Spectrum constructing with nonuniform samples using least-squares approximation by cosine polynomials

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The least-squares approximation of cosine polynomials is used to construct the spectrum from the simulated nonuniform samples of the interferogram given by a step-mirror-based static Fourier transform spectrometer. Numerical and experimental results show the stability of the algorithm and a spectrum-constructing error of 0.03%. © 2011 Optical Society of America

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1. Introduction

Nowadays spectrometers are wildly used in fields such as chemical analysis and environmental monitoring. Among various kinds of spectrometers, the Fourier transform spectrometer (FTS) is usually favored due to its high luminous flux and multichannel transmission. Today most of the industrialized FTSs are based on the classical Michelson interferometer. With a moving plane mirror, these FTSs sample the interferogram of the two incident beams at different optical path differences (OPDs), then the spectrum is achieved via Fourier transform. However, Fourier transform requires sampling at exactly equal intervals, and the obtained spectrum is crucially sensitive to the sampling errors. It has been presented in [1] that the theoretical maximum signal-to-noise ratio (SNR) relates to the sampling errors:

$$\mathrm{SNR}_{\max} = \frac{4}{\Delta x \tilde{v}_{\max}}, \tag{1}$$

where Δx is the RMS sampling error, $\tilde{v}_{\max}$ is the maximum wavenumber of the source. This means Δx should be less than 10 nm to achieve an SNR higher than 1000 when $\tilde{v}_{\max} = 4000\,\mathrm{cm}^{-1}$. Although this requirement can be easily met by laser referencing, in recent years, to meet the growing need for real-time and small-platform spectrum detection, many miniaturized FTSs without the laser referencing system have been studied [2–4]. For these time-modulated FTSs, movement precision and system stability are still big problems.

This problem can be solved by static FTSs. Until now, many space-modulated static FTSs have been proposed [5,6]. A step-mirror-based model was given by Moller [7] and later studied by some institutions including us [8–11]. This kind of FTS promises a stabile and portable instrument concept without a complex driving system. However, in practice, the manufacturing accuracy of the step heights requires sampling the interferogram with nonunique intervals.

A nonuniform sampling problem of the band-limited signals exists in many fields, such as astronomy, geography, and medical imaging areas. To deal with the nonuniform samples people usually refer to the approximation theory: use polynomials to approximate the unknown functions at the sampled points, thus achieving the "right" values at the

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desired positions. Most of the proposed approximation algorithms include two parts: the reconstruction of the signals and the resampling process. As to the reconstruction algorithms, there are iterative algorithms [12–14] and noniterative methods [15,16]. See [17,18] for more references on approximation theories and their applications.

In this paper, considering the interferogram is a periodic band-limited signal, we will show that using least-squares approximation by cosine polynomials, the spectrum can be directly constructed from the nonuniform sampled interferogram without the reconstruction and the resampling process.

In Section 2 we briefly introduce the principle of the step-mirror-based static FTS. Section 3 gives the algorithm of spectrum constructing with nonuniform sampled values using trigonometric polynomials. In Section 4 the numerical and experimental results are presented to show the stability and performance of the algorithm in our present designed FTS.

2. Principle of the Static FTS

Figure 1 shows the simplified configuration of the static FTS. The FTS is based on Michelson's interferometer with flat mirrors replaced by step mirrors. The two step mirrors each consisting of n steps are crossed to generate the interferometric samples of different OPDs. The total height of the steps of the lower one is equal to one step height of the higher one. Thus, the system gives $n \times n$ samples with a uniform sampling interval two times the lower step height. The spectrum can be obtained via Fourier transform with the sampled signal values.

