
UM-SJTU Joint Institute

Probabilistic Methods in Engineering
(VE401)

Term Project Report

Photolithography Overlay for Patterning of Integrated Circuitry

Instructed by

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1 Abstract

Photolithography is one of the key technologies that are used to create integrated circuits. Whether the different layers are perfectly aligned is crucial to the lithography process. Therefore, the machine alignment should be modified and the overlay error from the nominal coordinate should be precisely predicted and adjusted accordingly. There are several models to conclude the relation between the coordinate of the die (X, Y) , the nominal position within each die (x, y) and the deviation of real coordinates with the nominal ones (o_x, o_y) . Based on the collected data, this study mainly looks into one given multivariate polynomial model by calculating its coefficients and further explores other regression models that might be better fitting the data, such as the cubic polynomial model, the bi-quadratic polynomial model and the quadratic mixed polynomial model. Measures, such as the R^2 values, the t statistic, the Significance F, and the *PRESS* measure are used for testing the goodness of the models.

Key Words: Photolithography, Overlay error, Multiple regression model; Determination of coefficients; Improving model

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2 Introduction

Photolithography is the method that can create extremely small patterns, down to a few tens of nanometers in size. Also, it's an efficient and relatively economical method to provide precise control of the shape and size of the objects it creates; sometimes it creates the patterns over an entire wafer in just one single step. Photolithography is often used in integrated circuit manufacturing. Its general working principle is to use light to produce minutely patterned thin films of suitable materials over a substrate, such as a silicon wafer; this can well protect its selected areas during the operations of subsequent etching, deposition, and implantation. Typically, ultraviolet light is used to transfer a geometric design from an optical mask to a light-sensitive chemical, which we call photoresist, coated on the substrate. The photoresist either breaks down or hardens where it is exposed to light; then, we can create the patterned film by removing the softer parts of the coating with appropriate solvents.[3]

The process of Photolithography seems clear, but multiple factors may influence its precision. One most common factor is whether wafers are perfectly aligned during the whole photolithographing process. There are many reasons for this alignment deviation: it can be introduced by mask deformation or abnormal proportion, deformation of the wafer itself, distortion of the projection lens system of the lithography machine, or by the uneven movement of the wafer workpiece stage.[4]

Due to the multi-layer imprinting of the dies, it is crucial that we take this alignment deviation into consideration, so that we can get our expected final products.[2] Often, we use the overlay errors to describe the displacement errors between a present exposure layer and a preceding exposure layer; the overlay errors must be controlled to within the tolerance incorporated in the manufacturing to ensure the yield of products.

It is now of interest to model the overlay errors so that by adjusting the process machinery, the errors may be corrected. In this report, we firstly construct a full multivariate quadratic model and use the multi-linear regression method to calculate its coefficients. Then, we improve the model by checking whether some terms can be reduced so as to reach a greater R^2 .

2.1 Program Objectives

- Fit the coefficients of the given quadratic polynomial model using the raw data.
- Analyze the result of regression using qualities such as R^2 , *PRESS*, Variance Inflation Factor(*VIF*), Significance F, and t statistic.
- Simplify the resulting regression functions; Discover whether some terms may be eliminated from the full model.
- Improve the fit by adding mixed terms or high-order terms.

3 Coefficients for the Given Model

Since Photolithography is a two-dimensional problem, there will be errors occurring on both the X and Y coordinates. Therefore, the following table summarizes the notations for the factors that we have considered in this project.

Notation	Definition
(X,Y)	Position of the die
(x,y)	Nominal position within each die
(o_x, o_y)	Deviation of real coordinates with the nominal ones

Table 1: Notations for the multivariate quadratic model

3.1 Verification of the distribution for the response variables

To make sure that the response variables o_x and o_y are useful variables for our data analysis, we make the assumption that they should follow the normal distribution. First we look at the data of o_x . According to the histogram (Figure 1) and the boxplot (Figure 2), we can see that generally o_x follows a normal distribution. Although there are few outliers according to the boxplot, the number of data, which is 250, is large enough to accept these outliers.

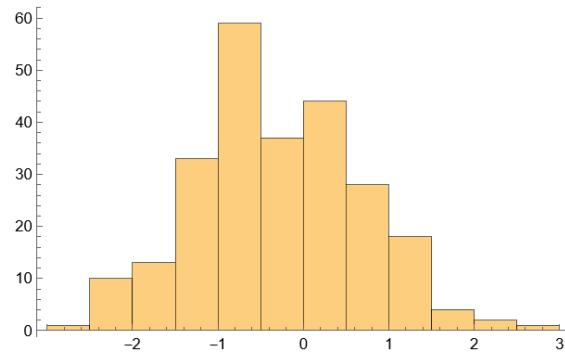


Figure 1: histogram of o_x

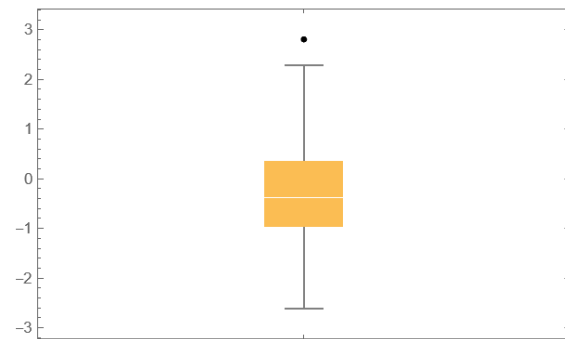


Figure 2: boxplot of o_x

Similarly, we can do this analysis to see whether o_y follows a normal distribution. From Figure 3 and Figure 4, This time, we can see there is no outlier according to the boxplot; also, the symmetric median line and equally long whiskers give more information that there is no evidence that o_y does not follow a normal distribution.

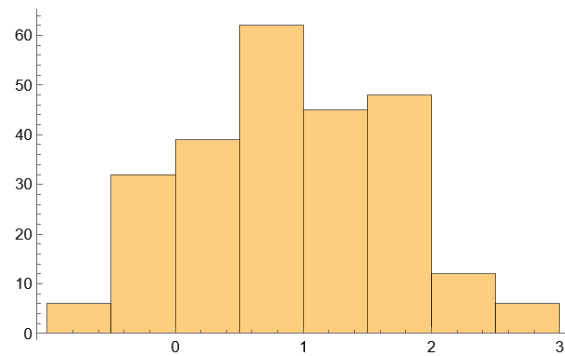


Figure 3: histogram of o_y

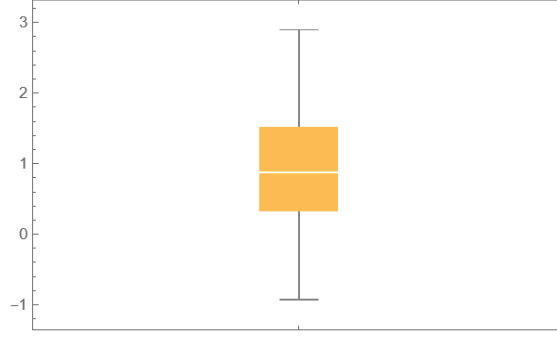


Figure 4: boxplot of o_y

3.2 Verification of using multilinear regression model

To fit the data to an appropriate model, we decide to use the multilinear model that is provided in the manual. To discuss these two models[2]

$$o_x(X, Y, x, y) = \alpha_0 + \alpha_1 X + \alpha_2 Y + \alpha_3 XY + \alpha_4 X^2 + \alpha_5 Y^2 + \alpha_6 x + \alpha_7 y + \alpha_8 xy + \alpha_9 x^2 + \alpha_{10} y^2 \quad (1)$$

$$o_y(X, Y, x, y) = \beta_0 + \beta_1 X + \beta_2 Y + \beta_3 XY + \beta_4 X^2 + \beta_5 Y^2 + \beta_6 x + \beta_7 y + \beta_8 xy + \beta_9 x^2 + \beta_{10} y^2 \quad (2)$$

we find an appropriate matrix formalism to define the variables.

