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The Fractal Characterization of Mechanical Surface Profile Based on Power Spectral Density and Monte-Carlo Method

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Abstract. The analysis of rough surface morphology plays an important role in the functional characteristics of the contact surface of mechanical parts. Fractal geometry method is more accurate and sensitive than classical statistics model. For fractal representation of rough surface, it is necessary to determine the proper fractal dimension calculation method. In this research, the effect of power spectral density method is studied based on Monte-Carlo method. The fractal dimensions are calculated, the theoretical and the calculated values are compared with paired samples. And the results are compared by non-parametric test. The result shows that power spectral density method has good characterization effect on fractal simulation contour curve. In addition, the precision of fractal dimension of power spectral density is related to fractal dimension of contour theory. The estimation methods of classical power spectral density have different application range.

1 Introduction

Contact mechanics of rough surfaces is important in studying and modeling physical phenomena such as thermal and electrical conductivity, friction, adhesion, wear, etc. Obviously, the ability to characterize surface profile by adequate parameters is crucial in these cases. The research of rough surface characteristics is one of the crucial subjects in engineering. The traditional surface morphology has many parameters. It can be divided into three types, geometric parameters, shape parameters and random process parameters [1,2]. The contour arithmetic mean deviation is a geometric parameter. It is the arithmetic mean value of absolute value of contour deviation in the sampling length. The disadvantage is that it can only describe the roughness of the same kind of surface obtained by the same processing method. The skewness and kurtosis coefficient are the shape parameter, which can reflect the shape of the convex peak, as shown in table 1 [3]. The structure function and power spectral density is parameter of random process. However, geometric parameters and shape parameters change as the sample size and measurement scale change. In other words, geometric parameters and shape parameters are parameters of scale. The fractal dimension of surface profile can effectively overcome scale correlation of traditional roughness parameters.

Table 1. Skewness And Kurtosis.

Coefficient	Value	Shape
Skewness	A negative number	The contour convex peak is blunt peak.
	Zero	The convex peak is a composite shape with a peak on the blunt peak.
	A positive number	The profile has a convex peak.
Kurtosis	Less than 3	Temple kurtosis
	Is equal to 3	Normal distribution
	More than 3	Leptokurtic

However, it is found that only fractal dimension cannot determine the unique surface, and the surface of different topography may have similar or even same contour fractal dimension. By measuring rough contour curve of grinding and turning surface, GE Shirong analyses fractal characteristics of rough surface. The results show that rough surface has fractal characteristics and fractal dimension can be calculated. The characteristic roughness is combined with similar

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measurement and absolute measurement. The numerical value can not only represent the scaling law characteristics of surface multi-scale measurement, but also can hold the sensitivity and accuracy [4]. In the study, ZHU Hua calculates the fractal dimension and scale coefficient of wear surface profile by structural function method. He gives the characteristic roughness calculation expression and does the wear test on the test machine. The results show that fractal dimension of feature roughness is more regular [5].

In order to apply the characteristic roughness parameter to the tribological research, the first step is to choose the appropriate fractal dimension calculation method. There are many different methods for calculating fractal dimension, such as box counting, root-mean-square method, structural function method and power spectrum method. In the book, GE Shirong points out that the method of root-mean-square method and structural function method have the highest calculation accuracy. In the literature, there are many applications of structural function method and fewer researches on power spectrum method relatively. The Monte-Carlo method is also called a stochastic simulation method, which can also be called a random sampling technique or a statistical experimental method. The basic idea of Monte-Carlo method is to establish a probabilistic model or stochastic process, to calculate the statistical characteristics of the desired parameters in the model sampling test, and to give the approximate value of the solution. Monte-Carlo method can solve the problems of physics, mathematics, engineering and so on. The accuracy of the solution can be expressed by the standard error of the estimate. The Monte-Carlo method solves the problem of randomness. The subjects studied were influenced more by randomness. In general, the direct simulation method is used which is a sampling experiment with a digital machine.

