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Generalized maximum entropy approach to unreplicated factorial experiments

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In the initial stage of developing an industrial process, experimental studies based on factorial designs are often used to determine which factors among a number of factors have an effect on the response variable. A large number of factors somehow may arise and a number of runs that grows exponentially with the number of factors to be analyzed. Therefore, researchers often design unreplicated factorial experiments. Furthermore, considering the cost of experimentation, time, effort, and/or limitation of data resources, unreplicated factorial designs can be adopted to reduce the number of runs. But, using ordinary least squares method to analyze unreplicated experimental data results in zero degrees of freedom for error term in regression analysis. Generalized maximum entropy approach which is a method of selecting among probability distributions to choose the distribution that maximizes uncertainty or uniformity remaining in the distribution, subject to information already known about the distribution, is an alternative way of analyzing the unreplicated experiments. In this paper, generalized maximum entropy approach is applied to an illustrative data set and a real-world example and results are compared to the alternatives with respect to their abilities to find active effects.

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1. INTRODUCTION

Design of Experiment (DoE) is one of the most common tools in statistics. It covers a wide range of applications from household works like food preparation to technological innovation, science, agriculture and so forth. Experimentation is used to comprehend and/or advance a system. It enables researchers to explore what results in a response (output) variable when the settings of the input variables in the system, the variables that are supposed to affect this output, are altered.

Managers and engineers of today's modern industrial world put an increased emphasis on achieving breakthroughs and improvements in productivity and quality of processes and products through the application of DoE and other statistical techniques. DoE provides a theoretical basis for experimentation for these reasons and is exclusively convenient for working simultaneously on several variables, in order to ascertain the input variables with the greatest effect on an output variable and the levels of these input variables, at which they should be kept to improve process or product performance. In factorial designs, the experimental runs are often replicated to obtain an estimate of experimental error which can be used to construct statistical tests for assessing factors' significance. However, when experiments are conducted in manufacturing facilities, the processes' complexity often makes the replication of physical experiments prohibitive, if not, impossible considering the cost of experimentation, time, effort, and/or limitation of data resources. Consequently, unreplicated factorial designs play an important role in process and product improvement.

Analysis of unreplicated factorial designs has been much studied, however, it still constitutes an open and active research field. As it was stated above, replication allows to estimate experimental error and as well as to increase power to detect important effects by decreasing the variance of the treatment effects estimates. When there is no estimate for experimental error, the high order interactions are often sacrificed for the estimate of error term, which cannot always be a good solution, assuming one of these interactions might be statistically significant. The most popular tool for identifying active effects in unreplicated factorial experimentations is the normal or half-normal probability plot of the factorial effects (Daniel (1959) [1]). Although several researchers are aware of that their interpretations are somewhat informal and subjective, these plot techniques have been applied to identify the active effects. It is not easy to identify and classify as inactive the effects that fall along a straight line and as active the ones that tend to "fall on the line". Thus, objective methods are preferable and numerous competing alternatives have been reported in the literature (Hamada and Balakrishnan (1998) [2]). It is important to avoid empirical practices and subjective analyses in experimental studies, reinforcing one important message: efficient methods whose interpretation is not subjective are more suitable and advisable, mainly for those who do not have enough background in DoE.

After the entropy concept is developed as a measure of uncertainty by Shannon (1948) [3], the maximum entropy

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principle was formulated by Jaynes (1957) [4] as a method for estimation and inference particularly for ill-posed and/or ill-conditioned problems. More recently, Golan et al. (1996) [5] develop the generalized maximum entropy (GME) estimator in the context of non-normal disturbances. Eruygur (2005) [6] compared the GME estimator of unknown parameters of the general linear models with the ordinary least squares (OLS) estimator by Monte Carlo simulations and concluded that the performance of the GME estimator is substantially good, especially when the sample size is small. Ciavolino and Al-Nasser (2009) [7] compared the GME estimator with the partial least squares estimator in the presence of missing data, outliers and multicollinearity by simulations and showed that the empirical results of GME outperform the partial least squares in the terms of mean squared error. All these papers pointed out that the GME method has several advantages over the traditional maximum likelihood and least squares formulations. Some of the most commonly cited advantages are that it is more efficient specifically whenever convergence rate is considered necessary, avoids strong parametric assumptions, works pretty well in small sample sizes, and uses prior information.