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 1 & X & \cdots & x^2 & y^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & X_n & \cdots & x_n^2 & y_n^2 \end{pmatrix} \quad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{10} \end{pmatrix} \quad \mathbf{E} = \begin{pmatrix} E_1 \\ \vdots \\ E_n \end{pmatrix}$$

Then we can write these two models as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\alpha} + \mathbf{E} \quad (3)$$

Defining

$$\hat{\boldsymbol{\alpha}} = \mathbf{b} := \begin{pmatrix} b_0 \\ \vdots \\ b_{10} \end{pmatrix}$$

By minimizing the SS_E , we can get the formula to calculate the regression coefficients, which is given by

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \quad (4)$$

3.3 Calculation for coefficients of o_x

In this project, we use the regression method implemented in excel to get the results of all the terms' coefficients and analysis quantities, such as R^2 and p – *value*. The following Table summarized the coefficients and p – *value* of Equation (1).

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-0.2624229	0.120665768	-2.17479	0.030627	-0.50013	-0.02472	-0.500127	-0.024719
x	0.06659785	0.00644279	10.3368	6.09E-21	0.053906	0.07929	0.0539059	0.0792898
X	0.00065211	0.000552347	1.180623	0.238926	-0.00044	0.00174	-0.000436	0.0017402
y	-0.0345959	0.003736687	-9.25845	1.23E-17	-0.04196	-0.02723	-0.041957	-0.027235
Y	0.00127669	0.000563458	2.265814	0.024358	0.000167	0.002387	0.0001667	0.0023867
X^2	-4.621E-05	7.86828E-06	-5.87297	1.43E-08	-6.2E-05	-3.1E-05	-6.17E-05	-3.07E-05
Y^2	-1.311E-05	7.71105E-06	-1.7007	0.090301	-2.8E-05	2.08E-06	-2.83E-05	2.076E-06
XY	-5.614E-05	8.54462E-06	-6.56986	3.12E-10	-7.3E-05	-3.9E-05	-7.3E-05	-3.93E-05
x^2	0.0029393	0.001264872	2.323789	0.020976	0.000448	0.005431	0.0004476	0.005431
y^2	0.00105152	0.000358667	2.931728	0.003698	0.000345	0.001758	0.000345	0.0017581
xy	-0.0003529	0.000564235	-0.62544	0.532278	-0.00146	0.000759	-0.001464	0.0007586

Figure 5: coefficients of o_x

Therefore, after plugging these coefficients to Equation (1), we can get the full equation of our quadratic model (the confidence 95% intervals for each coefficients are also in Figure 5.) :

$$\begin{aligned}
 o_x(X, Y, x, y) = & -0.262 + 0.001X + 0.001Y - 5.614 \times 10^{-5}XY - 4.621 \times 10^{-5}X^2 \\
 & - 1.311 \times 10^{-5}Y^2 + 0.067x - 0.035y - 3.529 \times 10^{-4}xy + 0.003x^2 \\
 & + 0.001y^2
 \end{aligned}
 \tag{5}$$

3.4 Calculation for coefficients of o_y

Using the same methods as what we did in section 2.3, we get the coefficients and p – *value* for o_y .

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0.70648086	0.116706149	6.053502	5.45E-09	0.476577	0.936385	0.4765768	0.9363849
x	0.01631079	0.006231372	2.617529	0.009422	0.004035	0.028586	0.0040354	0.02858622
X	0.00264355	0.000534222	4.948417	1.41E-06	0.001591	0.003696	0.0015912	0.00369594
y	0.01313946	0.003614069	3.63564	0.00034	0.00602	0.020259	0.00602	0.02025895
Y	0.00358417	0.000544968	6.576836	3E-10	0.002511	0.004658	0.0025106	0.00465772
X^2	5.5177E-06	7.61008E-06	0.725048	0.469132	-9.5E-06	2.05E-05	-9.47E-06	2.0509E-05
Y^2	-9.488E-06	7.45802E-06	-1.27214	0.204561	-2.4E-05	5.2E-06	-2.42E-05	5.2042E-06
XY	3.0456E-06	8.26423E-06	0.368525	0.712808	-1.3E-05	1.93E-05	-1.32E-05	1.9326E-05
x^2	-0.0033504	0.001223366	-2.73865	0.006634	-0.00576	-0.00094	-0.00576	-0.00094042
y^2	0.00265074	0.000346898	7.641262	5.19E-13	0.001967	0.003334	0.0019674	0.00333411
xy	0.00078755	0.000545719	1.443146	0.150289	-0.00029	0.001863	-0.000287	0.00186259

Figure 6: coefficients of o_y

Equation (2) can now be written as the following (the confidence 95% intervals for each coefficients are also in Figure 6.):

$$o_y(X, Y, x, y) = 0.706 + 0.003X + 0.004Y + 3.046 \times 10^{-6}XY + 5.518 \times 10^{-6}X^2 - 9.489 \times 10^{-6}Y^2 + 0.016x - 0.013y + 0.001xy - 0.003x^2 + 0.003y^2 \quad (6)$$

3.5 Analysis for the given model

To analyze the given model, we would like to use five important coefficients R^2 , *PRESS*, *VIF*, Significance F, and t statistic to see the performance of the model.

- R^2 is the coefficient of determination, which expresses the proportion of the total variation in Y that is explained by the linear model. Generally speaking, we expect to have a R^2 value that is close to 1, because this shows our built model has considered much of the variance and there are less differences between the model and the real situation. However, a close-to-one R^2 won't necessarily prove that our model is helpful, since it can also lead to an overfitting situation. The calculation formula of R^2 is listed below,[1]

$$R^2 := \frac{SS_T - SS_E}{SS_T} \quad (7)$$

where SS_T is the total response rate of Y and SS_E is the Error Sum of Squares, which is the variation of Y after we have applied the model.

- Significance F is used to determine whether the regression can be accepted from a macroscopic perspective. The calculation formula of significance F is listed below,[1]

$$F_{p,n-p-1} = \frac{SS_R/p}{SS_E/(n-p-1)} = \frac{SS_R/p}{S^2} \quad (8)$$

where SS_E and SS_T is shown above and

$$SS_R = SS_T - SS_E \quad (9)$$

In this project, if the significance F is smaller than 0.05, then we can say that our regression test is valid and acceptable.

- The t statistic is another inflection of the validity of the coefficients. It can be combined with the R^2 to better prove if our coefficients are acceptable. Let $0 < \alpha \leq 1$ and $\gamma > 0$. We define $t_{\alpha/2, \gamma} \geq 0$ by[1]

$$\int_{t_{\alpha/2, \gamma}}^{\infty} f_{T_{\gamma}}(t) dt = \alpha/2; \quad (10)$$

where f_{T_γ} is the density of the T-distribution with n degrees of freedom. For t statistic with different degrees of freedom, there will be a table for all the boundary value. In this project, if the t statistic for each coefficient is greater than the boundary values, then we can say that this item should be eliminated.

- *PRESS* is the abbreviation of the ***prediction sum of squares***, which is a coefficient to see if the model has been overfitted or not. That is to say, if the R^2 value is too large, we need to calculate the *PRESS* value to prevent overfitting. Its calculation formula is given below.[1]

$$PRESS := \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (11)$$

- As we haven't done the data analysis of the original dependent variables, we don't know whether they are linearly related, which is so called Multicollinearity. Multicollinearity may make the whole model completely different from the actual situation. Therefore, to prevent this situation, we use the ***Variance inflation factor***(VIF) to determine if there is multicollinearity among these variables. The formula of VIF is given below.[5]

$$VIF := \frac{1}{1 - R_i^2} \quad (12)$$

where R_i is the negative correlation coefficient of the variable on the remaining variables for regression analysis.

