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Fractional factorial designs for Fourier-cosine models

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Abstract
Fourier-cosine models, rooted in the discrete cosine transformation, are widely used in numerous applications in science and engineering. Because the selection of design points where data are collected greatly affects the modeling process, we study the choice of fractional factorial designs for fitting Fourier-cosine models. We propose a new type of generalized resolution and provide a framework for the construction of fractional factorial designs with the maximum generalized resolution. The construction applies level permutations to regular designs with a novel nonlinear transformation. A series of theoretical results are developed to characterize the properties of the level-permuted designs. Based on the theory, we further provide efficient methods for constructing designs with high resolutions without any computer search. Examples are given to show the advantages of the constructed designs over existing ones.

Keywords Discrete cosine transformation · Generalized wordlength pattern · Level permutation · Maximum resolution · Orthogonal array · Regular design

1 Introduction

The Fourier-cosine modeling (also called cosine modeling) method and its corresponding cosine expansion have been widely used for modeling or expanding a function. Vapnik (1998) proposed fitting a posterior probability by a truncated cosine model to map the output of support vector machines to some probabilities. Uenohara and Kanade (1998) proved that the eigenvalues of the vector inner product matrix of uniformly rotated images can be represented with a cosine series. Spurr et al. (2001) used the cosine expansion for the determination of solutions to the radiative transfer equation. Fang and Oosterlee (2008, 2009) developed an option pricing method by representing

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the probability density function of the log-asset price in terms of its cosine expansion. Ruijter and Oosterlee (2012) further proposed to use two-dimensional cosine expansion for pricing financial options. Expanding grid data with cosine series is equivalent to conducting discrete cosine transform (DCT) Ahmed et al. (1974) on the data. The DCT is a good approximation to Karhunen-Loeve transform, which is optimal in the sense that it completely decorrelates the data in the transformed domain. Therefore, any truncated cosine expansion has the minimum mean squared error (Rao and Yip 2014). Buckley (1994) showed that the solution to a penalized minimum mean squared error problem for grid data also has a cosine series form. Butler (2001) argued that a second-order cosine model is a good simulation model for computer experiments, because it provides a good approximation to a second-order polynomial model and at the same time provides a link with spatial processes.

When the observations are collected from a subset of grid points, the choice of design points is crucial as it can greatly affect the precision of parameter estimations. While much attention was paid to the application of cosine models, there is little work on the choice of design points. Butler (2001) and Yin and Liu (2013) considered constructing Latin hypercube designs for fitting second-order cosine models, where the number of levels for each factor is restricted to be the same as the number of design points.

In this paper, we study the construction of fractional factorial designs for fitting cosine models. Factorial designs provide the capability of studying complex factorial effects and interactions, a capability that Latin hypercube designs do not possess. Fractional factorial designs have been widely studied under the minimum aberration and maximum resolution criteria and their various generalizations for ANOVA and polynomial models; see Tang and Deng (1999), Xu and Wu (2001), Cheng and Ye (2004), Xu et al. (2009), Huang et al. (2012), Cheng (2014) and Xu (2015) for major developments and references. Here we propose a new type of generalized wordlength pattern, called the γ-wordlength pattern, and its related γ-resolution to select designs for cosine models. Designs with high γ-resolution not only perform well for cosine models, but remarkably also outperform available designs for polynomial models.

We propose to construct high γ-resolution designs via level permutations for regular designs. Both polynomial and cosine models have a special feature that level permutation of any factor can alter a design's geometrical structure and statistical properties. This enables us to improve the property of regular designs via level permutations, but the huge number of possible permutations substantially complicates the task. Using a naive enumeration, for a design with m q-level factors, one needs to account for all the $(q!)^m$ possible level permutations, making it a formidable task to choose the best permutation even for moderate m and q. Cheng and Wu (2001), Ye et al. (2007) and Tang and Xu (2014) restricted the search within linear permutations to improve properties of regular designs. Wang et al. (2018) considered the so called Williams transformation in addition to linear permutations for good lattice point designs. We provide a special nonlinear level permutation and develop a general theory on the obtained designs. Using the theory, we propose highly efficient constructions that require no computer search for generating designs. The obtained designs have better properties than regular designs and linearly permuted regular designs.

The rest of this paper is organized as follows. Section 2 introduces notation and backgrounds. Section 3 defines the γ-resolution and provides preliminary results. Section 4 provides the nonlinear level permutation and its nice properties for generating designs for cosine models. Section 5 presents main theoretical results and construction methods. Section 6 considers the application of the constructed designs. Section 7 gives concluding remarks. We defer all proofs to the "Appendix".

2 Notation and backgrounds

Let $Z_q = \{0, 1, \ldots, q-1\}$. For a vector $u = (u_1, \ldots, u_m) \in Z_q^m$, let $\|u\|_0$ be the number of its nonzero elements and $\|u\|_1 = \sum_{j=1}^m u_j$. A design with N points, m factors and q levels, is an $N \times m$ matrix $D = (x_{ij})$ over Z_q, where each row represents a design point and each column represents a factor. An orthogonal array (OA) of strength t is a design in which all possible level combinations for any t factors appear equally often. OAs include both regular and nonregular fractional factorial designs. They are widely used in physical and computer experiments; see Hedayat et al. (1999).

Let q be a prime. A regular q^{m-p} design is an OA with $m-p$ independent columns, denoted as $x_1, \ldots, x_{m-p}$, which form a full factorial design, and p dependent columns, denoted as $x_{m-p+1}, \ldots, x_m$, which can be specified by p linear equations:

$$\begin{cases} x_{m-p+1} = c_{11}x_1 + \cdots + c_{1,m-p}x_{m-p} + b_1, \\ \quad \cdots \quad \cdots \quad \cdots \\ x_m = c_{p1}x_1 + \cdots + c_{p,m-p}x_{m-p} + b_p, \end{cases} \tag{1}$$

where c_{ij} and b_i are constants in Z_q for $i = 1, \ldots, p$ and $j = 1, \ldots, m-p$. Denote $C = (c_{ij})$ and $b = (b_1, \ldots, b_p)'$. The matrix $G = [I_{m-p}, C']$ is called the generator matrix, where I_{m-p} is the $(m-p) \times (m-p)$ identity matrix. The linear space generated by row vectors of matrix $[C, (q-1)I_p]$ is called the defining contrast subgroup, denoted by L. Each vector (row) in $u \in L$ is called a word with wordlength $\|u\|_0$. For any given C, different choices of b lead to different fractions. All fractions share the same defining contrast subgroup. The one with $b = (0, \ldots, 0)'$ is called the principal fraction and other fractions are its cosets. One fraction can be obtained from another by linearly permuting the levels of factors (that is, replacing a column x of the design to $x + z \pmod q$ for some $z \in Z_q$).

