用 Zernike 多项式拟合干涉波面不同算法的等价性研究

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摘 要:通过严格证明在 Zernike 多项式拟合光学干涉波面时,求解拟合系数的2种典型算法即 最小二乘法和 Gram - Schimdt 算法的等价性,论证了求解 Zernike 多项式拟合系数的各种算法 在求解过程中具有相同的稳定性。研究发现当其中一种算法在求解过程因故中断或拟合的干 涉波面出现了突变,则另一种算法同样无法实现对该干涉波面的正确拟合。研究结果表明:用 Zernike 多项式拟合干涉波面,没有哪一种算法更优于其他算法,仅仅是求解过程不同而已,各 种算法的可靠性是等价的。

关键词:Zernike 多项式;干涉波面;最小二乘法;Gram-Schimdt 算法;算法等价性

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如何正确求解出 Zernike 多项式拟合干涉波面的拟合系数已成为现代数字化干涉精密检测技术的重要 组成部分^[1-8]。不同研究者都强调所采用算法的优势并都给出了充分的理由。然而,实践中不论采用哪一 种算法都无法绝对避免求解拟合系数过程中可能的失败或测量结果的突变。如何找到一个求解 Zernike 多 项式拟合系数的最佳算法,使得拟合系数的求解过程简洁快速且稳定,确保测量结果的可靠性,成为该领域 研究的重点。

求解 Zernike 多项式拟合系数的算法包括典型的最小二乘法和 Gram – Schimdt 方法以及 Householder 变换方法。实际上,在众多的算法中,只有 2 类基本算法,一类是直接应用最小二乘法求解 Zernike 多项式拟合系数,另一类则是利用 Zernike 多项式构造一个新的正交归一化的函数系,再对该新的函数系应用最小二乘法求解拟合系数^[9-11]。以下通过证明最小二乘法与 Gram – Schimdt 方法的等价性,说明各种算法之间是相通的,其收敛性是等价的。

1 求解 Zernike 多项式拟合系数的最小二乘法

Zernike 多项式用极坐标的具体表达为:

$$Z_n^l(\rho) = R_n^l(\rho) \Theta_n^l(\theta)$$

式中:n为多项式的"阶",取值为0,1,…;l为与阶数n相关的序号,l的值恒与n同奇偶性,且绝对值小于或等于阶数n。拟合时选取的阶n越大,加入拟合的多项式数量N将越多。用 Zernike 多项式表达的光学干涉 波面 W的函数为:

$$W(\boldsymbol{\rho},\boldsymbol{\theta}) = \sum_{k=0}^{\infty} a_k Z_n^l(\boldsymbol{\rho},\boldsymbol{\theta}) \qquad \vec{\mathfrak{R}} W(\boldsymbol{r}_j) = \sum_{k=0}^{\infty} a_k Z_k(\boldsymbol{r}_j)$$

式中: a_k 为拟合系数; r_j 为对干涉波面数字化后采样点的位置矢量,应用时常采用直角坐标系波函数 W(x, y),因此 Zernike 多项式为 $Z_k(x, y)$ 。根据最小二乘法原理,求解 a_k 的方法与过程如下:

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$$\Delta^2 = \sum_{j=1}^{M} \left[\sum_{i=1}^{N} a_i Z_i(\boldsymbol{r}_j) - \varphi(\boldsymbol{r}_j) \right]^2$$
(1)

式中: $\varphi(\mathbf{r}_i)$ 为干涉波面 \mathbf{r}_i 点的相位; $\sum_{j=1}^{M}$ 为对所有采样点求和, $\sum_{i=1}^{N}$ 为对多项式的所有项求和。又有:

$$\frac{\partial}{\partial a_k}(\Delta^2) = 2\sum_{i=1}^N \sum_{j=1}^M a_i Z_i(\mathbf{r}_j) Z_k(\mathbf{r}_j) - 2\sum_{j=1}^M \varphi(\mathbf{r}_j) Z_k(\mathbf{r}_j) = 0$$
(2)

$$\diamondsuit S_{i+k} = \sum_{j=1}^{m} Z_i(\mathbf{r}_j) Z_k(\mathbf{r}_j) , t_k = \sum_{j=1}^{m} \varphi(\mathbf{r}_j) Z_k(\mathbf{r}_j) , \text{M} \mathfrak{K}(2) \mathfrak{B} \mathfrak{K}:$$

$$\sum_{i=1}^{N} S_{i+k} a_i = t_k$$

$$(3)$$

式(3)为最小二乘法正则方程,将其展开便是关于 *a*_i 的线性方程组。*S*_{i+k} 系数方阵的性质表征了求解 *a*_i 的稳定性。实践表明,用最小二乘法求解多项式拟合系数,逻辑关系简洁,方法通用,收敛性令人满意。

2 求解 Zernike 多项式拟合系数的 Gram - Schimdt 正交化方法

Gram – Schimdt 正交化方法的基本思想是将线性独立函数系 Zernike 多项式进行线性组合,构成一组在干涉波面采样数据点上离散正交归一化的基底函数系[V_i],即:

$$\begin{bmatrix} V_i \end{bmatrix} = \begin{bmatrix} C_{ik} \end{bmatrix} \begin{bmatrix} Z_i \end{bmatrix}$$
(4)