The significance F for the above two multilinear regressions are the following:

$$F_{o_x,full} = 1.14683 \times 10^{-44} \quad (13)$$

$$F_{o_y,full} = 3.5136 \times 10^{-34} \quad (14)$$

We can see that the significance F is much smaller than 0.05, so our regression for the model is acceptable.

The R^2 for the above two multi-linear regressions are the following:

$$R_{o_x,full}^2 = 0.577611 \quad (15)$$

$$R_{o_y,full}^2 = 0.389161 \quad (16)$$

We can see that they are far from satisfaction. Therefore, there is no need to calculate the *PRESS* value. And the *VIF* value is given in the table below.

	X	Y	XY	X^2	Y^2	x	y	xy	x^2	y^2
VIF	2.35	2.31	2.01	2.07	2.34	1.64	1.74	2.36	2.31	2.29

Table 2: VIF of the o_x model

	X	Y	XY	X^2	Y^2	x	y	xy	x^2	y^2
VIF	1.48	1.39	1.64	1.63	1.63	1.60	1.55	1.62	1.59	1.31

Table 3: VIF of the o_y model

From the *VIF* value shown above, we can see that they are all much less than 10. Therefore, we can conclude that these variables are not linearly related; the model we choose is relatively reliable.

Also, after we throw away the items whose P-value is greater than 0.05, we found that the t statistic of the remaining items are all smaller than the boundary values that are gained from the t-value table.

4 Improvement for the Given Model

R^2 is definitely not the only quality to measure whether our model is helpful or not, but the above unsatisfied R^2 for our first models has indeed brought us to think whether we can improve them.

4.1 Simplification of models based on the $p - value$

Before finding ways to improve the model, the first step is to eliminate some unnecessary terms in the original equations. This can not only help us get a clearer and more simplified regression formula, but can also save much time in our later process of improving the model, which means we don't need to consider those terms that have already been discarded in previous steps. We can simplify models by considering the $p - value$ of each of those coefficients.

$P - value$ is the probability of obtaining the current measured value or a more extreme value.[1] For a $T - test$, which we have used in the above regressions, $p < 0.05$ means the significance level of this test is up to 95%. Therefore, we calculate the $p - value$ of each coefficient and decide to eliminate all those terms whose $p - value$ is greater than 0.05.

In the following sections, we will apply this model simplification method in the process of finding an improved model. We will first calculate the full model, which include all the terms, then using this method to get a simplified, or in other word, reduced version.

4.2 Eliminations of coefficients for o_x and o_y

We now go back to the Figure 5 and draw out all those terms whose $p - value$ is greater than 0.05. We can see that the $p - value$ of α_1 , α_5 and α_8 are greater than 0.05, thus enabling us to eliminate these three coefficients. After that, we get a new model:

$$o_x(X, Y, x, y) = -0.384 + 0.066x + 1 \times 10^{-4}X - 0.035y + 0.001Y - 4.1 \times 10^{-5}X^2 - 5.6 \times 10^{-5}XY + 0.003X^2 + 0.001y^2 \quad (17)$$

To test the whether the model is suitable to use, we again calculate the value of R^2 and we get

$$R_{ox, reduced}^2 = 0.571795 \quad (18)$$

which is a bit lower than the previous value shown in equation (15), but its value doesn't vary much, so that we can simplify our model in this way.

Similarly, according to the Figure 6, we may eliminate coefficients β_3 , β_4 , β_5 and β_8 . Then we get the new model:

$$o_y(X, Y, x, y) = 0.670 + 0.016x + 0.003X + 0.014y + 0.004Y - 0.003x^2 + 0.003y^2 \quad (19)$$

The new R^2 equals to

$$R_{oy, reduced}^2 = 0.375834 \quad (20)$$

and compared to what we got in equation (16), it is also an acceptable value. Hence we can simplify our model by eliminating some of their coefficients. Since

the R^2 value is not that high, it is unnecessary to consider the value of $PRESS$ as there is no evidence that the model overfits the data. At the same time, from the small R^2 value, we can know that this model is not good enough to fit the data. Therefore, we need to find a more powerful model.

4.3 Improved model: Cubic polynomial model

Considering cubic polynomial model, we can add elements like X^3 , X^2Y , XY^2 , Y^3 , x^3 , x^2y , xy^2 and y^3 . We calculate the coefficients for each term and summarize their values in the following figure.

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-0.380269	0.093287604	-4.07631	6.28E-05	-0.56406	-0.19647	-0.56406426	-0.1964742
x	0.0166285	0.019057021	0.872565	0.383799	-0.02092	0.054175	-0.02091761	0.05417459
X	-0.000308	0.001527506	-0.20154	0.84045	-0.00332	0.002702	-0.00331735	0.00270163
y	-0.040036	0.012637836	-3.16791	0.001741	-0.06493	-0.01514	-0.0649346	-0.0151365
Y	0.0030229	0.001556749	1.941829	0.053363	-4.4E-05	0.00609	-4.4163E-05	0.00609004
X^2	-4.12E-05	7.07409E-06	-5.82268	1.91E-08	-5.5E-05	-2.7E-05	-5.5128E-05	-2.725E-05
XY	-5.84E-05	8.2011E-06	-7.12574	1.28E-11	-7.5E-05	-4.2E-05	-7.4597E-05	-4.228E-05
x^2	0.0025958	0.001209144	2.146768	0.032845	0.000213	0.004978	0.000213499	0.004978
y^2	0.0012318	0.0003456	3.564115	0.000443	0.000551	0.001913	0.000550857	0.00191266
X^3	7.748E-09	1.03351E-07	0.074969	0.940304	-2E-07	2.11E-07	-1.9587E-07	2.1137E-07
X^2Y	2.176E-07	1.37212E-07	1.585547	0.114198	-5.3E-08	4.88E-07	-5.2779E-08	4.8789E-07
XY^2	2.565E-07	1.30115E-07	1.971035	0.049904	1.09E-10	5.13E-07	1.0895E-10	5.1281E-07
Y^3	-2.37E-07	1.03946E-07	-2.27939	0.023549	-4.4E-07	-3.2E-08	-4.4173E-07	-3.214E-08
x^3	0.0008605	0.000253825	3.390206	0.00082	0.00036	0.001361	0.000360433	0.0013606
x^2y	-6.68E-05	0.000100942	-0.66163	0.508865	-0.00027	0.000132	-0.00026566	0.00013209
xy^2	-6.89E-05	5.39898E-05	-1.27572	0.203325	-0.00018	3.75E-05	-0.00017525	3.7495E-05
y^3	3.133E-05	4.71734E-05	0.6641	0.507283	-6.2E-05	0.000124	-6.1613E-05	0.00012427

Figure 7: coefficients of cubic o_x model

However, according to Figure 7, we can observe that p-values of coefficient of x , X , X^3 , X^2Y , x^2y , xy^2 and y^3 are greater than 0.05, hence we need to eliminate these elements. After modification, we can get the cubic polynomial model for o_x

$$\begin{aligned}
o_{x,cubic}(X, Y, x, y) = & -0.380 + 0.003Y - 5.84 \times 10^{-5}XY - 4.12 \times 10^{-5}X^2 \\
& - 0.040y + 0.003x^2 + 0.001y^2 + 2.565 \times 10^{-7}XY^2 \\
& - 2.37 \times 10^{-7}Y^3 + 0.001x^3
\end{aligned} \quad (21)$$

After calculation, the $R^2_{o_{x,cubic}}$ of this model is 0.61277, which is greater than what we have calculated in equation (18) and is a satisfying result.