If D is the principal fraction of a regular q^{m-p} design, linearly permuting each column x to $x + (q-1)/2$ generates a mirror-symmetric fraction (Tang and Xu 2014). An $N \times m$ design D over Z_q is called mirror-symmetric if $(q-1)J - D$ is the same design as D, where J is an $N \times m$ matrix of ones. In spite of the common application of principal fractions in designing experiments (see Mukerjee and Wu 2006; Wu and Hamada 2009), Tang and Xu (2014) showed that mirror-symmetric fractions are better than principal fractions for fitting polynomial models.

3 The γ-resolution

For an $N \times m$ design $D = (x_{ij})$ over Z_q with observations y_i, $i = 1, \ldots, N$, a first-order cosine model can be expressed as

$$y_i = \mu_0 + \sqrt{2} \sum_{j=1}^{m} \mu_j \cos\left\{\frac{\pi(x_{ij} + 0.5)}{q}\right\} + \varepsilon_i, \tag{2}$$

and a second-order cosine model is of the form

$$\begin{aligned} y_i = \mu_0 &+ \sqrt{2} \sum_{j=1}^{m} \mu_j \cos\left\{\frac{\pi(x_{ij} + 0.5)}{q}\right\} + \sqrt{2} \sum_{j=1}^{m} \mu_{jj} \cos\left\{\frac{2\pi(x_{ij} + 0.5)}{q}\right\} \\ &+ 2 \sum_{j=1}^{m-1} \sum_{k=j+1}^{m} \mu_{jk} \cos\left\{\frac{\pi(x_{ij} + 0.5)}{q}\right\} \cos\left\{\frac{\pi(x_{ik} + 0.5)}{q}\right\} + \varepsilon_i, \end{aligned} \tag{3}$$

where $\varepsilon_i \sim N(0, \sigma^2)$. Note that the first-order terms in (2) and (3) complete only half a cycle from $x = 0$ to $x = q - 1$. Consequently, the terms are different from the trigonometric functions usually included in Fourier models such as in Riccomagno et al. (1997) and Xie et al. (2007). Generally, a full cosine model can be expressed in the following matrix form

$$Y = X_0\theta_0 + X_1\theta_1 + \cdots + X_K\theta_K + \varepsilon,$$

where $Y = (y_1, \ldots, y_N)'$, $K = m(q - 1)$, and for $k = 0, 1, \ldots, K$, X_k is an $N \times l_k$ matrix with the (i, u)-th element $(X_k)_{iu} = 2^{\|u\|_0/2} \prod_{j=1}^{m} \cos(u_j\pi(x_{ij} + 0.5)/q)$ for $i = 1, \ldots, N$ and $u \in Z_q^m$ with $\|u\|_1 = k$, l_k is the number of $u \in Z_q^m$ such that $\|u\|_1 = k$, θ_k is an $l_k \times 1$ vector of the kth-order frequencies in the frequency domain, and $\varepsilon \sim N(0, \sigma^2 I_N)$.

The higher-order frequencies in a cosine model have dramatically smaller variances or spectral densities than lower-order frequencies (Rao and Yip 2014), so they are typically cut off to obtain a truncated model or expansion for easy interpretation. When doing so, we expect that the omitted frequencies bring the minimum bias to the obtained truncated model. To measure such bias, we define the γ-wordlength pattern for an $N \times m$ design $D = (x_{ij})$ over Z_q as $(\gamma_1(D), \ldots, \gamma_K(D))$, where

$$\gamma_k(D) = N^{-2} \sum_{\|u\|_1 = k} 2^{\|u\|_0} \left| \sum_{i=1}^{N} \prod_{j=1}^{m} \cos(u_j\pi(x_{ij} + 0.5)/q) \right|^2$$

for $k = 1, \ldots, K$, where $K = m(q-1)$, $\|u\|_1 = \sum_{j=1}^{m} u_j$, and $\|u\|_0$ is the number of its nonzero elements. Then γ_k measures the aliasing between two frequencies whose orders sum up to k. A zero $\gamma_k(D)$ implies no aliasing between jth- and $(k-j)$th-order frequencies for all j with $0 \le j \le k$. Define the γ-resolution of a design D to be the smallest number $k > 0$ such that $\gamma_k(D) \neq 0$. Then for any desired design size, our goal is to find a design with maximum γ-resolution.

Because OAs are widely used in practice, we provide a preliminary result for OAs regarding the γ-resolution.

Lemma 1 *Suppose D is an OA with strength t, then* $\gamma_k(D) = 0$ *for* $k = 1, \ldots, t$.

Lemma 1 shows that the γ-resolution of an OA with strength t is at least $t + 1$, so that increasing the strength of OAs generate designs with higher γ-resolution. However, this way tends to generate designs with large run sizes, which is undesirable in designing experiments. A natural concern is whether it is possible to improve the performance of an OA, say reducing its γ_{t+1} value to zero, without increasing the run size. Let us first see an illustrative example.

Example 1 Let D be the principal fraction of a regular 5^{3-1} design with $x_3 = x_1 + x_2$, $D_1 = D + 2J$ (mod 5), which means D_1 is obtained from D by linearly permuting the levels (0, 1, 2, 3, 4) to (2, 3, 4, 0, 1) over Z_5, and D_2 be the design obtained from D by permuting levels (0, 1, 2, 3, 4) to (2, 4, 3, 1, 0). Each of the three designs is an OA of strength 2 and has $\gamma_1 = \gamma_2 = 0$ by Lemma 1. It can be verified that $\gamma_3(D) = 0.1278$ so that the γ-resolution of D is 3, $\gamma_3(D_1) = 0$ and $\gamma_4(D_1) = 0.96$ so that the γ-resolution of D_1 is 4, while $\gamma_3(D_2) = \gamma_4(D_2) = \gamma_5(D_2) = 0$ and $\gamma_6(D_2) = 2$ so that the γ-resolution of D_2 is 6. Design D_2 is much better than D and D_1. Under the second-order model in (3), the estimates of the parameters are correlated for D and D_1 but are uncorrelated for D_2.

Example 1 shows that permuting levels of a regular design can improve its performance without increasing its run size. Except for the linear level permutation proposed by Tang and Xu (2014), which leads to D_1 in Example 1, a nonlinear permutation, for example the permutation for D_2 in Example 1, may lead to a better design with a more significant improvement. We study this nonlinear permutation in detail in the next section.