In this paper, the simulated surface contour curve of different fractal dimension is based on W-M function, and the Monte-Carlo method. Meanwhile, statistical hypothesis tests are used to study the effect of power spectral density fractal characterization. The results can provide a theoretical reference for the accurate characterization of the characteristic roughness.

2 PSD Fractal Dimension Calculation Method

2.1 Power Spectral Density Method

The W-M function is introduced by Majumdar and Tien in 1989 to describe the height distribution function of surface topography[6,7]. The relational expression is given as

$$z(x) = G^{D-1}\sum_{n=n_1}^{\infty} \frac{\cos \pi\gamma^n x}{\gamma^{(2-D)n}}; 1<D<2, \gamma>1 \quad (1)$$

Where D denotes the similarity of functions $z(x)$ on different scales. G is the magnitude of the amplitude. V is the spectrum, generally $V = 1.5$. Therefore, D is one of the parameters of the decision. The power spectrum density method is derived to solve the fractal dimension of the isotropic rough surface.

The rough surface with fractal characteristics can be characterized by power spectrum density method. Autocorrelation function and power spectral density describes the statistical characteristics of stochastic process from two aspects, time domain and frequency domain. According to Wiener-Khinchin theorem, autocorrelation function and power spectral density function is a pair of Fourier transform. So the power spectral density of stationary random process is the Fourier transform of its autocorrelation function[8]. The relationship of autocorrelation function $R(\tau)$ and power spectral density function $S(\omega)$ is shown as

$$R(\tau) = \int_{-\infty}^{\infty} S(f) e^{j2\pi f\tau} df \quad (2)$$

$$S(f) = \int_{-\infty}^{\infty} R(\tau) e^{-j2\pi f\tau} d\tau \quad (3)$$

The two-dimensional autocorrelation function of isotropic rough surface is given by

$$R(\tau) = \lim_{L\to\infty} \tfrac{1}{L}\int_0^L z(x)z(x+\tau)dx \quad (4)$$

The Fourier transform of the autocorrelation function $R(\tau)$ is the discrete power spectral density. The approximate continuous power spectral density $\hat{S}(\omega)$ can be written simply as

$$\hat{S}(\omega) \propto \omega^{-(5-2D)} \quad (5)$$

Fitting the line $\lg S(\omega) - \lg \omega$, the slope of the linear region is α, then $D = (5+\alpha)/2$.

2.2 Classical Spectral Density Estimation

There are many techniques to estimate the power spectrum density. In addition to the autocorrelation method used here, there are also classical estimation methods such as periodogram method, Bartlett method, and Welch method.

The simulated rough surface profile height is a finite long random signal sequence. The direct method is to take the sampled data of the simulated rough surface profile to the Fourier transform to solve the power spectral density. The relationship between the Fourier transform and the power spectral density estimation $\hat{S}(\omega)$ is as follows

$$\hat{S}(x) = \frac{1}{N}\left|FFT[z(x)]\right|^2 \quad (6)$$

Where $FFT[z(x)]$ is Fourier transform of the sequence $z(x)$. This method is also known as the periodogram method. Because it is a fast Fourier transform to solve the power spectral density function with a finite long sample sequence, the result obtained is only an estimation way, and there will be a certain amount of error.

The Bartlett method is an improvement to the periodogram method. The sample data $z(x)$ of the rough surface profile height is divided into S segments that do not overlap each other (can be overlapped), and each segment has K sample value and $N = S \times K$. The power spectrum of each segment is calculated by the periodogram method. Then, the average of each segment is calculated. Finally, the average value is estimated as the power spectrum of the entire contour height sampling data $z(x)$. The computed result of the overlapping section is better than that of the non-overlapping section.

The Welch method develops Bartlett method. Firstly, the sample data of rough surface profile height is segmented. Then, the window function is used to preprocess each segment. Finally, the power spectral density function of the sampled data of the whole contour height is estimated by using the Bartlett method. Using the proper window function can improve the spectral resolution and reduce the error.