In this article, we use the GME estimation method for modelling unreplicated factorial designs and compare its ability to find the active effects with some well-known and mostly-used methods and some recent techniques, objectively selected from the literature. The use of the approach can be found in the session on the ENTROPY procedure of the SAS/ETS 9.3 User's Guide (2011) [18] and in Ying-Chao (2010) [15]. Ying-Chao (2010) [15] describes results of simulation studies and comparisons of the generalized maximum entropy approach and Lenth's method for analyzing unreplicated factorial designs. Since the thesis from the Chinese University may be a difficulty reading for many, other references on the use of entropy for analyzing experimental designs are Koukouvinos et al. (2011) [17] and Balakrishnan et al. (2012) [16].

The present study is structured into five chapters and organized as follows. In the following section we introduce GME approach in details, which has not been applied to unreplicated factorial effects, so far. Section 3 briefly discusses competing methods. In Section 4 and 5, we perform GME approach and all other methods on an illustrative example and a real-life experiment data set respectively, and active effects are obtained, and a discussion is given in the last section.

2. GENERALIZED MAXIMUM ENTROPY ESTIMATION

Let Y be $N \times 1$ dependent variable vector, X be the $N \times K$ known matrix that contains data on the explanatory variables. The linear regression model can be written as follows:

$$Y = X\beta + \varepsilon \tag{1}$$

where β is the $K \times 1$ vector of unknown parameters and ε is the $N \times 1$ vector of unknown errors (also called noise or disturbances). The standard least squares estimation of β vector of parameters is the solution of the following optimization problem:

$$min_\beta \left\{ \sum_{i=1}^{N} \varepsilon_i^2, \;\; \varepsilon_i = Y_i - X_i\beta, \;\; \forall i \right\} \tag{2}$$

Here, the objective is to minimize the quadratic sum of squares function for β. The maximum entropy approach is based on the entropy objective function $H(p)$ instead of quadratic sum of squares objective function given in Equation (2). In order to use Jaynes' maximum entropy principle for the estimation of regression parameters, the unknown parameter vector β should be written in terms of probabilities because of the fact that the arguments of the Shannon's maximum entropy function are probabilities. Each unknown parameters β_k is reparameterized for $M \geq 2$ as follows (Golan et al. (1996) [5]):

$$\beta_k = \sum_{m=1}^{M} z_{km} p_{km}, \;\; k = 1, 2, \ldots, K, \tag{3}$$

Let us define Z as $K \times KM$ block diagonal matrix of support points and p^β as $KM \times 1$ vector of probabilities or weights on support points. Now we can rewrite β in Equation (1) as,

$$\beta = Zp^\beta = \begin{bmatrix} z_1' & 0 & \ldots & 0 \\ 0 & z_2' & \ldots & . \\ . & . & \ldots & 0 \\ 0 & . & 0 & z_k' \end{bmatrix} \times \begin{bmatrix} p_1 \\ p_2 \\ . \\ p_k \end{bmatrix} \tag{4}$$

where $z_k' = [z_{k1}, z_{k2}, \ldots, z_{kM}]$ and $p_k = [p_{k1}, p_{k2}, \ldots, p_{kM}]'$ are M-dimensional vector of equally distanced discrete points (support space) and associated M-dimensional vector of proper probabilities, respectively. The implementation of the maximum entropy formalism allowing for unconstrained parameters starts by choosing a set of discrete points by researcher based on his a priori information about the value of parameters to be estimated (Eruygur (2005) [6]). If the researcher has no prior information about the sign and magnitude of the unknown β_k, support space should be defined uniformly symmetric around zero with end points of large magnitude. For instance, for $M = 5$ and for a scalar C, $z_k' = [-C, -C/2, 0, C/2, C]$.

Similarly, the unknown error vector ε is reparameterized for $J \geq 2$ as follows (Jaynes (1957) [4]):

$$\varepsilon_t = \sum_{j=1}^{J} v_{tj} p_{tj}, \;\; t = 1, 2, \ldots, T. \tag{5}$$

Define V as $T \times TJ$ block diagonal matrix of support points and p^ε as $TJ \times 1$ vector of probabilities or weights on support points. Now we can rewrite ε in Equation (1) as

$$\varepsilon = Vp^{\varepsilon} = \begin{bmatrix} v_1' & 0 & ... & 0 \\ 0 & v_2' & ... & . \\ . & . & ... & 0 \\ 0 & . & 0 & v_T' \end{bmatrix} \times \begin{bmatrix} p_1 \\ p_2 \\ . \\ p_T \end{bmatrix} \quad (6)$$

where $v_t' = [v_{t1}, v_{t2}, \ldots, v_{tJ}]$ and $p_t = [p_{t1}, p_{t2}, \ldots, p_{tJ}]'$ are J-dimensional vector of support space and associated J-dimensional vector of probabilities, respectively.