4 A level permutation

Let q be an odd prime. Define

$$\varphi(x) = \begin{cases} 2x + (q-1)/2, & \text{for } 0 \leq x < q/4; \\ -2x + (3q-1)/2, & \text{for } q/4 < x < 3q/4; \\ 2x - (3q+1)/2, & \text{for } 3q/4 < x < q. \end{cases} \tag{4}$$

Then φ defines a permutation for all $x \in Z_q$. For example, for $q = 3$, φ linearly permute the levels (0, 1, 2) to (1, 2, 0) over Z_3; for $q = 5$, φ is the permutation used for D_2 in Example 1. For $q \geq 5$, φ is nonlinear. Figure 1 shows the cases for $q = 5$ and 7. The permutation is well defined because for $x_1, x_2 \in Z_q$ and $x_1 \neq x_2$, $\varphi(x_1) \neq \varphi(x_2)$. In fact, for instance, if $0 \leq x_1 < q/4$, $q/4 < x_2 < 3q/4$ and $\varphi(x_1) = \varphi(x_2)$, then $q = 2(x_1 + x_2)$, which contradicts with the fact that q is odd. It

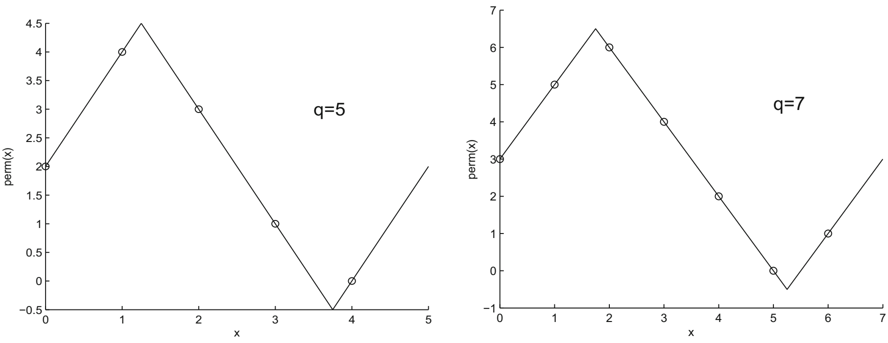

Fig. 1 The permutation $\varphi(x)$ in (4) for $q = 5$ and 7

is easy to see that the permutation has the property

$$\varphi(x) + \varphi(q - x) = q - 1 \pmod q. \tag{5}$$

Note that φ is in fact a piece-wise linear transformation, similar to the Williams transformation applied to the construction of Latin hypercube designs in Butler (2001) and Wang et al. (2018). However, φ is directly ready to use on regular designs and significantly improves their properties. Below is an important result on φ. For a $D = (x_{ij})$, denote $\varphi(D) = (\varphi(x_{ij}))$, the design obtained from D by permuting the levels with φ for all factors.

Theorem 1 *Let q be an odd prime. If D is the principal fraction of a regular q^{m-p} design, $\varphi(D)$ is mirror-symmetric.*

Theorem 1 is important because we have the following property for mirror-symmetric designs.

Theorem 2 *A design D is mirror-symmetric if and only if $\gamma_k(D) = 0$ for all odd $k > 0$.*

Theorems 1 and 2 guarantee that odd-order frequencies are not aliased with any even-order frequencies for $\varphi(D)$ if D is a principal fraction. Specifically, linear frequencies are not aliased with any even-order frequencies. In the next section, we will further discuss theoretical properties of $\varphi(D)$.

5 Theoretical results

We consider the construction of the maximum γ-resolution design among the class of all possible $\varphi(D)$ where D is a regular q^{m-p} design defined in (1). If D is an OA of strength t, so is $\varphi(D)$, then, by Lemma 1, $\gamma_k(\varphi(D)) = 0$ for $k = 1, \ldots, t$. So we consider the choice of C in the generator matrix and the vector b for determining D so that the strength of D and then the γ-resolution of $\varphi(D)$ are maximized. An exhaustive search for both C and b seems infeasible considering the number of candidates, $q^{p(m-p)}$ for C and q^p for b, which can be super large for even moderate q and m, and the high complexity of the computation of $\gamma_{t+1}(\varphi(D))$ (or further, $\gamma_{t+2}(\varphi(D)))$ for a single design. We provide a series of theoretical results and construction methods in this section so that no computer search is required for generating the maximum γ-resolution designs. First, we have the following result showing that it suffices to set $b = 0$ and restrict our search within principal fractions.

Theorem 3 *Let q be an odd prime, D be a principal q^{m-p} regular design with strength t and D_1 be one of its cosets.*

(i) If t is even, $\gamma_{t+1}(\varphi(D)) = 0$. Further, $\gamma_{t+2}(\varphi(D_1)) = 0$ implies $\gamma_{t+2}(\varphi(D)) = 0$.
(ii) If t is odd, $\gamma_{t+1}(\varphi(D_1)) = 0$ implies $\gamma_{t+1}(\varphi(D)) = 0$. Further, $\gamma_{t+2}(\varphi(D)) = 0$.

By Theorem 3, if any regular design permuted with φ has zero γ_{t+1} or γ_{t+2}, so does its principal fraction. So principal fractions seem to derive designs with at least the same performance as their cosets.

Example 2 Let D be the principal fraction of a regular 5^{3-1} design with $x_3 = x_1 + x_2$ and D_1 be its coset with $x_3 = x_1 + x_2 + 1$. Because both D and D_1 have strength $t = 2$, $\gamma_1 = \gamma_2 = 0$ for both $\varphi(D)$ and $\varphi(D_1)$. By Theorem 3(i), $\gamma_3(\varphi(D)) = 0$, while it can be verified that $\gamma_3(\varphi(D_1)) = 0.452 \neq 0$. Further, $\gamma_4(\varphi(D_1)) = 0$ and this implies that $\gamma_4(\varphi(D)) = 0$ by Theorem 3(i).

Example 2 shows that the γ-resolution of $\varphi(D)$ with D being a principal fraction is typically higher than that of $\varphi(D)$ with D being a coset. Also, recall the nice property that $\gamma_k(\varphi(D)) = 0$ for all odd k if D is a principal fraction (Theorems 1 and 2). For these reasons, we shall restrict our search within principal fractions and focus on the choice of C. The effect of C on the γ-resolution of $\varphi(D)$ is illustrated by the following example.

Example 3 Let D be the principal fraction of a regular 5^{3-1} design with $x_3 = 2x_1+2x_2$. It is straightforward to verify that $\gamma_1(\varphi(D)) = \gamma_2(\varphi(D)) = \gamma_3(\varphi(D)) = 0$ and $\gamma_4(\varphi(D)) = 0.5$ so that the γ-resolution of this $\varphi(D)$ is 4. Recall that for the principal fraction, also denoted by D, of a regular 5^{3-1} design with $x_3 = x_1 + x_2$ in Example 1, we have $\gamma_1(\varphi(D)) = \cdots = \gamma_5(\varphi(D)) = 0$ and the γ-resolution of this $\varphi(D)$ is 6. The two principal fractions differ merely in the generators of dependent columns while have significantly different γ-resolution.