The periodogram method, also called the direct method. This estimation method is simpler than the calculation of autocorrelation method. Bartlett method and Welch method are the improvement of the autocorrelation method and the periodogram method, and the estimation results are more accurate. Welch method makes two modifications to the Bartlett method. First, select the appropriate window function to make the spectrum estimation non-negative. The second is that there is overlap between the segments, so that the variance decreases. The power spectrum density method is suitable for self - affine fractal curve.

3 Characterization of Power Spectral Density Method

3.1 The Fractal Representation of Simulated Contour Curve

Based on the principle and application characteristics of Monte-Carlo method, the Monte-Carlo method is used to randomly simulate 300 numbers as D [9]. The value of contour height $z(x)$ is calculated with the given parameter, and the W-M function is given to simulate the rough contour curves of multiple groups, as shown in the Fig1-4. Given the fractal roughness $G = 0.01$, $\gamma = 1.5$, $n_1 = 1$, the simulation length is $L = 25mm$, and the rough contour curves are simulated.

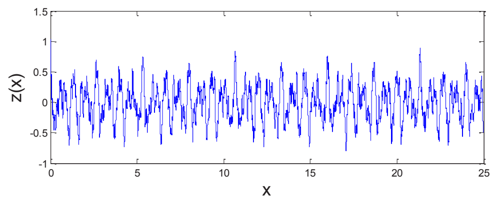


Fig. 1. The simulated contour curve($D = 1.2$).

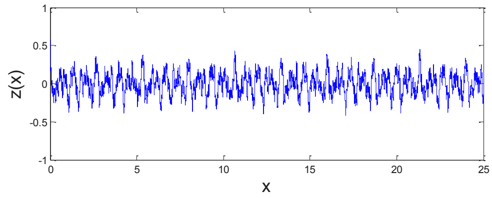


Fig. 2. The simulated contour curve($D = 1.4$).

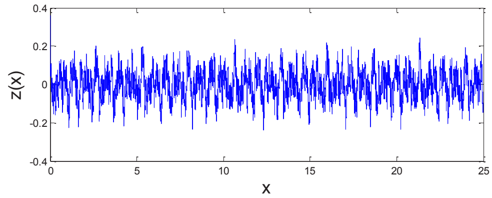


Fig. 3. The simulated contour curve($D = 1.6$).

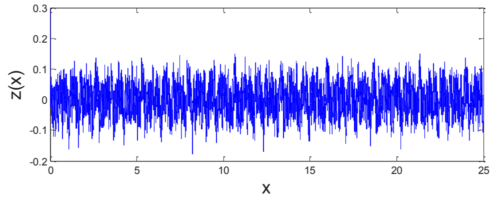
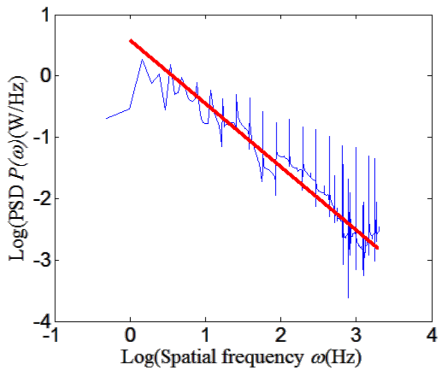


Fig. 4. The simulated contour curve($D = 1.8$).

3.2 Characterization Effect of Power Spectral Density Method

3.2.1 Power Spectral Density Method to Solve Fractal Dimension

The fractal dimension of simulation curves is calculated by power spectral density method. The sampling frequency is $fs = 1/0.00025$, the amounts of sampling points are $N = 2^{13}$. Sampling the above contour curves. The fractal dimension is calculated by using the power spectral density method, and the range of fractal features is determined. The theoretical and calculated values of fractal dimension are calculated and the outliers are filtered. The calculation results are obtained by MATLAB R2014a. We choose the classic power spectrum density estimation method of autocorrelation method, periodogram method, Bartlett method, and Welch method to estimate power spectral density. The estimation methods are shown in Fig. 5.