In practice, discrete support spaces for both parameters and errors, supplied by the researcher, are based on economic or other prior information. The support space of errors is defined according to Chebyshev's inequality $(-\upsilon\sigma, +\upsilon\sigma)$. Golan et al. (1996) [5] suggested using the "three-sigma rule" to establish bounds on the error components: the lower bound is taken as $-3\sigma_y$ and the upper bound is taken as $3\sigma_y$, there, σ_y is the standard deviation of the dependent variable. For example, if $J = 5$, then $v_t' = [-3\sigma_y, -1.5\sigma_y, 0, 1.5\sigma_y, 3\sigma_y]$ is used. With the assumption that unknown weights on the parameters and the error support for linear regression model are independent, the unknown parameters and errors are obtained by solving the constrained optimization problem $maxH(p^{\beta}, p^{\varepsilon}) = -p^{\beta\prime} \ln p^{\beta} - p^{\varepsilon\prime} \ln p^{\varepsilon}$ subject to $Y = X\beta + \varepsilon = XZp^{\beta} + Vp^{\varepsilon}$.

The data constrained GME estimator of the linear regression model is defined by the following maximum entropy problem (Golan et al. (1996) [5]):

(7)
$$maxH(p^{\beta}, p^{\varepsilon}) = -\sum_{k=1}^{K}\sum_{m=1}^{M} p_{km}^{\beta} \ln p_{km}^{\beta} - \sum_{t=1}^{T}\sum_{j=1}^{J} p_{tj}^{\varepsilon} \ln p_{tj}^{\varepsilon}$$

subject to constraints

$$\sum_{k=1}^{K}\sum_{m=1}^{M} x_{tk} z_{km} p_{km}^{\beta} + \sum_{j=1}^{J} v_{tj} p_{tj}^{\varepsilon} = y_t, \quad t = 1, 2, \ldots, T \quad (8)$$

$$\sum_{m=1}^{M} p_{km}^{\beta} = 1, \quad k = 1, 2, \ldots, K \quad (9)$$

$$\sum_{j=1}^{J} p_{tj}^{\varepsilon} = 1, \quad t = 1, 2, \ldots, T \quad (10)$$

Solution by the help of Lagrange multipliers (Eruygur (2005) [6]), we get the GME estimators of of β_k and ε_t as follows:

$$\hat{\beta}_k^{GME} = \sum_{m=1}^{M} \hat{p}_{km}^{\beta(GME)} z_{km}, \quad k = 1, 2, \ldots, K \quad (11)$$

$$\hat{\varepsilon}_t^{GME} = \sum_{j=1}^{J} \hat{p}_{tj}^{\varepsilon(GME)} v_{tj}, \quad t = 1, 2, \ldots, T \quad (12)$$

Under the conditions that support space is uniformly symmetric around zero and errors are independent, GME estimator is consistent and asymptotically normal (Joshi et al. (2010) [8]). In order to obtain the estimates of β_k^{GME} and ε_t^{GME} over Equations (11) and (12), numerical optimization techniques should be employed.

For the entropy problem, the estimate of asymptotic variance of the parameters is given by

$$\hat{Var}(\hat{\beta}^{GME}) = \frac{\hat{\sigma_{\gamma}^2}(\hat{\beta}^{GME})}{\hat{\psi^2}(\hat{\beta}^{GME})} (X'X)^{-1} \quad (13)$$

where,

$$\hat{\sigma_{\gamma}^2}(\hat{\beta}^{GME}) = \frac{1}{T}\sum_{t=1}^{T} {\gamma_t}^2 \quad (14)$$

and γ_t is the Lagrange multiplier associated with the tth row of the Vp^{ε} constraint matrix. Also,

(15)
$$\hat{\psi^2}(\hat{\beta}^{GME}) = \left[\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{j=1}^{J} v_{tj}^2 p_{tj}^{\varepsilon} - \left(\sum_{j=1}^{J} v_{tj} p_{tj}^{\varepsilon}\right)^2\right)^{-1}\right]^2$$

3. METHODS FOR IDENTIFYING THE SIGNIFICANT EFFECTS IN UNREPLICATED FACTORIAL DESIGNS

In this study, some popular methods utilized for analyzing unreplicated factorial designs are compared. In this section, we briefly discuss these methods.