 $[C_{ik}]$ 为变换方阵, $[V_i]$ 和 $[Z_i]$ 分别为 V_i 和 Z_i 构成的列向量。 $[V_i]$ 中的每一个元素均满足正交化条件:

$$\sum_{j=1}^{M} V_{i} V_{k} G = \begin{cases} 1 & , i = k \\ 0 & , i \neq k \end{cases}$$
(5)

 $\sum_{i=1}^{M}$ 为对所有采样点求和; G为非负的全函数, 一般取值为1。根据式(4)和(5)可得[V_i]和[Z_i]的关系:

$$V_{i} = \frac{Z_{i} - \sum_{r=1}^{M} V_{r} \sum_{j=1}^{M} Z_{i} V_{r}}{\left[\sum_{j=1}^{M} Z_{i}^{2} - \sum_{r=1}^{i-1} \left(\sum_{j=1}^{M} Z_{i} V_{r}\right)^{2}\right]^{1/2}}$$
(6)

变换矩阵[C_{ik}]为:

$$C_{ik} = \begin{cases} 0 , i < k \\ \left[\sum_{j=1}^{M} Z_{i}^{2} - \sum_{r=1}^{i-1} \left(\sum_{j=1}^{M} Z_{i} V_{r} \right)^{2} \right]^{1/2} , i = k \\ - \sum_{r=1}^{i-1} \left[\left(\sum_{j=1}^{M} Z_{i} V_{r} \right) C_{ii} C_{rk} \right] , i > k \end{cases}$$
(7)

被拟合的干涉波面F(r)用矩阵表示为:

$$F(\mathbf{r}) = [a_i]^{\mathrm{T}}[Z_i] = [a_i]^{\mathrm{T}}[C_{ik}]^{-1}[V_i] = [b_i]^{\mathrm{T}}[V_i] = \sum_{i=1}^{N} b_i V_i$$

$$(8)$$

式中 $\begin{bmatrix} b_i \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} a_i \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} C_{ik} \end{bmatrix}^{-1}$ 。

根据最小二乘法原理:

$$\Delta^{2} = \sum_{j=1}^{M} \left[F(\mathbf{r}_{j}) - \varphi(\mathbf{r}_{j}) \right]^{2} = \sum_{j=1}^{M} \left[\sum_{i=1}^{N} b_{i} V_{i}(\mathbf{r}_{j}) - \varphi(\mathbf{r}_{j}) \right]^{2} = \sum_{j=1}^{M} \left(\sum_{i=1}^{N} b_{i} V_{i}(\mathbf{r}_{j}) \right)^{2} - 2 \sum_{j=1}^{M} \varphi(\mathbf{r}_{j}) \sum_{i=1}^{N} b_{i} V_{i}(\mathbf{r}_{j}) + \sum_{j=1}^{M} \varphi(\mathbf{r}_{j})^{2}$$
(9)

利用式(5) 关于 V_i 的正交关系可得:

$$\Delta^{2} = \sum_{i=1}^{N} \left[b_{i}^{2} - 2b_{i} \sum_{j=1}^{M} \varphi(\mathbf{r}_{j}) V_{i}(\mathbf{r}_{j}) \right] + \sum_{j=1}^{M} \varphi(\mathbf{r}_{j})^{2}$$

 $\frac{\partial \Delta^2}{\partial b_i} = 2 \left[\sum_{i=1}^N b_i - \sum_{j=1}^M \varphi(\mathbf{r}_j) V_i(\mathbf{r}_j) \right] = 0$

故可得:

$$b_i = \sum_{j=1}^{M} \varphi(\mathbf{r}_j) \ V_i(\mathbf{r}_j)$$
(10)

把根据式(10) 求得的[b_i] 代回式(9) 中,便可得所需要的 Zernike 多项式拟合干涉波面的拟合系数 [a_i]。

3 最小二乘法与 Gram - Schimdt 方法的等价性证明

根据 Gram - Schimdt 正交化方法,在没有用到最小二乘法原理之前,由式(4) 和式(7) 可得:

$$Z_{i} = \sum_{k=1}^{i} C_{ik}^{-1} V_{i}$$
(11)

把式(11)代入式(8)中,得:

$$\sum_{i=1}^{N} a_{i} \left(\sum_{k=1}^{i} C_{ik}^{-1} V_{k} \right) = \sum_{i=1}^{N} b_{i} V_{i}$$

$$\sum_{i=1}^{M} \left[\sum_{i=1}^{N} a_{i} \left(\sum_{k=1}^{i} C_{ik}^{-1} V_{k} \right) V_{k} \right] = \sum_{j=1}^{M} \left(\sum_{i=1}^{N} b_{i} V_{i} \right) V_{k}$$
(12)