(a) Autocorrelation method

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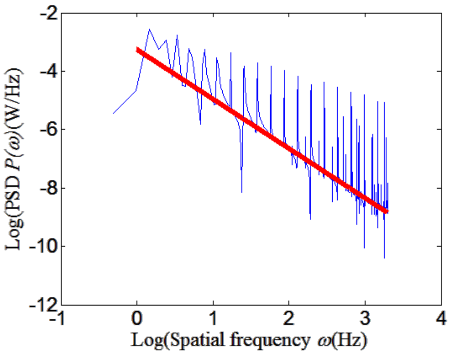
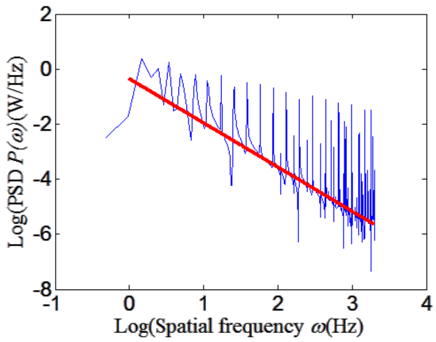
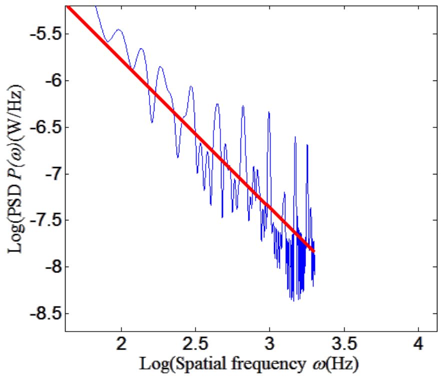


(b) Periodogram method



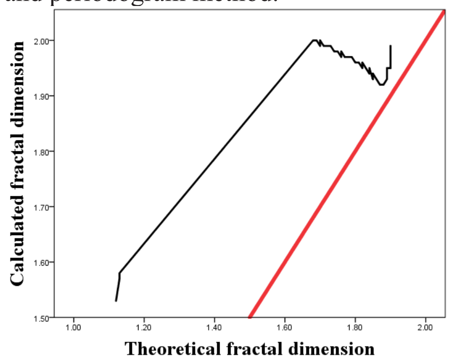
(c) Bartlett method



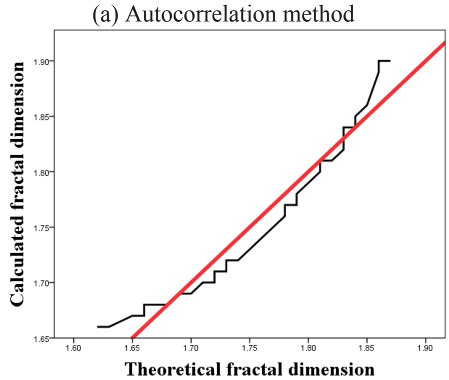
(d) Welch method

Fig. 5. The fractal dimension is calculated by PSD method.

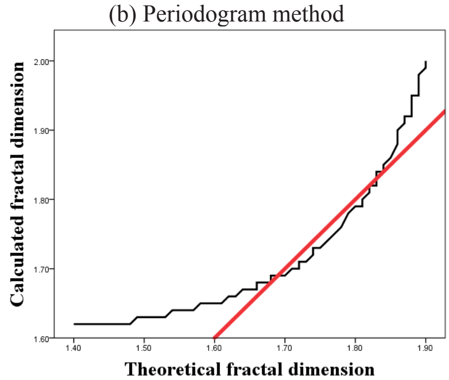
The calculated value of fractal dimension is the slope α of the straight line, $D=(5+\alpha)/2$. The simulation data is shown in fig. 6. The results illustrate that the estimation value of autocorrelation method is meticulous in the range of the theoretical fractal dimension between 1.6 and 1.9, and the calculated value is larger than theoretical value. The periodogram method is relatively accurate in the range of theoretical fractal dimension from 1.7 to 1.85, and the calculated value is smaller than theoretical value, and the calculated value of both ends is larger. The Bartlett method is correct in the theoretical fractal dimension and is estimated to be exact in the range of 1.7 to 1.9, and the calculated value of both ends is large. The Welch method is precise in the theoretical fractal dimension of 1.7 to 1.8, and the calculated value is small, and the calculated value of both ends is large. The estimation error of autocorrelation method is the largest in those methods. Although the calculation precision is high, the periodogram method has great fluctuation. The range that Bartlett method and Welch method can accurately estimate fractal dimension is larger than autocorrelation method and periodogram method.