The first method is based on the projection property of factorial designs, i.e., such designs can be projected into smaller designs by the significant factors. It was proposed by Angelopoulos et al. (2010) [9] and it is a two-step procedure. The authors proposed determining firstly a set of inactive effects in order to take advantage of the projective property and project the factorial design in those factors that appear to be active and use the classical *ANOVA* techniques to perform tests. Suppose that A is a set of all factorial effects of a factorial design with k main effects and $P_i, i = 1, \ldots, k$ be the k sets of all factorial effects obtained after projecting the unreplicated design into all possible choices of $k-1$ factors. Each projection design can be viewed as a new experiment that can be analyzed since there are 2^{k-1} degrees of freedom left to estimate the experimental error. Using classical analysis we can identify the active and inactive effects in each P_i. If a factorial effect is found to be active in any projection design analysis, then it appears to be a potential active effect for the original unreplicated design and vice versa. The authors also suggested that experimental errors should be controlled at a desired level and thus, the critical values should be selected following their procedure.

The second method used in this study is Lenth's method, which is one of the most popular tools, proposed by Lenth (1989) [10]. Let $\hat{\theta}_1, \ldots, \hat{\theta}_p$ denote p mutually orthogonal estimated factorial effects. Assuming that there are only a few active effects. Lenth used a pseudo standard error (PSE) to estimated the standard deviation of $\hat{\theta}_i$'s:

$$PSE = 1.5 \times \text{median}_{|\hat{\theta}_i|<2.5s_0} |\hat{\theta}_i| \tag{16}$$

where,

$$s_0 = 1.5 \times \text{median } |\hat{\theta}_i| \tag{17}$$

Lenth, then, obtained a margin error (ME) for contrasts. Contrasts that exceed the ME in absolute value are deemed active. Because with a large number of p contrasts, one can expect one or two estimates of inactive contrasts to exceed the ME leading to false conclusion, alternatively, one can compute simultaneous margin of error (SME) to account for this possibility. A contrast that extends beyond the SME is clearly considered as an active effect. ME and SME can be calculated as follows:

$$ME = t_{0.975;d} \times PSE \tag{18}$$

$$SME = t_{\gamma;d} \times PSE \tag{19}$$

where,

$$\gamma = \frac{(1 + 0.95^{1/p})}{2} \tag{20}$$

Here, $t_{0.975;d}$ and $t_{\gamma;d}$ are the 0.975th and the γth quantiles of a t distribution on d degrees of freedom, respectively.

Dong (1993) [11] also defined an estimator of contrast standard error as follows:

$$S_{\text{Dong}} = \sqrt{\frac{1}{p_{inactive}} \left(\sum_{|\hat{\theta}_i|<2.5s_0} \hat{\theta}_i^2 \right)} \tag{21}$$

where p is the number of factorial effects (contrasts), $p_{inactive}$ is the number of inactive contrasts characterized by $|\hat{\theta}_i| < 2.5s_0$, and $s_0 = 1.5 \cdot \text{median } |\hat{\theta}_i|$. A contrast is declared active if

$$|\theta_i| > t_{\gamma;p_{inactive}} \times S_{Dong} \tag{22}$$

where,

$$\gamma = \frac{(1 + 0.97^{1/p_{inactive}})}{2} \tag{23}$$

Here, we choose 0.97 because it will make the actual α-levels closer to those of Lenth's.

Ye et al. (2001) [12] proposed a step-down version of the Lenth's method for controlling experimental error rate (EER), which is the error rate of at least one inactive effect being declared active. Let $|\hat{\theta}|_{(1)} \leq |\hat{\theta}|_{(2)} \leq \ldots \leq |\hat{\theta}|_{(p)}$ be the order statistics of p absolute contrasts. Obtain the test statistics;

$$t_i = \frac{|\hat{\theta}|_{(i)}}{PSE_i}, \quad i = 1, \ldots p \tag{24}$$

where PSE_i is the pseudo standard error of $\hat{\theta}_{(1)}, \hat{\theta}_{(2)}, \ldots, \hat{\theta}_{(p)}$, the signed contrasts corresponding to the absolute contrasts $|\hat{\theta}|_{(1)}, |\hat{\theta}|_{(2)}, \ldots, |\hat{\theta}|_{(p)}$. Let C_α^i denote the critical value at significance level α of the original Lenth method with p contrasts. If $t_i > C_\alpha^i$ for all $i > p-k$, then the largest k factorial effects are declared active. Values of C_α^i for i between 4 and 35 are obtained by simulation and listed in Ye et al. (2001) [12]. The description of the simulation can be found in Ye et al. (2000) [13].