Configuration parameters are designed thus: the spectra wavelength range is 3.7–5 μm (wavenumber 2000–2700 cm^{-1}), the lower step height is 0.625 μm, the higher step height is 20 μm. The problem is, the high accuracy requirement of the step height indicated by Eq. (1) is hard to suit. At present the standard deviation of the step heights can be controlled around 0.1 μm for the lower step mirror, and 0.4 μm for the higher step mirror. According to Eq. (1), a

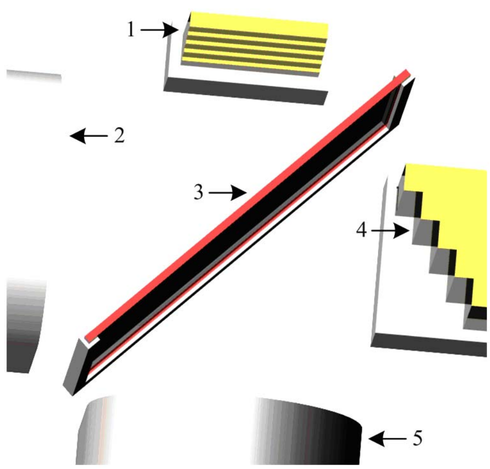

Fig. 1. (Color online) Simplified configuration of the static FTS. 1. lower step mirror; 2. collimator; 3. beam splitter (50% transmission, 50% reflection); 4. higher step mirror; 5. detecting system.

theoretically best SNR as low as 18 is predicted if Fourier transform is directly performed. Since the step heights can be accurately measured, the step height error can be partly made up by the least-squares approximation of trigonometric polynomials.

3. Theory

A. Spectrum Constructing with Least-Squares Approximation of Trigonometric Polynomials

Begin with considering the well-known least-squares approximation of a function known only at discrete data points. Assume $f(x) \in C[a,b]$, given a sampled nonuniform data series $\{y_i = f(x_i), i = 0, 1, \ldots n\}$ of $f(x)$, and $\varphi_0(x), \varphi_1(x), \ldots \varphi_m(x) \in C[a,b]$, find a $S^*(x)$ in $\varphi = \mathrm{span}\{\varphi_0(x), \varphi_1(x), \ldots \varphi_m(x)\}$, to minimize the discrete least-squares error

$$\| \to \delta \|_2^2 = \sum_{i=0}^{n} \delta_i^2 = \sum_{i=0}^{n} [S^*(x_i) - y_i]^2$$
$$= \min_{S(x)\in\varphi} \sum_{i=0}^{n} [S(x_i) - y_i]^2, \tag{2}$$

where

$$S(x) = a_0\varphi_0(x) + a_1\varphi_1(x) + \ldots + a_m\varphi_m(x) \quad (m < n).$$

Write

$$A = (a_0, a_1, \ldots a_m)^T, \tag{3}$$

$$Y = (y_0, y_1, \ldots y_n)^T, \tag{4}$$

$$\Phi_k = (\varphi_k(x_0), \varphi_k(x_2), \ldots \varphi_k(x_n))^T, \tag{5}$$

$$G = (\Phi_0, \Phi_1, \ldots \Phi_m). \tag{6}$$

One can obtain the coefficients $a_0, a_1, \ldots a_m$ by solving the normal equation

$$G^H G A = G^H Y, \tag{7}$$

where the matrix $G^H G$ is a Toeplitz matrix T with entries $T_{jk} = \Phi_{j-1}^H \Phi_{k-1}$.

The ideal interferometric function (AC components) of a source spectrally band-limited to $[\sigma_{\min}, \sigma_{\max}]$ is

$$I(\mathrm{OPD}) = \int_{\sigma_{\min}}^{\sigma_{\max}} 2I(\sigma)\cos(2\pi\sigma\mathrm{OPD})\mathrm{d}\sigma, \tag{8}$$

where σ is the wavenumber. In practice, the interferogram is sampled within a maximum OPD, and $I(\mathrm{OPD})$ is treated as a periodic function with period $2\mathrm{OPD}_{\max}$. Since $I(\mathrm{OPD})$ is a periodic band-limited function, in theory it can be approximated by the finite-dimensional trigonometric polynomials.