We next provide explicit formulas for computing γ_{t+1} and γ_{t+2} for principal fractions. For $d = 1, \ldots, m$, let N_d be the number of words $u \in L$ of length d with all components of u being 0, 1, or $q - 1$ (for example, $u = (1, 1, 4, 0)$ for a 5-level design), and M_d be the number of words $u \in L$ of length d with exactly one component being 2 or $q - 2$ and all other components being 0, 1 or $q - 1$ (for example, $u = (1, 2, 0, 4)$ for a 5-level design).

Theorem 4 *Let q be an odd prime and D be the principle fraction of a regular q^{m-p} design with strength t.*

(i) *If t is even, $\gamma_{t+1}(\varphi(D)) = 0$ and $\gamma_{t+2}(\varphi(D)) = 2^{-(t+1)} N_{t+2} + 2^{-t} M_{t+1}$.*
(ii) *If t is odd, $\gamma_{t+1}(\varphi(D)) = 2^{-t} N_{t+1}$ and $\gamma_{t+2}(\varphi(D)) = 0$.*

Theorem 4 provides a simple and fast computation of $\gamma_{t+1}(\varphi(D))$ and $\gamma_{t+2}(\varphi(D))$. For any possible t, we only need to compute either $\gamma_{t+1}(\varphi(D))$ or $\gamma_{t+2}(\varphi(D))$, and the computation only involves the counting of some words. The following example illustrate the use of Theorem 4.

Example 4 Let D be a regular 5^{4-2} design with $x_3 = x_1 + x_2$ and $x_4 = x_1 + 2x_2$, so that

$$C = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix},$$

the strength of D is $t = 2$, and the defining contrast subgroup is

$$L = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 0 & 1 & 2 & 3 & 4 & 0 & 1 & 2 & 3 & 4 & 0 & 1 & 2 & 3 & 4 & 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 0 & 2 & 3 & 4 & 0 & 1 & 3 & 4 & 0 & 1 & 2 & 4 & 0 & 1 & 2 & 3 \\ 0 & 4 & 3 & 2 & 1 & 1 & 0 & 4 & 3 & 2 & 2 & 1 & 0 & 4 & 3 & 3 & 2 & 1 & 0 & 4 & 4 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 4 & 4 & 4 & 4 & 3 & 3 & 3 & 3 & 3 & 2 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}'.$$

Then $M_3 = 4$ and $N_4 = 0$. By Theorem 4(i), $\gamma_3(\varphi(D)) = 0$ and $\gamma_4(\varphi(D)) = N_4/8 + M_3/4 = 1$.

Based on the above theoretical results, we propose two efficient methods for generating high γ-resolution designs among the class of $\varphi(D)$. By Theorem 3, we only consider D to be a principal fraction so that each dependent column is generated by $c_1x_1 + \cdots + c_{m-p}x_{m-p}$ with $c_1, \ldots, c_{m-p} \in Z_q$. These generators are determined so that the strength, t, of D is first maximized and then $\gamma_{t+1}(\varphi(D))$ or $\gamma_{t+2}(\varphi(D))$ could be zero, where $\gamma_{t+1}(\varphi(D))$ and $\gamma_{t+2}(\varphi(D))$ are considered or computed with Theorem 4.

We first provide a simple construction from regular q^{m-p} designs with $q \geq 5$ and $p = 1$. For convenience, let 0_n (and 1_n) be the $n \times 1$ vector of zeros (and ones). If m is odd, $C = 1'_{m-1}$ generates a principal fraction D with strength $t = m - 1$, which is the maximum possible strength. For design D, $L = \{0'_m, u, \ldots, (q-1)u\}$ where $u = (1'_{m-1}, q-1)$, and $N_{t+2} = M_{t+1} = 0$. Thus $\gamma_{t+2}(\varphi(D)) = 0$. From Theorem 4, $\varphi(D)$ has γ-resolution at least $m + 3$. For example, see the design D_2 in Example 1. If m is even, we can choose $C = (1'_{m-2}, 2)$. Then C generates a principal fraction D with resolution $t = m - 1$, $L = \{0'_m, u, \ldots, (q-1)u\}$ where $u = (1'_{m-2}, 2, q-1)$, and $N_{t+1} = 0$. Thus $\gamma_{t+1}(\varphi(D)) = 0$. From Theorem 4, $\varphi(D)$ has γ-resolution at least $m + 2$.

Theorem 5 *Suppose D is the principal fraction of a regular q^{m-1} design with a generator matrix $G = [I_{m-1}, C']$, where $q \geq 5$ is an odd prime.*

(i) *If m is odd and $C = 1'_{m-1}$, the γ-resolution of $\varphi(D)$ is at least $m + 3$.*
(ii) *If m is even and $C = (1'_{m-2}, 2)$, the γ-resolution of $\varphi(D)$ is at least $m + 2$.*

Recall that given a principal fraction D, $\tilde{D} = D + ((q-1)/2)J \pmod q$ obtained via linear level permutation is mirror-symmetric (Tang and Xu 2014). Suppose D is the principal fraction of a regular q^{m-1} design specified in Theorem 5. Table 1 compares the γ-resolutions of designs D, $\tilde{D}$ and $\varphi(D)$ for $q = 5, 7, 11$ and $m = 3, 4, 5$. It is

Table 1 The γ-resolutions for three types of q^{m-1} designs

(q, m)	(5,3)	(5,4)	(5,5)	(7,3)	(7,4)	(7,5)	(11,3)	(11,4)	(11,5)
D	3	4	5	3	4	5	3	4	5
$\tilde{D}$	4	4	6	4	4	6	4	4	6
$\varphi(D)$	6	6	8	6	8	10	6	10	10

easy to see that $\varphi(D)$ performs much better than the corresponding $\tilde{D}$ and D. Note that Theorem 5 does not hold for $q = 3$. This is because for three-level designs, $N_{t+1} = M_{t+1}$ and neither of them can be zero. Therefore, when $q = 3$, $\varphi(D)$ and $\tilde{D}$ has the same possible maximum γ-resolution, which is $m + 1$ for odd m and m for even m.