Table 1. Factors' level combinations and the response variable for the illustrative example

Run	A	B	C	D	E	y	Run	A	B	C	D	E	y
1	–	–	–	–	–	8.11	2	+	–	–	–	–	7.93
3	–	+	–	–	–	5.56	4	+	+	–	–	–	5
5	–	–	+	–	–	5.77	6	+	–	+	–	–	7.47
7	–	+	+	–	–	5.82	8	+	+	+	–	–	12.00
9	–	–	–	+	–	9.17	10	+	–	–	+	–	9.86
11	–	+	–	+	–	7.80	12	+	+	–	+	–	3.65
13	–	–	+	+	–	3.23	14	+	–	+	+	–	6.40
15	–	+	+	+	–	5.69	16	+	+	+	+	–	11.61
17	–	–	–	–	+	8.82	18	+	–	–	–	+	12.43
19	–	+	–	–	+	14.23	20	+	+	–	–	+	17.55
21	–	–	+	–	+	9.20	22	+	–	+	–	+	8.87
23	–	+	+	–	+	8.94	24	+	+	+	–	+	25.58
25	–	–	–	+	+	11.49	26	+	–	–	+	+	13.06
27	–	+	–	+	+	11.49	28	+	+	–	+	+	18.83
29	–	–	+	+	+	6.25	30	+	–	+	+	+	11.78
31	–	+	+	+	+	9.12	32	+	+	+	+	+	26.05

4. AN ILLUSTRATIVE EXAMPLE

The illustrative example is directly taken from Angelopoulos et al. (2010) [9]. For this example, SAS Base programming [18] has been used to find GME estimators. In this example, we will use a simulated example where five factors are investigated in order to identify if they have an effect on a response variable. The active effects are set to be A, B, E, AB, AC, AE, BC, BE, ABC and ABE. The true model under investigation will be $y = 10+2A+1.8B+3E+1.2AB+1.2AC+1.5AE+BC+1.8BE+1.1ABC+1.1ABE$. The scenario is as follows: no prior knowledge exists for the researcher, so all main effects and all interactions might influence the response. The number of experimental runs is limited to 32. So an unreplicated 2^5 full factorial design is employed. The experiment settings along with the response for each experimental run are presented in Table 1.

GME approach can directly estimate the full model without having to rely upon the probability plot for insight into which effects can be significant. The resulting GME estimates, t-values and p-values are shown in Table 2. Note that the parameter estimates associated with the A, B, E, AB, AC, AE, BC, BE, ABC, ABE effects are all statistically-significant.

Table 2. GME results for full design of the illustrative example

Factorial effect	Estimate	Approx. Std. Error	t-value	Approx. Pr > $\|t\|$	Factorial effect	Estimate	Approx. Std. Error	t-value	Approx. Pr > $\|t\|$
A	1.272714	0.2299	5.5	**<0.0001**	ABD	-0.00669	0.0123	-0.54	0.5896
B	0.702976	0.1621	4.34	**0.0001**	ABE	0.188356	0.0810	2.33	**0.0265**
C	0.000047	0.000480	0.10	0.9224	ACD	0.00166	0.00501	0.33	0.7426
D	-2.59E-6	0.000069	-0.04	0.9703	ACE	-0.00001	0.000204	-0.06	0.9488
E	2.170737	0.3159	6.87	**<0.0001**	ADE	0.019964	0.0239	0.83	0.4104
AB	0.257316	0.0949	2.71	**0.0107**	BCD	0.005263	0.0105	0.50	0.6206
AC	0.429341	0.1238	3.47	**0.0015**	BCE	-0.01342	0.0189	-0.71	0.4823
AD	0.009015	0.0148	0.61	0.5463	BDE	-0.00013	0.000934	-0.14	0.8906
AE	0.510293	0.1358	3.76	**0.0007**	CDE	0.009474	0.0152	0.62	0.5383
BC	0.395087	0.1185	3.33	**0.0022**	ABCD	-0.00251	0.00657	-0.38	0.7048
BD	-2.28E-7	0.000014	-0.02	0.9867	ABCE	0.023765	0.0265	0.90	0.3772
BE	0.748951	0.1681	4.46	**<0.0001**	ABDE	0.000654	0.00273	0.24	0.8120
CD	-0.00294	0.00728	-0.40	0.6888	ACDE	-0.00019	0.00122	-0.16	0.8760
CE	-1.04E-7	8.191E-6	-0.01	0.9899	BCDE	-0.00019	0.00120	-0.16	0.8777
DE	-1.47E-8	2.248E-6	-0.01	0.9948	ABCDE	-0.01612	0.0211	-0.76	0.4502
ABC	0.359115	0.1127	3.19	**0.0032**					