利用式(5),上式变成:

$$b_{k} = \sum_{i=1}^{N} a_{i} C_{ik}^{-1} , \quad j \le i$$
(13)

式(13)为从 Gram – Schindt 正交化方法推导出来的用最小二乘法原理进行 Zernike 多项式拟合的系数 [*a_i*]与用 Gram – Schindt 正交化方法进行拟合的系数[*b_i*]之间的变换关系。

反过来,也可以从最小二乘法原理出发,推导出2种方法所获得的拟合系数变换关系完全相同。由此充 分说明了2种拟合系数的求解算法是完全等价的。从最小二乘法原理出发的推导过程如下:

由最小二乘法获得的正则方程式(3) 可得:

$$\sum_{i=1}^{M} \left(\sum_{i=1}^{N} a_i Z_i(\boldsymbol{r}_j) Z_k(\boldsymbol{r}_j) \right) = \sum_{j=1}^{M} \varphi(\boldsymbol{r}_j) Z_k(\boldsymbol{r}_j)$$
(14)

$$\begin{split} \begin{split} &\Xi = \sum_{j=1}^{M} \left[\sum_{i=1}^{N} a_{i} \left(\sum_{n=1}^{i} C_{in}^{-1} V_{n} \right) \left(\sum_{m=1}^{k} C_{km}^{-1} V_{m} \right) \right] = \sum_{i=1}^{N} a_{i} \sum_{j=1}^{M} \left[\left(\sum_{n=1}^{i} C_{in}^{-1} V_{n} \right) \left(\sum_{m=1}^{k} C_{km}^{-1} V_{m} \right) \right] = \\ &\sum_{i=1}^{N} a_{i} \left(\sum_{m=1}^{k} C_{im}^{-1} C_{km}^{-1} \right) = \sum_{m=1}^{k} \left(\sum_{k=1}^{N} a_{i} C_{im}^{-1} \right) C_{km}^{-1} \quad , \quad n \leq i, \ m \leq k, \ k \leq i \end{split}$$

$$\overline{A} = \sum_{j=1}^{M} \varphi \left(\sum_{m=1}^{k} C_{km}^{-1} V_{m} \right) = \sum_{m=1}^{k} C_{km}^{-1} \left(\sum_{j=1}^{M} \varphi V_{m} \right) = \sum_{m=1}^{k} C_{km}^{-1} b_{m} \quad , \quad n \leq i, m \leq k, k \leq i$$

$$\overline{E} = \overline{A}, \overline{\eta} \overline{\Theta}:$$

$$b_m = \sum_{i=1}^{N} a_i C_{im}^{-1} , \quad m \le i$$
 (15)

4 结束语

采用 Zernike 多项式拟合干涉波面是现代数字化光学精密测量的核心技术之一。本文通过推导研究,澄 清了多年来有关求解 Zernike 多项式拟合系数的算法之争,明确了在同样条件下,任何算法都不可能比其他 算法具有更好的解的稳定性以及测量结果的可靠性。进一步的研究发现:只要在拟合时所选择的 Zernike 多 项式的阶小于被测干涉波面光瞳内干涉条纹的数量,不论采用何种算法,都可以确保 Zernike 多项式对采样 的拟合精度和拟合干涉波面函数的精度,从而确保检测系统测量结果的可靠性。可见.若被测干涉波面光瞳 内干涉条纹的数量足够多时(多于7根条纹以上),选择7阶(36项)以下 Zernike 多项式进行拟合都会得到 一致正确的测量结果。

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93

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The Research on Equivalence of the Algorithms in Fitting Interference Wave Surface with Zernike Polynomials

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Abstract: Through strictly proving the equivalence of the least squares method and Gram – Schimdt algorithm in fitting interference wave – front with Zernike polynomials, it is demonstrated that all algorithms of solving Zernike polynomial coefficients in the solving process are the same in stability. That is, when one of these algorithms is interrupted or a mutation appears in fitted interference wave – front in the solving process, then it is also not possible for the other algorithms to fit interference wave – front correctly. The research results show that no algorithm is superior to other algorithms in fitting the interference wave surface with Zernike polynomials. All these algorithms are equivalent in reliability except that their fitting processes are different.

Key words: Zernike polynomials; interference wave surface; least square method; Gram – Schimdt algorithm; algorithm equivalence

(上接第89页)

General Expressions of Constitutive Tensors of Irregular Prism Cloaks

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Abstract:Based on the coordinate transformation theory, the condition for irregular prism cloaks is deduced and the tensor expressions of electromagnetic parameters are obtained. By using the deduced tensor expressions of electromagnetic parameters, the effects of 3 – sided, 4 – sided and 6 – sided prism cloaks are verified through full – wave simulations. The results confirm the validity of the tensor expressions of electromagnetic parameters obtained. The cloaks designed by using the deduced expressions can surely make the electromagnetic wave transmit around the inner object and resume its primary transmission direction. The work done in this paper provided a theoretical basis for the design of two – dimensional baroque cloak.

Key words: coordinate transformation theory; irregular prism cloak; tensor expression; full - wave simulation