Similar process are conducted for o_y , and we get the regression results shown in Figure 8.

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0.6731746	0.071109752	9.466698	3.2E-18	0.533081	0.813269	0.5330805	0.8132686
x	0.0764202	0.016500907	4.63127	6.02E-06	0.043912	0.108929	0.0439116	0.1089288
X	0.0027608	0.001323672	2.085711	0.038084	0.000153	0.005369	0.000153	0.0053686
y	0.0308628	0.010955136	2.817198	0.005257	0.00928	0.052446	0.00928	0.0524456
Y	0.0052374	0.001349681	3.880453	0.000135	0.002578	0.007896	0.0025784	0.0078964
x^2	-0.002652	0.001047536	-2.53131	0.012017	-0.00472	-0.00059	-0.004715	-0.0005879
y^2	0.0026368	0.00029947	8.804914	2.91E-16	0.002047	0.003227	0.0020468	0.0032268
X^3	-5.71E-08	8.95666E-08	-0.63801	0.524091	-2.3E-07	1.19E-07	-2.34E-07	1.193E-07
X^2Y	5.614E-07	1.18922E-07	4.721043	4.03E-06	3.27E-07	7.96E-07	3.271E-07	7.957E-07
XY^2	1.283E-07	1.12725E-07	1.137762	0.256378	-9.4E-08	3.5E-07	-9.38E-08	3.503E-07
Y^3	-3.45E-07	9.0104E-08	-3.83098	0.000164	-5.2E-07	-1.7E-07	-5.23E-07	-1.677E-07
x^3	-0.001016	0.000219828	-4.61954	6.34E-06	-0.00145	-0.00058	-0.001449	-0.0005824
x^2y	8.639E-06	8.7348E-05	0.098903	0.9213	-0.00016	0.000181	-0.000163	0.0001807
xy^2	6.577E-05	4.67455E-05	1.407049	0.160734	-2.6E-05	0.000158	-2.63E-05	0.0001579
y^3	-7.52E-05	4.08981E-05	-1.83759	0.067386	-0.00016	5.42E-06	-0.000156	5.42E-06

Figure 8: coefficients of cubic o_y model

After deleting X^3, XY^2, x^2y, xy^2 and y^3 whose p-value of their coefficient are greater than 0.05, we get the following model:

$$\begin{aligned}
o_{y,cubic}(X, Y, x, y) = & 0.673 + 0.003X + 0.005Y + 0.076x - 0.031y - 0.003x^2 \\
& + 0.003y^2 + 5.614 * 10^{-7}X^2Y - 3.45 * 10^{-7}Y^3 - 0.001x^3
\end{aligned} \tag{22}$$

Again, we can calculate $R_{oy,cubic}^2$ to be 0.541273, which is already much higher than what we have calculated in equation (20).

4.4 Improved model: Bi-quadratic polynomial model

As we try to increase the degree of the elements to 4, which means we need to consider elements like $X^4, X^3Y, X^2Y^2, XY^3, Y^4, x^4, x^3y$ and so on, we find that almost all the $p - value$ of the coefficients of these elements are greater than 0.05 (shown in Figure 9).

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-0.113137	0.193451253	-0.58484	0.559222	-0.49427	0.267992	-0.494266	0.26799155
y	-0.033723	0.006652692	-5.06905	8.12E-07	-0.04683	-0.02062	-0.04683	-0.020616
Y	0.0046783	0.001460376	3.203477	0.001547	0.001801	0.007555	0.0018011	0.00755544
X^2	-4.1E-05	3.72891E-05	-1.09976	0.272568	-0.00011	3.25E-05	-0.000114	3.2456E-05
XY	-2.37E-05	2.07781E-05	-1.13857	0.256048	-6.5E-05	1.73E-05	-6.46E-05	1.7279E-05
x^2	-0.018705	0.010332253	-1.81031	0.071531	-0.03906	0.001652	-0.039061	0.00165157
y^2	0.0009538	0.000442357	2.156214	0.032087	8.23E-05	0.001825	8.231E-05	0.00182533
XY^2	5.433E-08	1.0676E-07	0.508867	0.611325	-1.6E-07	2.65E-07	-1.56E-07	2.6466E-07
Y^3	-3.17E-07	1.17814E-07	-2.69177	0.007621	-5.5E-07	-8.5E-08	-5.49E-07	-8.502E-08
x^2y	-6.98E-05	0.000123799	-0.56379	0.57344	-0.00031	0.000174	-0.000314	0.00017411
X^4	-1.64E-10	1.87878E-09	-0.08704	0.930711	-3.9E-09	3.54E-09	-3.87E-09	3.5379E-09
X^3Y	-4.27E-09	2.1933E-09	-1.94513	0.052958	-8.6E-09	5.49E-11	-8.59E-09	5.4895E-11
X^2Y^2	8.612E-10	2.42209E-09	0.35557	0.722483	-3.9E-09	5.63E-09	-3.91E-09	5.6331E-09
XY^3	-3.97E-10	6.36736E-10	-0.62289	0.533961	-1.7E-09	8.58E-10	-1.65E-09	8.5785E-10
Y^4	0	0	65535	#NUM!	0	0	0	0
x^4	0.000251	0.000111841	2.244278	#NUM!	3.07E-05	0.000471	3.066E-05	0.00047135
x^3y	-5.23E-06	9.28049E-06	-0.56373	0.573475	-2.4E-05	1.31E-05	-2.35E-05	1.3052E-05

Figure 9: coefficients of bi-quadratic o_x model

Also, this time the $R^2_{ox,bi-quadratic}$ for drops to 0.426302, which shows that the bi-quadratic polynomial model does not fit the real data of o_x well.

For o_y , its coefficients are summarized in Figure 10.

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0.1963565	0.169242904	1.160205	0.247148	-0.13708	0.529791	-0.137078	0.529791
x	0.0270416	0.02311993	1.169621	0.243343	-0.01851	0.072591	-0.018508	0.0725914
X	0.0026548	0.000453019	5.860216	1.56E-08	0.001762	0.003547	0.0017623	0.0035473
y	0.0142698	0.003136313	4.549876	8.62E-06	0.008091	0.020449	0.0080908	0.0204489
Y	0.0050237	0.001343533	3.739171	0.000232	0.002377	0.007671	0.0023767	0.0076707
x^2	0.0371185	0.01175339	3.158112	0.001797	0.013963	0.060275	0.0139625	0.0602745
y^2	0.0032355	0.000341973	9.461348	3.4E-18	0.002562	0.003909	0.0025618	0.0039093
X^2Y	5.861E-07	1.17561E-07	4.985659	1.2E-06	3.55E-07	8.18E-07	3.545E-07	8.177E-07
Y^3	-3.19E-07	9.08794E-08	-3.50873	0.00054	-5E-07	-1.4E-07	-4.98E-07	-1.4E-07
x^3	-7.01E-05	0.000355161	-0.19739	0.843696	-0.00077	0.00063	-0.00077	0.0006296
X^4	1.148E-10	3.79546E-10	0.302473	0.76256	-6.3E-10	8.63E-10	-6.33E-10	8.626E-10
X^3Y	7.37E-10	7.4162E-10	0.993779	0.321357	-7.2E-10	2.2E-09	-7.24E-10	2.198E-09
X^2Y^2	-1.24E-09	1.29793E-09	-0.9558	0.340161	-3.8E-09	1.32E-09	-3.8E-09	1.317E-09
XY^3	4.06E-11	3.92999E-10	0.103317	0.9178	-7.3E-10	8.15E-10	-7.34E-10	8.149E-10
Y^4	0	0	65535	#NUM!	0	0	0	0
x^4	-0.000445	0.00013027	-3.41787	#NUM!	-0.0007	-0.00019	-0.000702	-0.000189
x^3y	7.884E-06	6.34955E-06	1.241735	0.215577	-4.6E-06	2.04E-05	-4.63E-06	2.039E-05

Figure 10: coefficients of bi-quadratic o_y model

This time, $R^2_{oy,bi-quadratic}$ increases a little to 0.571302, compared to the previous one. However, since the $p - value$ for these new-added elements' coefficients are still too large, then we consider this model unhelpful.