Table 3. OLS estimates for reduced model of the illustrative example

Variable	Estimate	Std. Err.	t-value	Pr > $\|t\|$
Intercept	10.18594	0.21988	46.33	<.0001
A	2.19344	0.21988	9.98	<.0001
B	1.62156	0.21988	7.37	<.0001
E	2.99406	0.21988	13.62	<.0001
AB	1.03281	0.21988	4.70	0.0001
AC	1.29031	0.21988	5.87	<.0001
AE	1.39531	0.21988	6.35	<.0001
BC	1.24344	0.21988	5.66	<.0001
BE	1.67219	0.21988	7.61	<.0001
ABC	1.19219	0.21988	5.42	<.0001
ABE	0.90719	0.21988	4.13	0.0005

It is worth noting that GME approach identified the active effects in the model. We also analyzed the same example with other methods. Projection property method gave us the same results. However, Lenth's method identified only 7 out of 10 true active effects, which are A, B, E, AC, AE, BC and BE. Dong's method identifies as active effects A, B, E, AC, AE, BE, meaning that it fails to identify four real active effects. Additionally, step-down Lenth method could identify as active effects A, B, E, BE, AE, AC, BC, ABC, AB but not ABE.

Right after determining active effects, we perform regression analysis in order to find how OLS and GME estimates of the parameters and their corresponding standard errors change. OLS and GME results for reduced model are given in Table 3 and 4 for both estimation methods.

As can be seen in these tables, GME estimation can produce markedly different standard errors. However, with OLS estimation, we obtain the same standard error for each parameters in the regression model.

Table 4. GME estimates for reduced model of the illustrative example

GME-NM Variable Estimates				
Variable	Estimate	Approx. Std. Error	t-value	Approx. Pr > $\|t\|$
Intercept	9.788972	0.4816	20.33	<.0001
A	1.229109	0.2156	5.70	<.0001
B	0.718196	0.1673	4.29	0.0002
E	2.05426	0.2816	7.30	<.0001
AB	0.307867	0.1185	2.60	0.0140
AC	0.469957	0.1398	3.36	0.0020
AE	0.544113	0.1485	3.66	0.0009
BC	0.438357	0.1360	3.22	0.0029
BE	0.759729	0.1715	4.43	0.0001
ABC	0.40482	0.1317	3.07	0.0043
ABE	0.239894	0.1078	2.22	0.0333

Note: GME-NM estimation refers to normed moment generalized maximum entropy estimation method.

5. A REAL-LIFE EXAMPLE

Montgomery (2012) proposed a problem for understanding the use and analysis of 2^k factorial designs as it was described in a paper published in *Solid State Technology* (Orthogonal Design for Process Optimization and Its Application in Plasma Etching, 1987, 127–132). This paper describes the application of factorial designs in developing a nitride etch process on a single-wafer plasma etcher. The process uses C_2F_6 as a reactant gas. Four factors are of interest: anode-cathode gap (A), pressure in reactor chamber (B), C_2F_6 gas flow (C) and power applied to the cathode (D). The response variable is the etch rate of silicon nitride. A single replicate of 2^4 factorial design is run and the data are shown in Table 5.

Table 5. Factor's level combinations and the response variable for the real-life data set

Run	A	B	C	D	y	Run	A	B	C	D	y
1	−	−	−	−	550	2	+	−	−	−	669
3	−	+	−	−	604	4	+	+	−	−	650
5	−	−	+	−	663	6	+	−	+	−	642
7	-	+	+	−	601	8	+	+	+	−	642
9	−	−	−	+	1037	10	+	−	−	+	749
11	−	+	−	+	1052	12	+	+	−	+	868
13	−	−	+	+	1075	14	+	−	+	+	860
15	−	+	+	+	1063	16	+	+	+	+	729