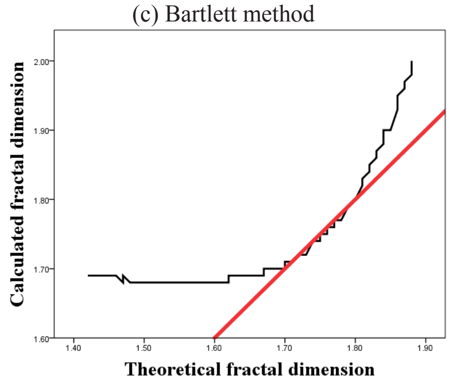
(a) Autocorrelation method



(b) Periodogram method



(c) Bartlett method



(d) Welch method

Fig. 6. Comparison between theoretical value and fractal dimension.

3.2.2 Statistical Testing of Characterization Results

A batch of theoretical values and calculated values are listed below. The outliers is cleaned. Because of the large amount of data, part of the data is shown here, as shown in table 2. D is theoretical value, $D^{'}$ is calculated value.

Table 2. Partial Data of Fractal Dimension.

	Autocorrelation method		Periodogram method		Bartlett method		Welch method	
	D	$D^{'}$	D	$D^{'}$	D	$D^{'}$	D	$D^{'}$
1	1.80	1.96	1.51	1.63	1.77	1.75	1.67	1.69
2	1.84	1.94	1.49	1.63	1.48	1.62	1.67	1.70
3	1.69	2.00	1.88	1.93	1.68	1.68	1.53	1.68
4	1.87	1.92	1.35	1.61	1.42	1.62	1.46	1.69
5	1.90	1.99	1.45	1.62	1.47	1.62	1.58	1.68
6	1.13	1.58	1.96	2.32	1.56	1.64	1.58	1.68
7	1.83	1.95	1.04	1.60	1.85	1.86	1.72	1.72
8	1.80	1.96	1.97	2.36	1.41	1.62	1.86	1.93
9	1.69	2.00	1.19	1.60	1.46	1.62	1.77	1.76
10	1.80	1.96	1.67	1.68	1.83	1.82	1.62	1.68
11	1.74	1.98	1.59	1.65	1.52	1.63	1.60	1.68
12	1.80	1.96	1.68	1.68	1.74	1.72	1.70	1.71
13	1.82	1.96	1.36	1.61	1.57	1.64	1.74	1.74
14	1.12	1.53	1.62	1.66	1.82	1.82	1.47	1.68
15	1.82	1.95	1.81	1.80	1.65	1.67	1.65	1.69
16	1.90	1.95	1.02	1.60	1.48	1.62	1.52	1.68
17	1.76	1.98	1.08	1.60	1.47	1.62	1.65	1.69
18	1.86	1.93	1.97	2.37	1.54	1.64	1.86	1.94
19	1.73	1.99	1.65	1.67	1.66	1.67	1.62	1.68
20	1.84	1.94	1.23	1.60	1.89	1.96	1.83	1.86
21	1.83	1.95	1.40	1.62	1.44	1.62	1.66	1.69
22	1.13	1.57	1.12	1.60	1.61	1.65	1.55	1.68
23	1.88	1.92	1.27	1.61	1.55	1.64	1.63	1.69
24	1.69	2.00	1.26	1.61	1.83	1.83	1.76	1.75
25	1.73	1.99	1.33	1.61	1.84	1.84	1.47	1.68
26	1.89	1.95	1.15	1.60	1.83	1.83	1.81	1.83
27	1.71	1.99	1.35	1.61	1.54	1.64	1.48	1.68
28	1.87	1.92	1.12	1.60	1.87	1.92	1.88	1.98
29	1.75	1.98	1.88	1.95	1.86	1.88	1.64	1.69
30	1.70	2.00	1.09	1.60	1.90	2.00	1.69	1.70
31	1.68	2.00	1.93	2.12	1.47	1.62	1.50	1.68
32	1.85	1.93	1.40	1.62	1.84	1.84	1.76	1.76
33	1.90	1.97	1.05	1.60	1.47	1.62	1.73	1.72
34	1.70	1.99	1.34	1.61	1.41	1.62	1.70	1.71
35	1.86	1.93	1.74	1.72	1.50	1.63	1.46	1.69
36	1.74	1.98	1.79	1.78	1.87	1.91	1.58	1.68
37	1.85	1.94	1.54	1.64	1.60	1.65	1.51	1.68
38	1.68	2.00	1.69	1.69	1.86	1.90	1.83	1.87