In conclusion, the biquadratic polynomial model does not fit the real data better than cubic polynomial model.

4.5 Improved model: Quadratic mixed polynomial model

We can also consider mixed terms, such as xX, yY, xY , and yX . To see whether including these terms increase the R^2 of our model, we use multilinear regression method to calculate the coefficients of all the terms. They are listed in Figure 11.

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-0.2106217	0.130788251	-1.6104	0.108652	-0.46829	0.047046	-0.468289	0.0470456
x	0.066969	0.006443834	10.39273	4.62E-21	0.054274	0.079664	0.0542739	0.0796641
X	0.00071072	0.000553822	1.283301	0.200651	-0.00038	0.001802	-0.00038	0.0018018
y	-0.0341741	0.003725383	-9.17332	2.41E-17	-0.04151	-0.02683	-0.041514	-0.026835
Y	0.00128213	0.000562012	2.281319	0.023425	0.000175	0.002389	0.0001749	0.0023894
X^2	-5.111E-05	8.68454E-06	-5.88542	1.36E-08	-6.8E-05	-3.4E-05	-6.82E-05	-3.4E-05
Y^2	-1.718E-05	9.00924E-06	-1.90704	0.057735	-3.5E-05	5.68E-07	-3.49E-05	5.683E-07
XY	-6.367E-05	9.31955E-06	-6.83173	7.13E-11	-8.2E-05	-4.5E-05	-8.2E-05	-4.53E-05
x^2	0.00272647	0.001314685	2.073861	0.039182	0.000136	0.005317	0.0001364	0.0053165
y^2	0.00093979	0.000385324	2.438954	0.015471	0.000181	0.001699	0.0001807	0.0016989
xy	-0.0007154	0.000605318	-1.18192	0.238431	-0.00191	0.000477	-0.001908	0.0004771
xX	-9.964E-05	9.62181E-05	-1.03559	0.301459	-0.00029	8.99E-05	-0.000289	8.992E-05
xY	-4.623E-05	9.22642E-05	-0.50102	0.616826	-0.00023	0.000136	-0.000228	0.0001355
yX	-0.0001136	5.15675E-05	-2.20389	0.028503	-0.00022	-1.2E-05	-0.000215	-1.21E-05
yY	-4.356E-05	6.06473E-05	-0.71827	0.473303	-0.00016	7.59E-05	-0.000163	7.592E-05

Figure 11: coefficients of o_x model with mixed terms

After extracting terms with a greater-than-0.05 p - value, we get the following model.

$$\begin{aligned}
 o_{x,mixed}(X, Y, x, y) = & -0.391 - 0.037y + 0.064x - 4.158 \times 10^{-5}x^2 \\
 & + 0.003x^2 + 0.001y^2 - 6.182 \times 10^{-5}XY - 9.487 \times 10^{-5}yX
 \end{aligned}
 \tag{23}$$

The $R^2_{ox,mixed} = 0.567215$ is smaller than the R^2 for the reduced model, which is shown in Equation (18); it's also smaller than the R^2 for cubic model. We conclude that it's not as effective as representing our data as the cubic model does.

For o_y , we repeat the above steps and get the coefficients for all terms listed in Figure 12.

	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0.7819555	0.12654991	6.179029	2.82E-09	0.532638	1.031273	0.5326383	1.0312728
x	0.015826	0.006235014	2.538253	0.011788	0.003542	0.02811	0.0035424	0.0281097
X	0.0026515	0.000535875	4.948002	1.43E-06	0.001596	0.003707	0.0015958	0.0037072
y	0.0131301	0.003604658	3.642525	0.000332	0.006028	0.020232	0.0060285	0.0202316
Y	0.0035186	0.000543799	6.470334	5.63E-10	0.002447	0.00459	0.0024472	0.0045899
X^2	3.911E-06	8.4031E-06	0.465404	0.642073	-1.3E-05	2.05E-05	-1.26E-05	2.047E-05
Y^2	-1.85E-05	8.71729E-06	-2.12483	0.034645	-3.6E-05	-1.3E-06	-3.57E-05	-1.35E-06
XY	7.436E-06	9.01754E-06	0.824659	0.410402	-1E-05	2.52E-05	-1.03E-05	2.52E-05
x^2	-0.003504	0.001272081	-2.75421	0.006344	-0.00601	-0.001	-0.00601	-0.000997
y^2	0.0023669	0.000372837	6.348234	1.11E-09	0.001632	0.003101	0.0016323	0.0031014
xy	0.0009753	0.000585702	1.665223	0.097201	-0.00018	0.002129	-0.000179	0.0021292
xx	2.654E-05	9.31001E-05	0.285102	0.775817	-0.00016	0.00021	-0.000157	0.00021
xy	7.504E-05	8.92743E-05	0.840548	0.401455	-0.0001	0.000251	-0.000101	0.0002509
yx	4.161E-05	4.98964E-05	0.833891	0.405189	-5.7E-05	0.00014	-5.67E-05	0.0001399
yy	-0.000124	5.8682E-05	-2.1162	0.035379	-0.00024	-8.6E-06	-0.00024	-8.57E-06

Figure 12: coefficients of o_y model with mixed terms

The formula for our model is:

$$o_{y,mixed}(X, Y, x, y) = 0.802 + 0.002X + 0.013y + 0.004Y - 2 \times 10^{-5}Y^2 - 0.003x^2 + 0.002y^2 - 1 \times 10^{-4}yY \quad (24)$$

In this case, $R_{oy,mixed}^2 = 0.378573$, which is greater than the R^2 of reduced model (Equation (20)), but is still smaller than that of the cubic model.

5 Model Two Variables Simultaneously

As a practical problem, we shouldn't just focus on o_x and o_y separately, but to consider the practical meaning behind it.

5.1 Methods Clarification

During the production in real life, we would like to focus on the the distance between the actual point to ideal point. Therefore, we introduce a new concept o_d

$$o_d = \sqrt{o_x^2 + o_y^2} \quad (25)$$

According to the given model of o_x and o_y whose highest degree term is the quadratic term, we can just assume that the model of o_d as follows

$$o_d(X, Y, x, y) = \gamma_0 + \gamma_1X + \gamma_2Y + \gamma_3XY + \gamma_4X^2 + \gamma_5Y^2 + \gamma_6x + \gamma_7y + \gamma_8xy + \gamma_9x^2 + \gamma_{10}y^2 \quad (26)$$

5.2 Analysis for o_d

Using the same methods as what we did in section 2.3, we get the coefficients and p -value for o_d . Then we eliminate all those terms whose p -value are smaller than 0.05, we now get the following reduced model.