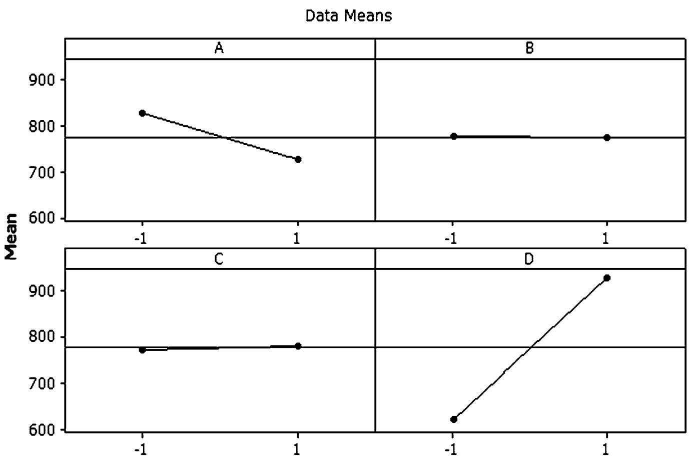

Figure 1. Main Effects Plot.

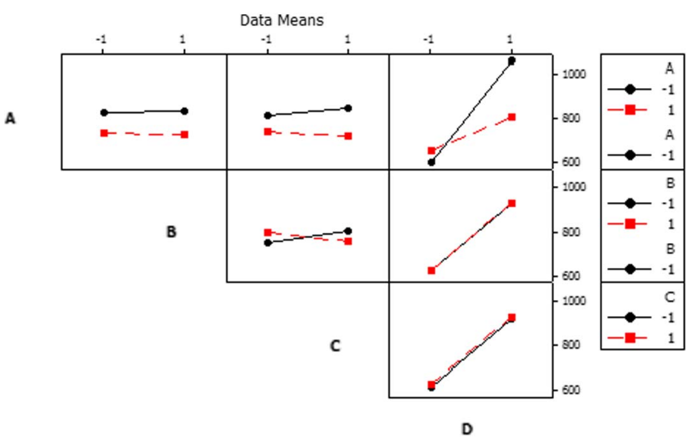

Figure 2. Interactions Plot.

Before analyzing this unreplicated factorial design, we can create factorial plots for main effects and interactions to draw some preliminary conclusions, i.e., important factors and interactions and best setting, given in Figure 1 and Figure 2, respectively.

From Figure 1 and Figure 2, we can subjectively conclude that main effects, anode-cathode gap (A) and the power (D), plus, interactions, anode-cathode gap/power (AD) and

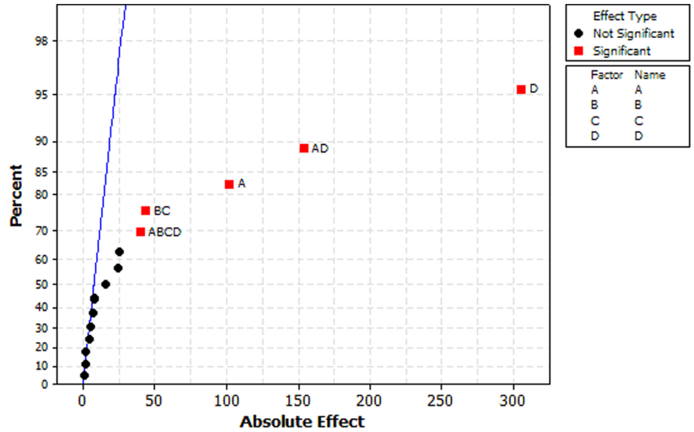

Figure 3. Half-normal plot of the effects.

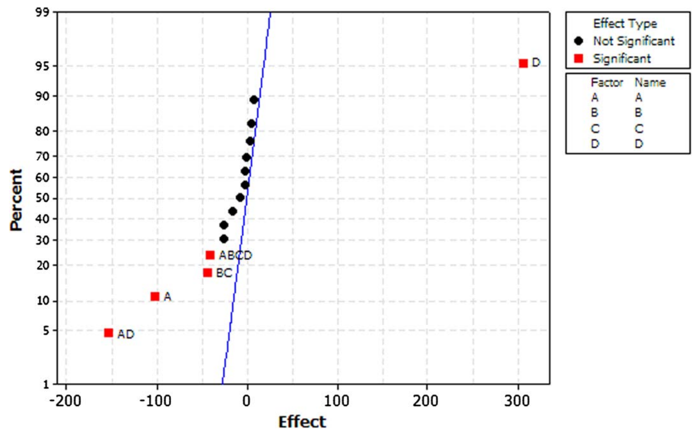

Figure 4. Normal plot of the effects.

pressure/gas flow (BC) might be important for the etch rate of silicon nitride.