The simulation results are estimated and the results are demonstrated in table 3. The calculation results and confidence range of fractal dimension are different with different estimation methods. The calculated value of the Periodogram method is the closest to the theoretical value.

Table 3. Fractal Dimension And Its Estimation.

Test		Autocorrelation method		Periodogram method		Bartlett method		Welch method	
		D	$D^{'}$	D	$D^{'}$	D	$D^{'}$	D	$D^{'}$
Mean		1.80	1.96	1.51	1.63	1.77	1.75	1.67	1.69
confidence interval	Upper limit	1.84	1.94	1.49	1.63	1.48	1.62	1.67	1.70
	Lower limit	1.69	2.00	1.88	1.93	1.68	1.68	1.53	1.68

In order to verify the validity of the calculation method, we test whether the theoretical value and the calculated value are consistent. And we can use the Paired Sample T test [10]. Null hypothesis is that there is no significant difference between the calculated value and the theoretical value. Alternative hypothesis is that there is a significant difference between the calculated value and the theoretical value. Inspection statistics is given as

$$y_i = x_{1i} - x_{2i} (i = 1,2,\cdots n) \quad (7)$$

$$t = \frac{\bar{y}}{s_y / \sqrt{n-1}} \sim t(n-1) \quad (8)$$

Table 4. Paired Sample T Test.

Test	Mean	Standard deviation	standard error of the mean	95% confidence interval for the difference		t	P
				Lower limit	Upper limit		
Autocorrelation method	-0.165	0.105	0.011	-0.187	-0.142	-14.593	0.000
Periodogram method	-0.002	0.017	0.002	-0.006	0.001	-1.190	0.238
Bartlett method	-0.065	0.068	0.005	-0.075	-0.054	-12.163	0.000
Welch method	-0.085	0.079	0.007	-0.099	-0.072	-12.807	0.000

The results of the paired sample test showed that $P = 0.238 > 0.05$, when the periodogram method is adopted. At the significance level of 0.05, we could not reject the null hypothesis. There is no significant difference between the calculated value and the theoretical value. The theoretical data is mainly concentrated in $[1.6, 1.8]$. This indicates that the fractal dimension calculation of rough contour curves in this range is practically no difference with the theoretical value.

K-S testing method can use sample data to infer whether sample from the overall to obey a certain distribution theory, is a kind of goodness-of-fit test method, applicable to explore the distribution of continuous random variables. The K-S test can not only test whether a single population is subject to a theoretical distribution, but also can test whether there are significant differences between the two general distributions.The data does not obey the normal distribution. So the theoretical values and calculated values are respectively tested by Wilcoxon Signed Rank Test in non-parametric tests.

Table 5. Wilcoxon Signed Rank Test

Test	null hypothesis	Test	p	Decision
Periodogram method	The median of the difference between the theoretical and the calculated values is equal to 0	Wilcoxon Signed Rank Test	0.482	Accept the null hypothesis
Autocorrelation method			0.000	
Bartlett method			0.000	Reject the null hypothesis
Welch method			0.000	

There are no basic assumptions about non-parametric methods. The test results show that the null hypothesis cannot be rejected when the periodogram method is adopted and the significance level is 0.05. There is no significant difference between the calculated value and the theoretical value. The accuracy of the fractal dimension calculation of rough contour curves is also verified by the PSD method.

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