	Coefficients	Stand deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95%	Upper 95%
Intercept	0.655173093	0.018428213	35.5527189	6.536E-99	0.6188759	0.6914703	0.6188759	0.6914703
y	0.001971682	0.000914179	2.15677941	0.03199207	0.0001711	0.0037723	0.0001711	0.0037723
X*X	0.299677484	0.005426928	55.2204618	1.278E-140	0.2889883	0.31036666	0.2889883	0.31036666
y*y	0.000269524	9.6508E-05	2.79276536	0.00563679	7.944E-05	0.00045961	7.944E-05	0.00045961

Figure 13: coefficients of o_d

The equation for o_d can now be written as the following (the confidence 95% intervals for each coefficients are also in Figure 6.):

$$o_d(X, Y, x, y) = 0.00197X^2 + 0.29968y + 0.00027y^2 \quad (27)$$

Also, we can find the significance F and R^2 as following:

$$R_{o_d, reduced}^2 = 0.936035 \quad (28)$$

$$F_{o_d, reduced} = 1.6423 \times 10^{-146} \quad (29)$$

Since the R^2 value may be too large and Significance F is much smaller than 0.05, we need to judge whether the model has been overfitted by calculating the *PRESS* value. According to [6], we can find the *PRESS* value:

$$PRESS = 6.9964 \quad (30)$$

According to the definition of *PRESS*, the average error of every data is about 0.167, which is sufficiently small. Therefore, the model is relatively acceptable.

6 Conclusion

In this project, we dive a little bit deeper into the topic of Photolithography, and try to model the overlay errors using the actual experimental data. In the first step, we aim to fit the coefficients of the given multivariate quadratic equations. Since their constructions are quite similar to the multilinear regression model we have learnt in class, we decide to try using this approach; we calculate the Variance Inflation Factor (*VIF*) for each term and find that they are actually not linearly related. Therefore, we prove that the multilinear regression model will be an appropriate approach. This means that we will treat each term as independent new variables containing the original variables X, Y, x and y .

By using multilinear regression tools built in excel, we get the coefficients for both the o_x and o_y equations.

$$\begin{aligned} o_{x,full}(X, Y, x, y) = & -0.262 + 0.001X + 0.001Y - 5.614 \times 10^{-5}XY \\ & - 4.621 \times 10^{-5}X^2 - 1.311 \times 10^{-5}Y^2 + 0.067x - 0.035y \quad (31) \\ & - 3.529 \times 10^{-4}xy + 0.003x^2 + 0.001y^2 \end{aligned}$$

$$\begin{aligned} o_{y,full}(X, Y, x, y) = & 0.706 + 0.003X + 0.004Y + 3.046 \times 10^{-6}XY + 5.518 \times 10^{-6}X^2 \\ & - 9.489 \times 10^{-6}Y^2 + 0.016x - 0.013y + 0.001xy - 0.003x^2 \\ & + 0.003y^2 \end{aligned} \quad (32)$$

In the second step, we check which terms can be eliminated by calculating their p -value. If the p -value for the coefficient is greater than 0.05, we say that it's not significant and can be eliminated. We also calculate the R^2 for both the full and the reduced model of o_x and o_y and find that they don't vary much; therefore, our elimination of these terms is appropriate. The reduced equation for o_x and o_y is listed below.

$$\begin{aligned} o_{x,reduced}(X, Y, x, y) = & -0.384 + 0.066x + 1 \times 10^{-4}X - 0.035y + 0.001Y \\ & - 4.1 \times 10^{-5}X^2 - 5.6 \times 10^{-5}XY + 0.003X^2 + 0.001y^2 \end{aligned} \quad (33)$$

$$\begin{aligned} o_{y,reduced}(X, Y, x, y) = & 0.670 + 0.016x + 0.003X + 0.014y + 0.004Y - 0.003x^2 \\ & + 0.003y^2 \end{aligned} \quad (34)$$

Since the R^2 for both the full and reduced model are not high enough to reach our expectation (please refer to Equation (18) and Equation (20)), we try to improve the current model by adding cubic, bi-quadratic or mixed terms to the original ones. We can see from the above equations that only in the cubic model, the R^2 value is greater than the original-reduced value for o_x , while in both the models with bi-quadratic terms or mixed terms, their R^2 value seems to present that they are no better than the original one. For o_y , we can see an increase of R^2 in both the cubic and mixed-term models, but still the cubic model has a higher R^2 . Therefore, we conclude that the cubic model is the most helpful model. The o_x and o_y equations can be presented as below. From Figure 17 and Figure 21 in Appendices, we can also see that both their t statistic and Significance F is quite small, then we conclude it's an appropriate model.

$$\begin{aligned} o_{x,cubic}(X, Y, x, y) = & -0.380 + 0.003Y - 5.84 \times 10^{-5}XY - 4.12 \times 10^{-5}X^2 - 0.04y \\ & + 0.003x^2 + 0.001y^2 + 2.565 \times 10^{-7}XY^2 - 2.37 \times 10^{-7}Y^3 \\ & + 0.001x^3 \end{aligned} \quad (35)$$

$$\begin{aligned} o_{y,cubic}(X, Y, x, y) = & 0.673 + 0.003X + 0.005Y + 0.076x - 0.031y \\ & - 0.003x^2 + 0.003y^2 + 5.614 \times 10^{-7}X^2Y - 3.45 \times 10^{-7}Y^3 \\ & - 0.001x^3 \end{aligned} \quad (36)$$

In the third step, we consider o_x and o_y together, because from the practical meaning of Photolithography, we would like to know the overlay error of o_x and o_y as a whole. Therefore, we introduce the concept o_d , which represents the distance between the actual point to the ideal point of the die. Using similar approach, we get the reduced model for o_d .

$$o_d(X, Y, x, y) = 0.00197X^2 + 0.29968y + 0.00027y^2 \quad (37)$$

From Equation (28), its R^2 reaches 0.936035, while its *PRESS* value still remain low (Equation (30)), therefore, we say our regression for this model is acceptable; it's a helpful model without over-fitting.

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7 Appendices

This section summarizes all the regression results we got from the excel tool.

SUMMARY OUTPUT								
回归统计								
Multiple R	0.562675302							
R Square	0.316603495							
Adjusted R Square	0.288009499							
Standard Deviation	0.548112701							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	10	33.26446811	3.32644681	11.0723767	1.7469E-15			
残差	239	71.80218028	0.30042753					
总计	249	105.0666484						
	Coefficients	Standard Deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95%	Upper 95%
Intercept	0.96036064	0.102803024	9.3417548	6.92118E-18	0.75784491	1.16287637	0.75784491	1.16287637
x	0.005398628	0.005489033	0.98352991	0.326341294	-0.0054144	0.01621169	-0.0054144	0.01621169
X	0.000780456	0.000470581	1.65849618	0.098529138	-0.0001466	0.00170747	-0.0001466	0.00170747
y	0.012590543	0.003183527	3.95490353	0.00010093	0.00631919	0.0188619	0.00631919	0.0188619
Y	0.002054906	0.000480047	4.28063765	2.69919E-05	0.00110924	0.00300057	0.00110924	0.00300057
X*X	2.73486E-05	6.7035E-06	4.07975578	6.14649E-05	1.4143E-05	4.0554E-05	1.4143E-05	4.0554E-05
Y*Y	6.6154E-06	6.56955E-06	1.00697883	0.314963346	-6.326E-06	1.9557E-05	-6.326E-06	1.9557E-05
X*Y	2.76496E-05	7.27972E-06	3.79817179	0.000184927	1.3309E-05	4.199E-05	1.3309E-05	4.199E-05
x*x	-2.1475E-05	0.001077627	-0.019928	0.984117435	-0.0021443	0.00210138	-0.0021443	0.00210138
y*y	0.001997748	0.000305572	6.53772762	3.74573E-10	0.00139579	0.00259971	0.00139579	0.00259971
x*y	-0.00125973	0.000480708	-2.6205618	0.009341118	-0.0022067	-0.0003128	-0.0022067	-0.0003128