Secondly, half-normal and normal plots of this unreplicated factorial design can be seen in Figure 3 and 4, respectively.

In addition to factorial plots, from the half-normal/normal plots above, we can see that the highest-order interaction $ABCD$ might be statistically-significant.

GME approach can directly estimate the full model without having to rely upon the probability plot for insight into which effects can be significant. The resulting GME estimates, t-values and p-values are shown in Table 6. Note that the parameter estimates associated with the A, D, AD, BC, $ABCD$ effects are all significant.

GME approach identifies the active effects in the model and seems to confirm the results of those obtained with factorial plots and half-normal/normal plots. Analyzing the same example with other methods, projection property method gives the active effects as A, D and AD. Lenth's method similarly identified the active effects, which those are A, D and AD. Dong's method gives the same results

Table 6. GME results for full design of real-life data set

Factorial effect	**Estimate**	**Approx. Std. Error**	**t-value**	**Approx. Pr > $\|t\|$**	**Factorial effect**	**Estimate**	**Approx. Std. Error**	**t-value**	**Approx. Pr > $\|t\|$**
A	-34.4979	5.0007	-6.90	**<0.0001**	BD	-0.00003	0.000914	-0.04	0.9724
B	-0.00056	0.00616	-0.09	0.9284	CD	-0.00126	0.0105	-0.12	0.9063
C	0.051531	0.1210	0.43	0.6758	ABC	-0.44982	0.4646	-0.97	0.3437
D	146.3858	8.4137	17.40	**<0.0001**	ABD	0.009177	0.0392	0.23	0.8178
AB	-0.06234	0.1370	-0.46	0.65528	ACD	0.023086	0.0719	0.32	0.7522
AC	-1.58821	0.9359	-1.70	0.1091	BCD	-1.6719	0.9621	-1.74	0.1015
AD	-64.2565	6.8994	-9.31	**<0.0001**	ABCD	-5.20849	1.7199	-3.03	**0.0080**
BC	-6.4127	1.9130	-3.35	**0.0040**					

Table 7. Parameter Estimates by GME Approach

GME-NM Variable Estimates				
Variable	**Estimate**	**Approx. Std. Error**	**t-value**	**Approx. Pr > $\|t\|$**
Intercept	774.1117	9.0065	85.95	< .0001
A	-34.538	5.0889	-6.79	< .0001
D	144.342	8.3330	17.32	< .0001
AD	-62.5826	6.6303	-9.44	< .0001
BC	-8.59879	2.8668	-3.00	0.0085
ABCD	-7.36329	2.7155	-2.71	0.0154

Note: GME-NM estimation refers to normed moment generalized maximum entropy estimation method.

with projection property method and Lenth's method. However, step-down Lenth method could identify as active effects A, D, AD and plus, BC.

The resulting GME estimates for reduced model are shown in Table 7. Note that the parameter estimates associated with the A, D, AD, BC and $ABCD$ effects are still all statistically-significant.

6. CONCLUSION

It is attempted to compare the results of generalized maximum entropy estimation with traditional estimation methods in order to investigate the advantages of the generalized maximum entropy approach for determining the active effects in unreplicated factorial design. For this reason, we use two data sets. For both data sets, those who uses OLS estimation method, id est, Lenth's method, Dong's method and step-down Lenth method failed to determine the active effects. However, projection property method can identify the variables with the greatest effect on response variable for the illustrative example, albeit, it can not for the real-life data set. Therefore, GME approach can find active effects truly and efficiently for both.

In the literature, it has been shown that the GME estimator is more precise than the OLS, because GME combines prior information with observed data. Moreover, using OLS method to analyze the unreplicated experimental data gives zero degrees of freedom for error term. The half-normal/normal plot method unlike other methods has disadvantages in terms of subjectivity. Whereas the OLS method gives constant standard error for each parameter estimates, the GME method gives distinct standard errors for each of the parameters for the reduced model.

The main advantages of using GME estimation method (Golan et al. (1996) [5], Eruygur (2005) [6]) can be summarized as: The GME approach uses all the data information and does not require any imposition on distributional error assumptions. The GME is robust and may be used when the sample is small. Therefore the GME works well in case of ill-posed data such as unreplicated factorial designs. Consequently, the GME estimator can be used as an alternative method and our results show that it is worthwhile to consider the idea of GME estimation method. Note that our conclusions are merely based on the data sets, a further study, in particular a simulation study can be conducted to make more general inferences.

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