We will show that the discrete Fourier transform is in fact a special case of Eq. (7) when one approximate the $I(\mathrm{OPD})$ by trigonometric polynomials and requires uniform sampling both in the time domain and the frequency domain.

Rescale and expand $I(\mathrm{OPD})$ across the boundaries into a periodic function with period 2π. Sample $I(\mathrm{OPD})$ in $[0, 2\pi]$ for N samples at

$$x_j = \frac{2\pi}{N} j \quad (j = 0, 1, \cdots N-1), \tag{9}$$

and choose

$$\Phi_k = (\exp(ikx_0), \exp(ikx_1), \ldots \exp(ikx_{N-1}))^T, \quad (k = 0, 1, \cdots N-1). \tag{10}$$

Obviously Φ_k are orthogonal with each other and T is a $N \times N$ matrix with entries

$$T_{jk} = \begin{cases} 0, j \neq k \\ N, j = k \end{cases}. \tag{11}$$

In this situation Eq. (7) describes the Fourier transform, which gives the least-squares solution with regularly sampled signals. The least-squares solution is the so called "spectrum".

However, in a nonuniform sampling situation, $x_j \neq \frac{2\pi}{N} j$, and the Fourier transform loses its precondition. But, theoretically, as long as the sampling locations are exactly known, Eq. (7) works. Thus, one can still obtain the least-squares solution by solving Eq. (7). What should be noticed is: since for nonuniform sampling Φ_k described by Eq. (10) are no longer orthogonal with each other, the least-squares solution does not gives the spectrum, indicating a difference from the real spectrum that we call the "spectrum-constructing error (SCE)". We will show in Section 4 that this constructing error is acceptably small when the cosine-type polynomials are used to approximate the interferogram.

Note: Eq. (7) can also be given as a result of the iterative algorithm (see [12,14]). The least-squares approximation by trigonometric polynomials has long been studied and used as a signal reconstruction method (see [18] for reference). Reference [18] also provides another noniterative least-squares approximation by solving a Vandermonde-type system and comparing between the two methods. The Toeplitz type is preferred here as it has the same form of the Fourier transform when it comes to uniform sampling.

B. Problems in Applying the Least-Squares Approximation

The following problems are concerned most in performing the spectrum constructing by solving the normal equation:

1. Can $I(\mathrm{OPD})$ be uniquely determined by its nonuniform samples?
2. If $I(\mathrm{OPD})$ can be uniquely determined, is the Toeplitz matrix T invertible, thus the solution of Eq. (7) exist?
3. Stability of the algorithm
4. Operational requirements of the algorithm

Problem 1. It has been proved in [19] that a band-limited signal is uniquely determined by its nonuniform samples as long as the average sampling rate exceeds the Nyquist rate. This requirement can be well suited as our average sampling interval is $1.25\,\mu$m compared with the Nyquist interval $1.85\,\mu$m.

Problem 2. Reference [18] proves T is invertible if and only if the number of sampling points is greater than the dimension of the space. This can be suited by controlling the dimension of the trigonometric polynomials.

Problem 3. For the stability of the algorithm, we refer to the condition number of T. The condition number measures the sensitivity of the solution of a system of linear equations to the errors or noises in the data. For a linear system $AX = B$, assume A is accurate, B has errors (or noises) δb, bringing a corresponding error δx in the solution X. Then the error estimates are

$$\frac{\|\delta x\|}{\|X\|} \leq c \frac{\|\delta b\|}{\|B\|}, \tag{12}$$

where c is the condition number of the matrix A. In practice, even if T is invertible and ensures a solution, the inversion problem usually requires large order of the trigonometric polynomials and a large condition number may appear, indicating a solution very sensitive to the changing of the input signal values.