We now provide a general method for generating high γ-resolution designs among the class of $\varphi(D)$. We first illustrate the method with designs of q^2 runs and then provide a general result. Denote D as a regular design with q^2 runs, then D has two independent columns x_1 and x_2. We still only consider D to be a principal fraction so that each dependent column is generated by $c_1x_1 + c_2x_2$ with $c_1, c_2 \in Z_q$. If D has $m \le q + 1$ columns (that is, less than $q - 1$ dependent columns), the maximum possible strength of D is $t = 2$, and the columns of D can be generated by sequentially choosing columns of G_2 as generators, where

$$G_2 = \begin{pmatrix} 1 & 0 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 1 & 2 & \cdots & q-1 \end{pmatrix}.$$

By Theorem 4(i), these designs derive $\varphi(D)$ with $\gamma_1 = \gamma_2 = \gamma_3 = 0$, that is, the γ-resolution of $\varphi(D)$ is at least 4. For $m > q + 1$, the maximum possible strength of D is $t = 1$. Define

$$G = [G_2, 2G_2, \ldots, ((q-1)/2)G_2].$$

For a regular design D with G as its generator matrix, $N_2 = 0$. By Theorem 4(ii), $\gamma_2(\varphi(D)) = 0$. Therefore, sequentially choosing columns of G generates the regular design D such that $\gamma_2(\varphi(D)) = 0$ and the γ-resolution of $\varphi(D)$ is at least 4.

Using this method, we catalogue a list of 5-level designs $\varphi(D)$ with 25 runs and up to 12 columns. Table 2 shows that the γ-resolution of $\varphi(D)$ is always larger than that of D and is larger than that of $\tilde{D}$ for $m > 6$. Specifically, for $m = 3, \ldots, 6$, the γ-resolutions of $\varphi(D)$ and $\tilde{D}$ are the same and they are both larger than that of D. For $m = 7, \ldots, 12$, the γ-resolutions of D and $\tilde{D}$ decrease to 2, which means that linear frequencies would be aliased with each other if either of these two designs is used for a cosine model, while the γ-resolution of $\varphi(D)$ stays at 4, making linear frequencies uncorrelated if $\varphi(D)$ is used. In addition, linear frequencies are uncorrelated with second-order frequencies with $\varphi(D)$. The 7-level designs with 49 runs listed in Table 3 show the same trend. Note that the maximum possible γ-resolution is 4 for 25-run designs with $m \ge 6$ factors and 49-run designs with $m \ge 9$ factors, which is achieved by $\varphi(D)$.

Table 2 The γ-resolutions for three types of 25-run designs with $m = 3, \ldots, 12$ columns

m	3	4	5	6	7	8	9	10	11	12
D	3	3	3	3	2	2	2	2	2	2
$\tilde{D}$	4	4	4	4	2	2	2	2	2	2
$\varphi(D)$	6	4	4	4	4	4	4	4	4	4

Table 3 The γ-resolutions for three types of 49-run designs with $m = 3, \ldots, 24$ columns

m	3	4	5	6	7	8	9	10	11	$12\cdots24$
D	3	3	3	3	3	3	2	2	2	2
$\tilde{D}$	4	4	4	4	4	4	2	2	2	2
$\varphi(D)$	6	4	4	4	4	4	4	4	4	4

Generally, for $k \geq 3$, we recursively define the generator matrix G_k of a saturated regular design with q^k runs and strength $t \geq 2$ as follows:

$$G_k = \begin{pmatrix} G_{k-1} & 0_{k-1} & G_{k-1} & G_{k-1} & \cdots & G_{k-1} \\ 0'_\nu & 1 & 1'_\nu & 2 \cdot 1'_\nu & \cdots & (q-1) \cdot 1'_\nu \end{pmatrix},$$

where $\nu = (q^{k-1} - 1)/(q - 1)$. Note that G_k has k rows and $(q^k - 1)/(q - 1)$ columns, and the columns of G_k are arranged in the Yates order. We can move the column $(0'_{k-1}, 1)'$ forward so that the first k columns of G_k form an identity matrix. Denote

$$G = [G_{m-p}, 2G_{m-p}, \ldots, ((q-1)/2)G_{m-p}]. \tag{6}$$

Then G has $m - p$ rows and $(q^{m-p} - 1)/2$ columns. Based on the above discussion, we have the following general result.

Theorem 6 *Suppose D is the principal fraction of a regular q^{m-p} design generated by G in (6). Then $\varphi(D)$ has $(q^{m-p} - 1)/2$ columns and its γ-resolution is at least 4.*

It should be noted that designs constructed using Theorem 6 have the maximum possible number of columns that a design with γ-resolution 4 can have. So Theorem 6 generates designs that can accommodate the maximum number of factors.

6 Applications

Consider applying two 5^{3-1} mirror-symmetric designs $\tilde{D}$ and $\varphi(D)$ in Table 1 to study three five-level quantitative factors with the second-order cosine model

$$y = \beta_0 + \sum_{j=1}^{3} f_1(x_j)\beta_j + \sum_{j=1}^{3} f_2(x_j)\beta_{jj} + \sum_{j=1}^{2} \sum_{k=j+1}^{3} f_1(x_j) f_1(x_k)\beta_{jk} + \varepsilon, \tag{7}$$

Table 4 Information matrices $M'M/25$ for $\tilde{D}$ and $\varphi(D)$ under a second-order cosine model

$\tilde{D}$						$\varphi(D)$					
1	0	0	0	0	−0.566	1	0	0	0	0	0
0	1	0	0	−0.566	0	0	1	0	0	0	0
0	0	1	0.566	0	0	0	0	1	0	0	0
0	0	0.566	1	−0.4	−0.4	0	0	0	1	0	0
0	−0.566	0	−0.4	1	0.4	0	0	0	0	1	0
−0.566	0	0	−0.4	0.4	1	0	0	0	0	0	1

where $f_u(x) = \sqrt{2}\cos(u\pi(x+0.5)/5)$ for $u = 1, 2$, $x_1, x_2, x_3 \in Z_5$ are levels for the three factors, β_0, β_j, β_{jj}, and β_{jk} are the intercept, linear, quadratic and bilinear terms, respectively, and $\varepsilon \sim N(0, \sigma^2)$. Since both designs have $\gamma_1 = \gamma_2 = \gamma_3 = 0$, the intercept and all of the linear terms can be estimated independently. For either design, let M denote the model matrix corresponding to the 3 quadratic and 3 bilinear terms: β_{11}, β_{22}, β_{33}, β_{12}, β_{13} and β_{23}. Table 4 shows the information matrix $M'M/25$ for both designs. The covariance matrix of the estimates of parameters for these terms is $\sigma^2(M'M)^{-1}$. For each quadratic term (β_{11}, β_{22} and β_{33}), the variance of the estimate is $0.0734\sigma^2$ for $\tilde{D}$ vs. $0.04\sigma^2$ for $\varphi(D)$, and for each bilinear term (β_{12}, β_{13} and β_{23}), the variance of the estimate is $0.1042\sigma^2$ for $\tilde{D}$ vs. $0.04\sigma^2$ for $\varphi(D)$. The estimates are correlated for $\tilde{D}$ while they are uncorrelated for $\varphi(D)$. The orthogonality of $\varphi(D)$ greatly improves the accuracy of the estimates. In addition, the above discussion on second-order models assumes that all third- or higher-order terms are negligible. It is possible, however, that some third-order terms are not negligible. Design $\varphi(D)$ ensures that all of the estimates for the model are not contaminated by nonnegligible third-order terms (as $\gamma_5(\varphi(D)) = 0$), so the estimates are robust against model uncertainty.