Figure 14: results for full model of o_d

SUMMARY OUTPUT								
回归统计								
Multiple R	0.967488996							
R Square	0.936034956							
Adjusted R Square	0.935254895							
标准误差	0.165286063							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	3	98.34605566	32.7820186	1199.95019	1.64E-146			
残差	246	6.72059274	0.02731948					
总计	249	105.0666484						
	Coefficients	Stand deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95%	Upper 95%
Intercept	0.655173093	0.018428213	35.5527189	6.536E-99	0.6188759	0.6914703	0.6188759	0.6914703
y	0.001971682	0.000914179	2.15677941	0.03199207	0.0001711	0.0037723	0.0001711	0.0037723
X*X	0.299677484	0.005426928	55.2204618	1.278E-140	0.2889883	0.31036666	0.2889883	0.31036666
y*y	0.000269524	9.6508E-05	2.79276536	0.00563679	7.944E-05	0.00045961	7.944E-05	0.00045961

Figure 15: results for o_d after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.756171							
R Square	0.571795							
Adjusted R Square	0.557581							
标准误差	0.645072							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	8	133.9129	16.73911	40.22686	2.4E-40			
残差	241	100.2844	0.416118					
总计	249	234.1972						
	Coefficients	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%	上限 95.0%
Intercept	-0.38431	0.097486	-3.94225	0.000106	-0.57635	-0.19228	-0.57635	-0.19228
x	0.066385	0.006459	10.27852	8.73E-21	0.053663	0.079108	0.053663	0.079108
X	0.000646	0.000554	1.16566	0.244904	-0.00045	0.001736	-0.00045	0.001736
y	-0.03451	0.003736	-9.23791	1.36E-17	-0.04187	-0.02715	-0.04187	-0.02715
Y	0.001237	0.000564	2.193933	0.029196	0.000126	0.002348	0.000126	0.002348
X*X	-4.1E-05	7.38E-06	-5.58908	6.16E-08	-5.6E-05	-2.7E-05	-5.6E-05	-2.7E-05
X*Y	-5.6E-05	8.55E-06	-6.60943	2.46E-10	-7.3E-05	-4E-05	-7.3E-05	-4E-05
x*x	0.00325	0.001254	2.591594	0.010136	0.00078	0.00572	0.00078	0.00572
y*y	0.001083	0.000359	3.018996	0.002809	0.000376	0.00179	0.000376	0.00179

Figure 16: results for quadratic o_x model after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.782796131							
R Square	0.612769782							
Adjusted R Square	0.598248649							
标准误差	0.614709416							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	9	143.508978	15.94544205	42.1984824	1.14683E-44			
残差	240	90.6882399	0.377867666					
总计	249	234.197218						
	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95%	Upper 95%
Intercept	-0.382677719	0.09292863	-4.11797425	5.2614E-05	-0.565737614	-0.1996178	-0.565738	-0.199618
y	-0.036564024	0.00358967	-10.1859029	1.751E-20	-0.043635305	-0.0294927	-0.043635	-0.029493
Y	0.004676112	0.00117176	3.990683876	8.7564E-05	0.00236787	0.00698435	0.0023679	0.0069844
X*X	-4.07415E-05	7.0404E-06	-5.78679421	2.2301E-08	-5.46104E-05	-2.687E-05	-5.46E-05	-2.69E-05
X*Y	-5.74678E-05	8.149E-06	-7.05213872	1.8683E-11	-7.35205E-05	-4.142E-05	-7.35E-05	-4.14E-05
x*x	0.002595083	0.00120037	2.161895182	0.03161513	0.000230469	0.0049597	0.0002305	0.0049597
y*y	0.001216868	0.00034188	3.55937807	0.00044801	0.000543406	0.00189033	0.0005434	0.0018903
X*Y*Y	2.28752E-07	8.769E-08	2.608646364	0.00966071	5.60118E-08	4.0149E-07	5.601E-08	4.015E-07
Y*Y*Y	-3.10407E-07	9.3457E-08	-3.32137433	0.00103541	-4.94508E-07	-1.263E-07	-4.95E-07	-1.26E-07
x*x*y	0.000969028	8.4714E-05	11.43885598	1.8042E-24	0.000802151	0.00113591	0.0008022	0.0011359

Figure 17: results for cubic o_x model after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.652918							
R Square	0.426302							
Adjusted R Square	0.385253							
标准误差	0.757748							
观测值	250							
方差分析								
	df	SS	MS	F	gnificance F			
回归分析	16	99.83875	6.239922	11.59201	6.26E-22			
残差	234	134.3585	0.574181					
总计	250	234.1972						
	Coefficient	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%	上限 95.0%
Intercept	-0.11314	0.193451	-0.58484	0.559222	-0.49427	0.267992	-0.49427	0.267992
y	-0.03372	0.006653	-5.06905	8.12E-07	-0.04683	-0.02062	-0.04683	-0.02062
Y	0.004678	0.00146	3.203477	0.001547	0.001801	0.007555	0.001801	0.007555
X*X	-4.1E-05	3.73E-05	-1.09976	0.272568	-0.00011	3.25E-05	-0.00011	3.25E-05
X*Y	-2.4E-05	2.08E-05	-1.13857	0.256048	-6.5E-05	1.73E-05	-6.5E-05	1.73E-05
x*x	-0.0187	0.010332	-1.81031	0.071531	-0.03906	0.001652	-0.03906	0.001652
y*y	0.000954	0.000442	2.156214	0.032087	8.23E-05	0.001825	8.23E-05	0.001825
X*Y*Y	5.43E-08	1.07E-07	0.508867	0.611325	-1.6E-07	2.65E-07	-1.6E-07	2.65E-07
Y*Y*Y	-3.2E-07	1.18E-07	-2.69177	0.007621	-5.5E-07	-8.5E-08	-5.5E-07	-8.5E-08
x*x*y	-7E-05	0.000124	-0.56379	0.57344	-0.00031	0.000174	-0.00031	0.000174
X*X*X*X	-1.6E-10	1.88E-09	-0.08704	0.930711	-3.9E-09	3.54E-09	-3.9E-09	3.54E-09
X*X*X*Y	-4.3E-09	2.19E-09	-1.94513	0.052958	-8.6E-09	5.49E-11	-8.6E-09	5.49E-11
X*X*Y*Y	8.61E-10	2.42E-09	0.35557	0.722483	-3.9E-09	5.63E-09	-3.9E-09	5.63E-09
X*Y*Y*Y	-4E-10	6.37E-10	-0.62289	0.533961	-1.7E-09	8.58E-10	-1.7E-09	8.58E-10
Y*Y*Y*Y	0	0	65535	#NUM!	0	0	0	0
x*x*x*x	0.000251	0.000112	2.244278	#NUM!	3.07E-05	0.000471	3.07E-05	0.000471
x*x*x*y	-5.2E-06	9.28E-06	-0.56373	0.573475	-2.4E-05	1.31E-05	-2.4E-05	1.31E-05

Figure 18: results for bi-quadratic σ_x model after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.74893757							
R Square	0.560907484							
Adjusted R Square	0.550065694							
标准误差	0.65052763							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	6	131.3629726	21.89382876	51.73568733	8.96735E-41			
残差	243	102.8342458	0.423186197					
总计	249	234.1972184						
	Coefficients	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%	上限 95.0%
Intercept	-0.384689902	0.098303927	-3.913270951	0.000118265	-0.57832646	-0.19105334	-0.57832646	-0.19105334
y	-0.03706987	0.003578084	-10.36025742	4.55051E-21	-0.044117888	-0.03002185	-0.04411789	-0.03002185
x	0.064533146	0.00632487	10.20307909	1.41789E-20	0.05207458	0.076991713	0.05207458	0.076991713
X*X	-4.13883E-05	7.44584E-06	-5.558577318	7.14008E-08	-5.60549E-05	-2.6722E-05	-5.6055E-05	-2.6722E-05
x*x	0.003271268	0.001264289	2.587436073	0.010251186	0.000780903	0.005761633	0.000780903	0.005761633
y*y	0.001111962	0.0003617	3.074267434	0.002351151	0.000399495	0.00182443	0.000399495	0.00182443
X*Y	-5.59467E-05	8.61673E-06	-6.492801854	4.70616E-10	-7.29197E-05	-3.8974E-05	-7.292E-05	-3.8974E-05