Giving an accurate theory to describe the relationship between the sampling methods and the condition numbers is a hard task. Until now, there have only been reports on estimating the condition number of T under particular assumptions. In [12] H. G. Feichtinger *et al.* give an estimate of the condition number assuming that the maximal sampling interval is no larger than the Nyquist interval. They mention an adaptive weights method to improve the condition number under this condition. In [20] the condition number is estimated for a totally random sampled data that is uniformly distributed over the sampling span. Both of the two studies pointed out that a higher oversampling rate improves the condition number.

Unfortunately, none of the mentioned situations suits our sampling process. In Section 4, we will show that our maximum sampling interval is much larger than the Nyquist interval. Also, our sampling points are not truly random distributed but a uniform sampling set with perturbations. A statistical result on the condition numbers under our present sampling method will be given in Section 4.

Problem 4. In $G^H G A = G^H Y$:

1. $G^H G$ is independent of the sampled signals. After the system is assembled, $G^H G$ need to be calculated only once and stored for further use
2. $G^H Y$ can be calculated with the nonuniform fast Fourier transform (NUFFT) algorithm developed by Q. H. Liu *et al.* [21], which requires $O(\alpha N \log_2(\alpha N))$, where $\alpha \geq 2$ is the oversampling factor.
3. There are already Toeplitz solvers that can solve the normal equation with $O(M \log_2 M)$ operations, where M is the size of the Toeplitz matrix.

4. Numerical and Experimental Result

A. Stability and the SCE of the Algorithm

The stability and the SCE will be given by simulation and numerical test.

Assume the step heights error obeys the normal distribution. At present the standard deviation σ is around $0.1\,\mu$m for the lower step mirror, and $0.4\,\mu$m for the higher step mirror. Generating a pair of arrays of 31 random numbers obeying the normal distribution with corresponding mean values of $20\,\mu$m, $0.625\,\mu$m, and standard deviations of $0.4\,\mu$m, $0.1\,\mu$m, we can simulate a pair of step mirrors and test the spectrum-constructing algorithm with them.

In practice, the phase correction requires a short double-sided sampling of the interferogram from $\mathrm{OPD} = -\Delta$ to $\mathrm{OPD} = \Delta$. Thus, totally 1024 points of different OPDs are sampled, in which 128 points between $[-\Delta, 0]$ and 897 points between $[0, \mathrm{OPD}_{\max}]$. For the benefit of discussion, we assume there is no phase effect and use the large single-sided 897 points to generate a double-sided interferogram of 1793 sampling points. By zeros-filling, the samples of the interferogram are expanded to 2048 points with the maximum $\mathrm{OPD} = 1.25 \times 1024 = 1280\,\mu$m. A source of continuous spectrum band-limited to 2000–2700 cm^{-1} is chosen as the testing source.

To be consistent with the discrete Fourier transform in the frequency domain, considering the interferogram is band-limited to 2000–2700 cm^{-1},

$$\Phi_k = \left(\exp\left(ik\frac{2\pi}{2048}\frac{x_0}{1.25}\right), \exp\left(ik\frac{2\pi}{2048}\frac{x_1}{1.25}\right), \ldots \exp\left(ik\frac{2\pi}{2048}\frac{x_{2047}}{1.25}\right)\right)^T$$
$$(k = 500, 501, \cdots, 700, 1348, \cdots, 1547, 1548) \quad (13)$$

is chosen to cover a wavenumber band 1950–2730 cm^{-1}.

Repeat the step-mirror-generating and spectrum-constructing process for 2000 times, we obtain a statistical result.

Two parameters are calculated:

1. The condition number of the matrix T. ($T \geq 1$, smaller T, better stability.) The result is given in Fig. 2, having a maximum value of 2.57, a minimum of 1.32, and an average of 1.64
2. The SCE

$$\mathrm{SCE} = \frac{\sum_{k=0}^{n} |I_{\mathrm{real}}(k) - I_{\mathrm{ideal}}(k)|}{\sum_{k=0}^{n} I_{\mathrm{ideal}}(k)}, \quad (14)$$

where $I_{\mathrm{real}}(k)$ is the constructed spectrum from nonuniform samples via the tested constructing method, $I_{\mathrm{ideal}}(k)$ is the constructed spectrum from uniform samples via the traditional fast Fourier transform (FFT) method. The result is given in Fig. 3, having a maximum value of 41%, a minimum of 1.89%, and an average of 9.93%.