Now consider fitting data with a traditional second-order polynomial model by replacing $f_1(x)$ and $f_2(x)$ in (7) with $p_1(x) = \sqrt{2}(x-2)/2$ and $p_2(x) = \sqrt{5/14}((x-2)^2-2)$. The intercept and all of the linear terms can also be estimated independently. Still let M be the model matrix corresponding to the 3 quadratic and 3 bilinear terms. The information matrices for the designs $\tilde{D}$ and $\varphi(D)$ are shown in Table 5. It is easy to verify that for each quadratic term, the variance of the estimate is $0.0583\sigma^2$ for $\tilde{D}$ vs. $0.0404\sigma^2$ for $\varphi(D)$, and for each bilinear term, the variance of the estimate is $0.0803\sigma^2$ for $\tilde{D}$ vs. $0.0409\sigma^2$ for $\varphi(D)$. Furthermore, the correlations between the estimates are smaller for $\varphi(D)$ than $\tilde{D}$. Therefore, $\varphi(D)$ is also better than $\tilde{D}$ for fitting a polynomial model, although $\varphi(D)$ is constructed for the cosine model in (7).

The good performance of $\varphi(D)$ for polynomial models does not occur by chance. In fact, the relationship between the cosine and polynomial models is highlighted by the inner products

$$\int_{-0.5}^{q-0.5} -p_1(x)f_1(x)dx = 0.993\left\{\int_{-0.5}^{q-0.5} p_1(x)^2dx\right\}^{\frac{1}{2}}\left\{\int_{-0.5}^{q-0.5} f_1(x)^2dx\right\}^{\frac{1}{2}},$$

Table 5 Information matrices $M'M/25$ for $\tilde{D}$ and $\varphi(D)$ under a second-order polynomial model

$\tilde{D}$						$\varphi(D)$					
1	0	0	0	0	−0.478	1	0	0	0	0	0.096
0	1	0	0	−0.478	0	0	1	0	0	0.096	0
0	0	1	0.478	0	0	0	0	1	−0.096	0	0
0	0	0.478	1	−0.4	−0.4	0	0	−0.096	1	0.08	0.08
0	−0.478	0	−0.4	1	0.4	0	0.096	0	0.08	1	−0.08
−0.478	0	0	−0.4	0.4	1	0.096	0	0	0.08	−0.08	1

$$\int_{-0.5}^{q-0.5} p_2(x) f_2(x) dx = 0.961 \left\{ \int_{-0.5}^{q-0.5} p_2(x)^2 dx \right\}^{\frac{1}{2}} \left\{ \int_{-0.5}^{q-0.5} f_2(x)^2 dx \right\}^{\frac{1}{2}},$$

for general orthonormal polynomials $p_1(x) = c_1[x-(q-1)/2]$ and $p_2(x) = c_2[(x-(q-1)/2)^2-(q^2-1)/12]$, where c_1 and c_2 are constants, and $f_u(x) = \sqrt{2}\cos(u\pi(x+0.5)/q)$ for $u = 1, 2$. The integral interval is set to $(-0.5, q-0.5)$ because it covers the set $Z_q = \{0, \ldots, q-1\}$ and takes $(q-1)/2$ as the middle point. The above equations indicate that the leading terms of cosine and polynomial models are very close. This consistency brings about the general good performance of the constructed designs in this paper for polynomial models.

7 Concluding remarks

In this paper, we study the choice of fractional factorial designs for Fourier-cosine models and propose the γ-resolution. We provide a nonlinear level permutation and obtain a series of theoretical results for constructing high γ-resolution design via permuting levels for regular designs. Using the theory, we further provide highly efficient methods for constructing designs without any computer search. The construction methods are simple but provide much better designs than available ones for Fourier-cosine modeling. In addition, the obtained designs also perform well for fitting polynomial models.

The present work leads to an open issue which concerns a comprehensive study of nonregular designs with the maximum γ-resolution. While this is likely to be very hard in general, one may consider some nonlinear permutations like φ on regular designs and develop theories for these resulting designs. Any future work about this issue will be illuminating.

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Declaration

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

Appendix: Proofs

Proof of Lemma 1 The result is obvious by noting that

$$\sum_{i=1}^{N} \prod_{j=1}^{m} \cos(u_j\pi(x_{ij}+0.5)/q) = \prod_{j=1}^{m} \left\{ \sum_{i=1}^{N} \cos(u_j\pi(x_{ij}+0.5)/q) \right\} = 0$$

for $\|u\|_1 \leq t$ if $D = (x_{ij})$ is an OA of strength t. □

Proof of Theorem 1 Suppose D is a principal fraction defined in (1) with $b_1 = \cdots = b_p = 0$. It is obvious that for any point $x = (x_1, \ldots, x_m) \in D$, $q - x_{m-p+i} = c_{i1}(q - x_1) + \cdots + c_{i,m-p}(q - x_{m-p}) \pmod q$ for $i = 1, \ldots, p$, thus $q - x \in D$. Therefore, $qJ - D$ is the same design as D.

