, 4, 2]. The estimated coefficients of the fitted mean response function, $\hat{m}(x)$ and the fitted variance response function, $\hat{v}(x)$ using OLS and WLS methods are exhibited in Table 6. The OLS and WLS with LT optimization scheme and the newly proposed PFO optimization scheme were applied to the data. The results of the OLS method based on LT optimization and WLS method based on our proposed PFO optimization scheme are presented in Table 7. It can be observed from Table 7 that the $\boldsymbol{WLS_{LT}}$ is more efficient compared to $\boldsymbol{OLS_{LT}}$ which have smaller bias, variance, and RMSE. Nevertheless, it is interesting to observe that our proposed $\boldsymbol{WLS_{PFO}}$ is superior and more reliable compared to$\boldsymbol{WLS_{LT}}$.

TABLE 5. Case study data from Cho and Park (2005)

index	x_1	x_2	y_{ij}							$\bar{y}$	s_i^2
1	1	-1	84.30	57.00	56.50					65.93	253.06
2	0	-1	75.70	87.10	71.80	43.80	51.60			66.00	318.28
3	1	-1	65.59	47.90	63.30					59.03	94.65
4	1	0	51.00	60.10	69.70	84.80	74.74			68.06	170.35
5	0	0	53.10	36.20	61.80	68.60	63.40	48.60	42.5	53.46	139.89
6	1	0	46.50	65.90	51.80	48.40	64.40			55.40	83.11
7	1	1	65.70	79.80	79.10					74.87	63.14
8	0	1	54.40	63.80	56.2	48.00	64.50			57.38	47.54
9	1	1	50.70	68.30	62.90					60.63	81.29

TABLE 6. Estimated coefficients of the fitted mean response function, and the fitted variance response function, using OLS and WLS methods

Coefficients	OLS		WLS	
	$\hat{m}(x)$	$\hat{v}(x)$	$\hat{m}(x)$	$\hat{v}(x)$
$\hat{\beta}_0$	55.61	160.65	55.08	154.26
$\hat{\beta}_1$	-5.63	-37.92	-5.76	-39.34
$\hat{\beta}_2$	0.32	-79.00	-0.52	-93.09
$\hat{\beta}_{11}$	5.04	-44.30	5.51	-38.31
$\hat{\beta}_{22}$	5.00	11.88	5.47	17.87
$\hat{\beta}_{12}$	-1.84	44.14	-1.84	44.14

TABLE 7. Estimated optimum settings, Bias, Variance and RMSE of the optimum mean response with OLS and WLS methods

Method	Optimal Settings	Bias	Var	RMSE
OLS_{LT}	(1.00, 1.00)	8.45	55.45	11.30
OLS_{PFO}	(1.00,0.94)	7.98	56.12	10.96
WLS_{LT}	(1.00, 1.00)	7.93	45.66	10.42
WLS_{PFO}	(1.00,0.99)	7.89	45.59	10.39

CONCLUSION

The problem of unbalanced design data lead to non-constant error variances in the response observation. The method of least squares combined with LT optimization scheme ($\boldsymbol{OLS_{LT}}$) gives less efficient results in solving these problems, while the integration of WLS concepts into robust design with LT optimization ($\boldsymbol{WLS_{LT}}$) has improved the estimated mean response. However, the overall results show that incorporating the WLS with our proposed PFO optimization scheme ($\boldsymbol{WLS_{PFO}}$) provide the most efficient results as it has the smallest bias, SE, and RMSE. Hence, the newly proposed scheme can be a good alternative method in dealing with robust design optimization problem with unbalanced data points.

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