Judging from the condition number, the algorithm is stable enough (insensitive to the errors and noises of the samples). However, when it comes to the SCE, the average 9.93% indicates a 9.93% constructing error. The standard deviations of 0.4 and $0.1\,\mu$m of the higher step heights and the lower step heights give statically 1% of the sampling intervals larger than the Nyquist interval and 0.1% percent two times larger than the Nyquist interval. It seems under this sampling situation the algorithm failed to offer an acceptable SCE. Since the approximation quality by polynomials is closely related to the form of the polynomials chosen, we decide to add more restrictions on the approximation polynomials to provide

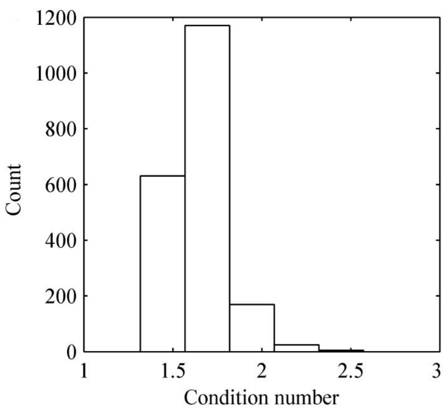

Fig. 2. Distribution of the 2000 condition numbers.

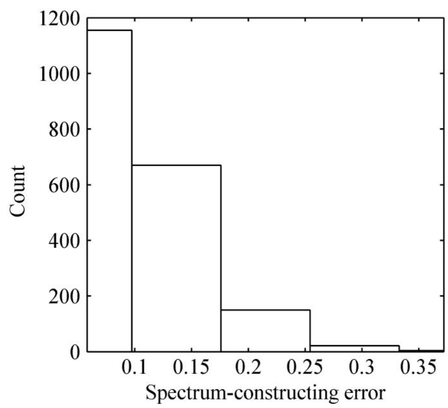

Fig. 3. Distribution of the 2000 SCEs.

the normal equation Eq. (7) with more information about the spectrum. Considering Eq. (8),

$$\Phi_k = \left(\cos\left(k\frac{2\pi}{2048}\frac{x_0}{1.25}\right),\right.$$
$$\left.\cos\left(k\frac{2\pi}{2048}\frac{x_1}{1.25}\right), \ldots \cos\left(ik\frac{2\pi}{2048}\frac{x_{2047}}{1.25}\right)\right)^T$$
$$(k = 500, 501, \cdots, 700) \qquad (15)$$

is chosen. That is, using the cosine polynomials to approximate the interferogram.

However, a practical interferogram always contains phase errors. This problem should be considered when using cosine polynomials. An obvious advantage of the algorithm above is that it allows adding phase information into the polynomials, such as

$$\Phi_k = \left(\cos\left(k\frac{2\pi}{2048}\frac{x_0}{1.25} + \varphi(k)\right),\right.$$
$$\left.\cos\left(k\frac{2\pi}{2048}\frac{x_1}{1.25} + \varphi(k)\right), \ldots\right)^T, \qquad (16)$$

when considering a wavenumber-related phase error $\varphi(k)$. This allows us to correct the phase directly in the spectrum constructing process. Thus, it is possible to use the cosine polynomials to approximate a practical interferogram with phase error as long as the error is known.

For the step-mirror-based spectrometer, once the system is assembled, the phase error is fixed. Thus, the phase error measuring process needs to be done only once. For this we refer to the signal reconstruction method mentioned in [16]. This method allows obtaining the uniform sampled signals if the average sampling interval is smaller than the Nyquist interval, which is proved to be available by numerical results. Thus, one can measure the phase error using the traditional phase correction method.