From (5), we know that $\varphi(D) = (q-1)J - \varphi(qJ - D)$, then $\varphi(D)$ and $(q-1)J - \varphi(D)$ are the same design, that is, $\varphi(D)$ is mirror-symmetric. □

Proof of Theorem 2 Let $f_0(x) = 1$ and $f_u(x) = \sqrt{2}\cos(u\pi(x + 0.5)/q)$ for $u = 1, \ldots, q-1$, then $\{f_0(x), f_1(x), \ldots, f_{q-1}(x)\}$ forms a set of orthonormal contrasts

$$\sum_{x \in Z_q} f_u(x) f_v(x) = \begin{cases} 0, \text{ if } u \neq v; \\ q, \text{ if } u = v, \end{cases}$$

and

$$f_u(q-1-x) = \begin{cases} -f_u(x), & \text{if } u \text{ odd}; \\ f_u(x), & \text{if } u \text{ even}. \end{cases}$$

The proof of Theorem 2 is similar to the proof of Theorem 2 of Tang and Xu (2014). □

To prove Theorem 3, we need some notation and the following Lemma 2. For a regular design D defined in (1), each word $u = (u_1, \ldots, u_m) \in L$ corresponds to a number in Z_q, denoted by b_u, such that $u_1x_1 + \cdots + u_mx_m + b_u = 0$. For example, suppose D is a regular 5^{3-1} design with $x_3 = x_1 + x_2 + 1$, then $u = (1, 1, 4)$ is a word and $b_u = 1$ because $x_1 + x_2 + 4x_3 + 1 = 0$. For $d = 1, \ldots, m$, let H_d be a subset of L containing all words u of length d with $u_j = 0, 1,$ or $q-1$ for $j = 1, \ldots, m$, W_d a subset of L containing all words u of length d with exactly one $j_0 \in \{1, \ldots, m\}$ such that $u_{j_0} = 2$ or $q-2$, and $u_j = 0, 1$ or $q-1$ for all $j \neq j_0$, $j = 1, \ldots, m$. For any $b \in Z_q$, let $N_{d,b}$ and $M_{d,b}$ be the number of words u in H_d and W_d respectively such that $u_1x_1 + \cdots + u_mx_m + b = 0$. For $b = 1, \ldots, q-1$, if $b_u = b$ then $b_{q-u} = q - b$, thus $N_{d,b} = N_{d,q-b}$ and $M_{d,b} = M_{d,q-b}$. Note that N_d and M_d are the number of words in H_d and W_d, respectively, so that $\sum_{b=0}^{q-1} N_{d,b} = N_d$ and $\sum_{b=0}^{q-1} M_{d,b} = M_d$.

Lemma 2 *Let q be an odd prime and D be a regular q^{m-p} design defined in (1) with strength t.*

(i) *If t is even, then*

$$\gamma_{t+1}(\varphi(D)) = 2^{-(t-1)} \sum_{b=1}^{(q-1)/2} N_{t+1,b} \sin^2(2\pi b/q), \text{ and}$$
$$\gamma_{t+2}(\varphi(D)) = 2^{-(t+1)} N_{t+2,0} + 2^{-t} M_{t+1,0} + 2^{-t} \sum_{b=1}^{(q-1)/2} (N_{t+2,b} + 2M_{t+1,b}) \cos^2(2\pi b/q).$$

(ii) *If t is odd, then*

$$\gamma_{t+1}(\varphi(D)) = 2^{-t} N_{t+1,0} + 2^{-(t-1)} \sum_{b=1}^{(q-1)/2} N_{t+1,b} \cos^2(2\pi b/q), \text{ and}$$

$$\gamma_{t+2}(\varphi(D)) = 2^{-t} \sum_{b=1}^{(q-1)/2} (N_{t+2,b} + 2M_{t+1,b}) \sin^2(2\pi b/q).$$

Proof of Lemma 2 From (4), it is easy to see that for $u = 1, \ldots, q-1$,

$$\cos(u\pi(\varphi(x) + 0.5)/q) = \begin{cases} (-1)^{(u+1)/2} \sin(2\pi ux/q), & \text{for odd } u; \\ (-1)^{u/2} \cos(2\pi ux/q), & \text{for even } u. \end{cases}$$

Denote $t_u(x) = \sqrt{2}\sin(2\pi ux/q)$ for odd u, $t_u(x) = \sqrt{2}\cos(2\pi ux/q)$ for even positive u, and $t_0(x) = 1$, then we have

$$\gamma_k(\varphi(D)) = N^{-2} \sum_{\|u\|_1=k} \left| \sum_{i=1}^{N} \prod_{j=1}^{m} t_{u_j}(x_{ij}) \right|^2 \text{ for } k = 1, \ldots, K. \tag{8}$$

Denote $D = (x_{kj})$ and $e_u(x) = \exp(i\theta ux)$ where $\theta = 2\pi/q$. For odd u, $t_u(x) = \sqrt{2}\sin(\theta ux) = \sqrt{2}(e_u(x) - e_{q-u}(x))/2i$; for even $u > 0$, $t_u(x) = \sqrt{2}\cos(\theta ux) = \sqrt{2}(e_u(x) + e_{q-u}(x))/2$. Since D is a regular design, if $u = (u_1, \ldots, u_m)$ is a word, $\sum_{k=1}^{N} \prod_{j=1}^{m} e_{u_j}(x_{kj}) = N\exp(-i\theta b_u)$; otherwise, $\sum_{k=1}^{N} \prod_{j=1}^{m} e_{u_j}(x_{kj}) = 0$. Since D has strength t, then for any $l \le t$, $0 \le j_1 < \cdots < j_l \le m$ and $u_1, \ldots, u_l \in Z_q$, $\sum_{k=1}^{N} t_{u_1}(x_{kj_1}) \cdots t_{u_l}(x_{kj_l}) = 0$. From (8),

$$\begin{aligned} \gamma_{t+1}(\varphi(D)) &= N^{-2} \sum_{\|u\|_1=t+1} \left| \sum_{k=1}^{N} \prod_{j=1}^{m} t_{u_j}(x_{kj}) \right|^2 \\ &= N^{-2} \sum_{1 \le j_1 < \cdots < j_{t+1} \le m} \left| \sum_{k=1}^{N} t_1(x_{kj_1}) \cdots t_1(x_{kj_{t+1}}) \right|^2 \\ &= N^{-2} 2^{-(t+1)} \sum_{1 \le j_1 < \cdots < j_{t+1} \le m} \left| \sum_{u \in H_{t+1}^{j_1 \cdots j_{t+1}}} \sum_{k=1}^{N} (-1)^{\zeta(u)} \prod_{j=1}^{m} e_{u_j}(x_{kj}) \right|^2 \end{aligned} \tag{9}$$

where $\zeta(u)$ is the number of elements of $u = (u_1, \ldots, u_m)$ satisfying $u_j = q-1$ for $j = 1, \ldots, m$, and for given $1 \le j_1 < \cdots < j_{t+1} \le m$, $H_{t+1}^{j_1 \cdots j_{t+1}} = \{u = (u_1, \ldots, u_m) \in H_{t+1} : u_j = 0 \text{ for } j \ne j_1, \ldots, j_{t+1}\}$. For any $1 \le j_1 < \cdots < j_{t+1} \le m$, we conclude that $H_{t+1}^{j_1 \cdots j_{t+1}}$ contains exactly two words, denoted by v and