Figure 19: results for reduced quadratic σ_x model with mixed terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.613053037							
R Square	0.375834026							
Adjusted R Square	0.36042252							
标准误差	0.623792553							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	6	56.93544	9.489239	24.38659	1.4774E-22			
残差	243	94.55547	0.389117					
总计	249	151.4909						
	Coefficients	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%	上限 95.0%
Intercept	0.670235722	0.082928	8.082125	3E-14	0.506885959	0.83358549	0.50688596	0.8335855
x	0.01643364	0.006241	2.633191	0.009001	0.004140357	0.02872692	0.00414036	0.0287269
X	0.00265161	0.000536	4.951574	1.38E-06	0.001596779	0.00370644	0.00159678	0.0037064
y	0.013708422	0.003612	3.795115	0.000186	0.006593354	0.02082349	0.00659335	0.0208235
Y	0.003520077	0.000545	6.458484	5.71E-10	0.002446488	0.00459367	0.00244649	0.0045937
x*x	-0.003154508	0.001211	-2.60431	0.009773	-0.005540425	-0.0007686	-0.0055404	-0.000769
y*y	0.00268	0.000347	7.726972	2.89E-13	0.001996809	0.00336319	0.00199681	0.0033632

Figure 20: results for quadratic o_y model after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.73571225							
R Square	0.54127252							
Adjusted R Square	0.52407024							
标准误差	0.53810253							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	9	81.99786262	9.11087362	31.46516	5.05716E-36			
残差	240	69.49304086	0.28955434					
总计	249	151.4909035						
	Coefficients	Standard deviation	t Stat	P-value	Lower 95%	Upper 95%	Lower 95%	Upper 95%
Intercept	0.67777393	0.071559745	9.47144139	2.749E-18	0.536808557	0.8187393	0.53680856	0.8187393
x	0.08371022	0.015859102	5.27837093	2.916E-07	0.052469415	0.11495103	0.05246941	0.11495103
X	0.00266039	0.000462481	5.75243527	2.667E-08	0.001749351	0.00357143	0.00174935	0.00357143
y	0.01399957	0.003186221	4.39378565	1.673E-05	0.007723043	0.0202761	0.00772304	0.0202761
Y	0.0052257	0.001359329	3.84431987	0.0001549	0.002547957	0.00790344	0.00254796	0.00790344
x*x	-0.0027383	0.001053712	-2.5987353	0.0099361	-0.004814023	-0.0006626	-0.004814	-0.0006626
y*y	0.00263486	0.000300031	8.78193304	3.098E-16	0.002043824	0.00322589	0.00204382	0.00322589
X*x*y	5.6472E-07	1.19649E-07	4.71982338	4.013E-06	3.29025E-07	8.0042E-07	3.2903E-07	8.0042E-07
Y*y*y	-3.442E-07	9.07012E-08	-3.7950594	0.0001869	-5.22889E-07	-1.655E-07	-5.229E-07	-1.655E-07
x*x*x	-0.0010059	0.000220371	-4.5647145	7.991E-06	-0.001440042	-0.0005718	-0.00144	-0.0005718

Figure 21: results for cubic o_y model after reducing unnecessary terms

SUMMARY OUTPUT							
回归统计							
Multiple R	0.755845						
R Square	0.571302						
Adjusted R Square	0.539547						
标准误差	0.526819						
观测值	250						
方差分析							
	df	SS	MS	F	Significance F		
回归分析	16	86.547	5.409187	20.78922	2.49E-36		
残差	234	64.9439	0.277538				
总计	250	151.4909					
	Coefficient	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%
Intercept	0.196356	0.169243	1.160205	0.247148	-0.13708	0.529791	-0.13708
x	0.027042	0.02312	1.169621	0.243343	-0.01851	0.072591	-0.01851
X	0.002655	0.000453	5.860216	1.56E-08	0.001762	0.003547	0.001762
y	0.01427	0.003136	4.549876	8.62E-06	0.008091	0.020449	0.008091
Y	0.005024	0.001344	3.739171	0.000232	0.002377	0.007671	0.002377
x*x	0.037119	0.011753	3.158112	0.001797	0.013963	0.060275	0.013963
y*y	0.003236	0.000342	9.461348	3.4E-18	0.002562	0.003909	0.002562
X*X*Y	5.86E-07	1.18E-07	4.985659	1.2E-06	3.55E-07	8.18E-07	3.55E-07
Y*Y*Y	-3.2E-07	9.09E-08	-3.50873	0.00054	-5E-07	-1.4E-07	-5E-07
x*x*x	-7E-05	0.000355	-0.19739	0.843696	-0.00077	0.00063	-0.00077
X*X*X*X	1.15E-10	3.8E-10	0.302473	0.76256	-6.3E-10	8.63E-10	-6.3E-10
X*X*X*Y	7.37E-10	7.42E-10	0.993779	0.321357	-7.2E-10	2.2E-09	-7.2E-10
X*X*Y*Y	-1.2E-09	1.3E-09	-0.9558	0.340161	-3.8E-09	1.32E-09	-3.8E-09
X*Y*Y*Y	4.06E-11	3.93E-10	0.103317	0.9178	-7.3E-10	8.15E-10	-7.3E-10
Y*Y*Y*Y	0	0	65535	#NUM!	0	0	0
x*x*x*x	-0.00045	0.00013	-3.41787	#NUM!	-0.0007	-0.00019	-0.0007
x*x*x*y	7.88E-06	6.35E-06	1.241735	0.215577	-4.6E-06	2.04E-05	-4.6E-06

Figure 22: results for bi-quadratic o_y model after reducing unnecessary terms

SUMMARY OUTPUT								
回归统计								
Multiple R	0.61528278							
R Square	0.3785729							
Adjusted R Square	0.36059774							
标准误差	0.6237071							
观测值	250							
方差分析								
	df	SS	MS	F	Significance F			
回归分析	7	57.35035	8.192907	21.0608874	4.58354E-22			
残差	242	94.14055	0.389011					
总计	249	151.4909						
	Coefficients	标准误差	t Stat	P-value	Lower 95%	Upper 95%	下限 95.0%	上限 95.0%
Intercept	0.80162692	0.100284	7.993567	5.3724E-14	0.604085957	0.9991679	0.604086	0.99916788
X	0.00233779	0.00052	4.495714	1.0758E-05	0.001313476	0.0033621	0.0013135	0.0033621
y	0.01345494	0.003614	3.7229	0.00024502	0.006335829	0.0205741	0.0063358	0.02057406
Y	0.00351104	0.000546	6.429407	6.7703E-10	0.002435342	0.0045867	0.0024353	0.00458674
Y*Y	-2.024E-05	8.03E-06	-2.52009	0.01237722	-3.60637E-05	-4.42E-06	-3.61E-05	-4.42E-06
x*x	-0.0032209	0.001216	-2.64887	0.00860766	-0.005616172	-0.000826	-0.005616	-0.0008257
y*y	0.0023679	0.000372	6.359511	1.0012E-09	0.001634459	0.0031013	0.0016345	0.00310134
y*Y	-0.0001364	5.8E-05	-2.35242	0.01945345	-0.000250672	-2.22E-05	-0.000251	-2.219E-05

Figure 23: results for reduced quadratic o_y model with mixed terms