Results when cosine polynomials are used are as follows: The condition number of the matrix T is given in Fig. 4, having a maximum value of 2.68, a minimum of 1.39, and an average of 1.78. The SCE is given in Fig. 5, having a maximum value of 0.023%, a minimum of 0.0028%, and an average of 0.01%

Although the condition number is not improved, the SCE is much smaller than pervious, giving an acceptable average error 0.01%.

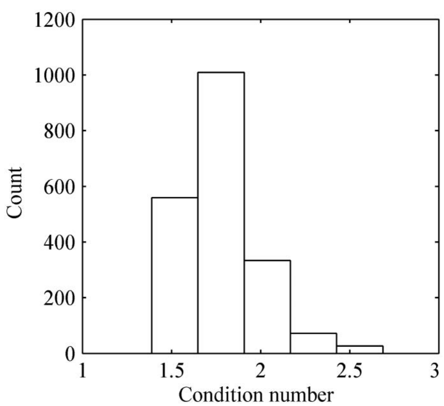

Fig. 4. Distribution of the 2000 condition numbers when cosine polynomials are used.

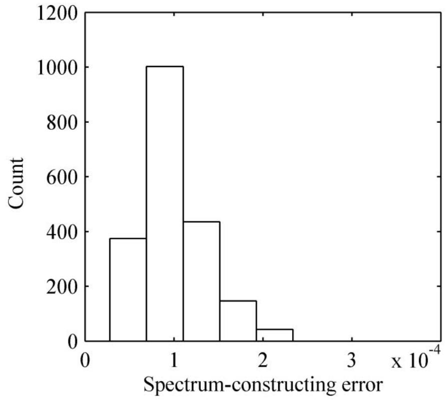

Fig. 5. Distribution of the 2000 SCEs when cosine polynomials are used.

B. Experimental Result

Figures 6 and 7 shows the steps of a higher and a lower step mirror manufactured. Heights testing details are given in Table 1.

The heights test gives a maximum sampling interval of 5.002 μm, a minimum of 0.584 μm, and an average of 1.291 μm. Twenty-seven intervals are larger than the Nyquist interval, in which eight are two times larger than the Nyquist interval.


Fig. 6. (Color online) Steps of a higher step mirror.

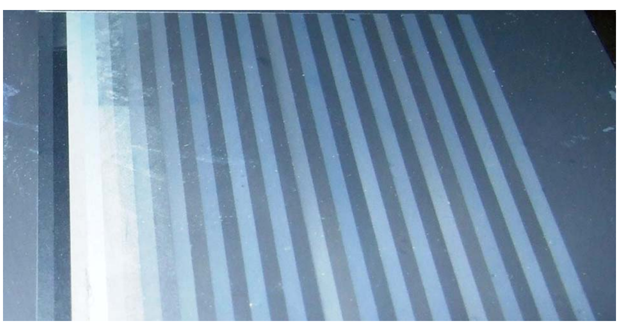
Fig. 7. (Color online) Steps of a lower step mirror.

Table 1. Testing Results of the Step Heights of the Step Mirrors

Steps	Aver. Height	Max. Height	Min. Height	σ
Higher steps	20.643 μm	21.520 μm	19.780 μm	0.422 μm
Lower steps	0.614 μm	0.878 μm	0.292 μm	0.113 μm