$(q-1)v$. Otherwise, suppose $u \in H_{t+1}^{j_1\cdots j_{t+1}}$, $u \neq v$ or $(q-1)v$, then $v+u$ is a word and $0 < \|v+u\|_0 \leq t$, which contradicts with the fact that the strength of D is t. Note that $b_{(q-1)v} = q - b_v$ and $\zeta(v) + \zeta((q-1)v) = t+1$. Thus

$$\left|\sum_{u\in H_{t+1}^{j_1\cdots j_{t+1}}}\sum_{k=1}^{N}(-1)^{\zeta(u)}\prod_{j=1}^{m}e_{u_j}(x_{kj})\right| = \begin{cases} N\left|\exp(i\theta b_v) - \exp(-i\theta b_v)\right|, & \text{if } t \text{ is even;}\\ N\left|\exp(i\theta b_v) + \exp(-i\theta b_v)\right|, & \text{if } t \text{ is odd.}\end{cases}$$
$$= \begin{cases} 2N\left|\sin(\theta b_v)\right|, & \text{if } t \text{ is even;}\\ 2N\left|\cos(\theta b_v)\right|, & \text{if } t \text{ is odd.}\end{cases}$$

There are $N_{t+1,0}/2$ choices of $j_1, \ldots, j_{t+1}$ such that $b_v = 0$, and $N_{t+1,b}$ choices of $j_1, \ldots, j_{t+1}$ for $b_v = 1, \ldots, q-1$. Then from (9), if t is even, $\gamma_{t+1}(\varphi(D)) = 2^{-(t-1)}\sum_{b=1}^{(q-1)/2} N_{t+1,b}\sin^2(2\pi b/q)$, and if t is odd, $\gamma_{t+1}(\varphi(D)) = 2^{-t}N_{t+1,0} + 2^{-(t-1)}\sum_{b=1}^{(q-1)/2} N_{t+1,b}\cos^2(2\pi b/q)$.

Now consider $\gamma_{t+2}(\varphi(D))$. From (8) and also because D has strength t, we have $\gamma_{t+2}(\varphi(D)) = N^{-2}\sum_{\|u\|_1=t+2}|\sum_{i=1}^{N}\prod_{j=1}^{m}t_{u_j}(x_{ij})|^2 = E_1 + E_2$, where

$$E_1 = N^{-2}\sum_{1\leq j_1<\cdots<j_{t+2}\leq m}\left|\sum_{k=1}^{N}t_1(x_{kj_1})\cdots t_1(x_{kj_{t+2}})\right|^2, \text{ and}$$

$$E_2 = N^{-2}\sum_{1\leq j_1<\cdots<j_t\leq m}\ \sum_{j_{t+1}\neq j_1,\ldots,j_t}\left|\sum_{k=1}^{N}t_1(x_{kj_1})\cdots t_1(x_{kj_t})t_2(x_{kj_{t+1}})\right|^2.$$

Similar to the discussion for $\gamma_{t+1}(\varphi(D))$, for E_1, we have

$$E_1 = \begin{cases} 2^{-(t+1)}N_{t+2,0} + 2^{-t}\sum_{k=1}^{(q-1)/2} N_{t+2,k}\cos^2(2\pi k/q), & \text{if } t \text{ is even;}\\ 2^{-t}\sum_{k=1}^{(q-1)/2} N_{t+2,k}\sin^2(2\pi k/q), & \text{if } t \text{ is odd.}\end{cases}$$

For E_2, we have

$$E_2 = N^{-2}2^{-(t+1)}\sum_{1\leq j_1<\cdots<j_t\leq m}\ \sum_{j_{t+1}\neq j_1,\ldots,j_t}\left|\sum_{u\in W_{t+1}^{j_1\cdots j_{t+1}}}\sum_{k=1}^{N}(-1)^{\zeta(u)}\prod_{j=1}^{m}e_{u_j}(x_{kj})\right|^2, \tag{10}$$

where $W_{t+1}^{j_1\cdots j_{t+1}} = \{u = (u_1, \ldots, u_m) \in W_{t+1} : u_{j_{t+1}} = 2 \text{ or } q-2, u_j = 0 \text{ for } j \neq j_1, \ldots, j_{t+1}\}$. We can also conclude that $W_{t+1}^{j_1\cdots j_{t+1}}$ contains exactly two words, denoted by w and $(q-1)w$. Otherwise, there will be a word of length less than $t+1$. Note that $\zeta(w) + \zeta((q-1)w) = t$. We have

$$\left| \sum_{u \in W_{t+1}^{j_1 \cdots j_{t+1}}} \sum_{k=1}^{N} (-1)^{\zeta(u)} \prod_{j=1}^{m} e_{u_j}(x_{kj}) \right| = \begin{cases} 2N \left|\cos(\theta b_w)\right|, & \text{if } t \text{ is even;} \\ 2N \left|\sin(\theta b_w)\right|, & \text{if } t \text{ is odd.} \end{cases}$$

Then from (10),

$$E_2 = \begin{cases} 2^{-t} M_{t+1,0} + 2^{-(t-1)} \sum_{b=1}^{(q-1)/2} M_{t+1,b} \cos^2(2\pi b/q), & \text{if } t \text{ is even;} \\ 2^{-(t-1)} \sum_{b=1}^{(q-1)/2} M_{t+1,b} \sin^2(2\pi b/q), & \text{if } t \text{ is odd.} \end{cases}$$

This completes the proof of Lemma 2. □

Proof of Theorem 3 (i) If t is even, $t+1$ is odd. By Theorems 1 and 2, $\gamma_{t+1}(\varphi(D)) = 0$. Further, if $\gamma_{t+2}(\varphi(D_1)) = 0$, then by Lemma 2, D_1 has $N_{t+2,b} = M_{t+1,b} = 0$ for $b = 0, \ldots, q-1$ so $N_{t+2} = M_{t+1} = 0$. Note that D_1 and D have the same N_{t+2} and M_{t+1}, so D also has $N_{t+2} = M_{t+1} = 0$. Therefore, D also has $N_{t+2,b} = M_{t+1,b} = 0$ for $b = 0, \ldots, q-1$. By Lemma 2, $\gamma_{t+2}(\varphi(D)) = 0$.

(ii) The proof is similar to part (i) and omitted.

□

Proof of Theorem 4 By Theorems 1 and 2, $\gamma_{t+1}(\varphi(D)) = 0$ if t is even and $\gamma_{t+2}(\varphi(D)) = 0$ if t is odd. For a principal fraction D_0, $b_u = 0$ for all $u \in L$ where L is the defining contrast subgroup of D_0. So for $d = 1, \ldots, m$, $N_{d,b} = M_{d,b} = 0$ for $b \neq 0$, $N_{d,0} = N_d$ and $M_{d,0} = M_d$. Then Theorem 4 follows from Lemma 2. □

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