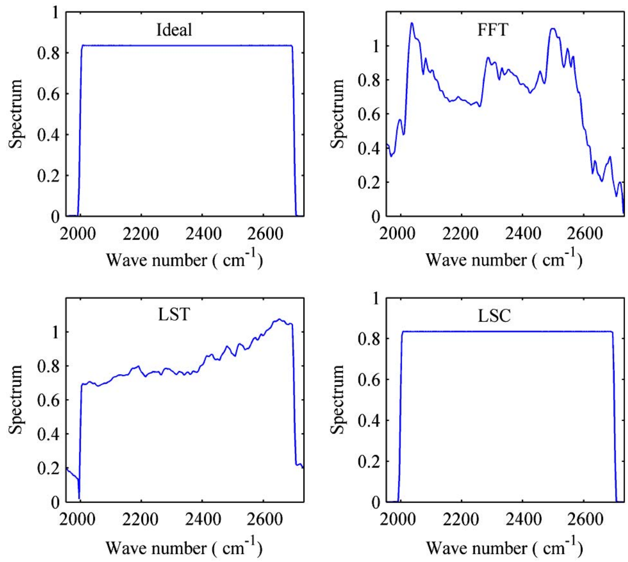

Fig. 8. (Color online) Constructed spectrum with different constructing methods (SC source).

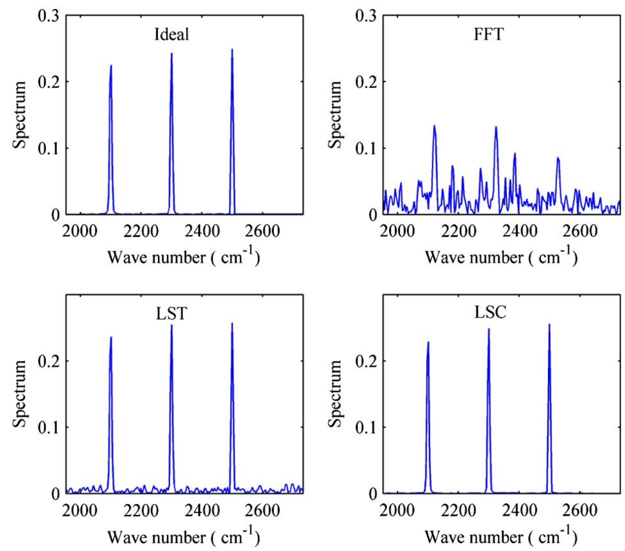

Fig. 9. (Color online) Constructed spectrum with different constructing methods (SD source).

We have simulated the same source of continuous spectrum (SC source) used above and a source of discrete wavenumbers 2100 2300 2500 cm^{-1} (SD source) to test the algorithm's performance. We compared the performance of the FFT, the least-squares approximation by trigonometric polynomials (LST), and the least-squares approximation by cosine polynomials (LSC). Results are given in Figs. 8 and 9, and in Table 2.

The LSC method gives a fairly good SCE $= 0.03\%$ for a continuous source. Although the corresponding SCE for the discrete source 5.28% is a bit larger, see Fig. 9, it successfully distinguishes the three spectral lines.

5. Discussion

It is impossible for FTS to sample the interforgram at exactly uniform points. See [22–25] for discussions on the sampling errors and their effects. Although now one can precisely control the sampling interval by laser referencing, there are other factors that prevent us from uniform sampling. For instance, E. Sarkissian *et al.* point out in [26] that a frequency-dependent Doppler shift caused by the off-axis of the detectors can be treated as a nonuniform sampling problem. Or, the phase error can be also treated as a nonuniform sampling problem. So, it seems even for the time-modulated FTS, spectrum constructing with trigonometric polynomials is a better choice than the FFT method, considering

1. it allows nonuniform sampling both in the time domain and the frequency domain as one wish, and can give the same result of the FFT method when required. Thus, it can handle the nonuniform-related problems, such as the Doppler shift and the phase effect all in one by adding information in the approximation polynomials;
2. since the spectrometers deal with 1D data, FFT shows no significant advantage in computational requirements. The computational requirements of the approximation by trigonometric polynomials can be easily met by today's computational processor.

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Table 2. Testing Results for SC and SD Sources with Different Constructing Methods

	FFT(SC)	LST(SC)	LSC(SC)	FFT(SD)	LST(SD)	LSC(SD)
Con. num.		2.14	2.35		2.14	2.35
SCE	24.24%	14.40%	0.03%	359.9%	54.43%	5.28%

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