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Letter to the Editor

Nonlinear inversion of a band-limited Fourier transform

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Discrete Fourier transform
Windows
Filtering
Approximation by exponentials
Approximation by rational functions

abstract

We consider the problem of reconstructing a compactly supported function with singularities either from values of its Fourier transform available only in a bounded interval or from a limited number of its Fourier coe cients. Our results are based on several observations and algorithms in [G. Beylkin, L. Monzón, On approximation of functions by exponential sums, Appl. Comput. Harmon. Anal. 19 (1) (2005) 17–48]. We avoid both the Gibbs phenomenon and the use of windows or filtering by constructing approximations to the available Fourier data via a short sum of decaying exponentials. Using these exponentials, we extrapolate the Fourier data to the whole real line and, on taking the inverse Fourier transform, obtain an e cient rational representation in the spatial domain. An important feature of this rational representation is that the positions of its poles indicate location of singularities of the function. We consider these representations in the absence of noise and discuss the impact of adding white noise to the Fourier data. We also compare our results with those obtained by other techniques. As an example of application, we consider our approach in the context of the kernel polynomial method for estimating density of states (eigenvalues) of Hermitian operators. We briefly consider the related problem of approximation by rational functions and provide numerical examples using our approach.

1. Introduction

We consider the problem of reconstructing a compactly supported function with singularities from values of its Fourier transform available only in a bounded interval, or from a limited number of its Fourier coe cients. The singularities that

As a representative example, let us consider a compactly supported real-valued function with Fourier transform of the form

$$\hat{}(\xi) = \sum_{=1} |\xi|^{-\alpha} \varphi \xi, \quad (2)$$

where $\mathbb{C}$

optimal approximation by decaying exponentials to approximate ˆ in the form (3). We note that trying to recover ˆ in the form (2) leads to a complicated system of nonlinear equations [7].

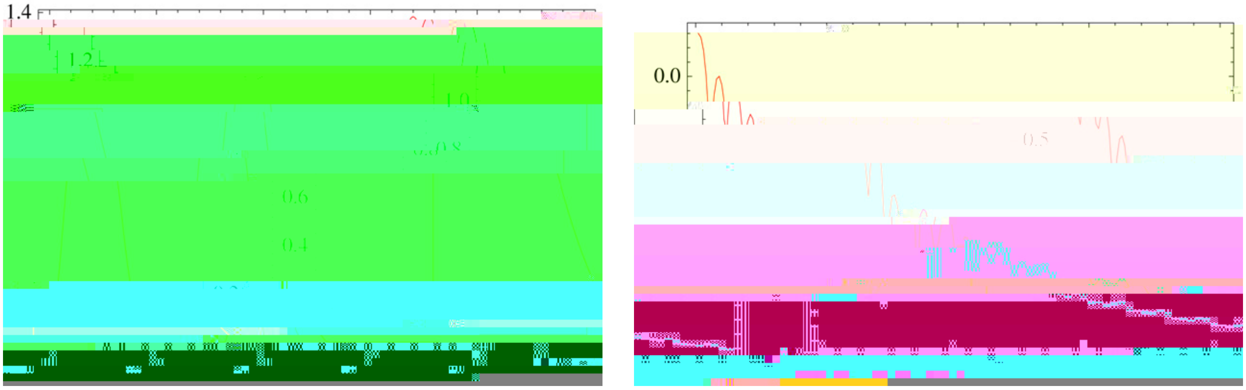
- Given the samples ˆ($\frac{}{2}$), = 0, 1, . . . , 2 , and assuming that they provide a su cient oversampling of the function ˆ(ξ) in [−, ,], the algorithm in [5] allows us to construct an approximation with a near optimal (minimal) number ofnum215.54

where is very close to provided that the function is appropriately sampled in (6) to justify local interpolation.

The steps to achieve the approximation (6) are as follows:

- Build the $+ 1 \times$ $+ 1$ Hankel matrix $\mathbf{H} = \; +$ using the samples $= \; (\frac{}{2})$, $0 \leqslant \; \leqslant 2$.
- Find a vector $\mathbf{u} = (\;_0, \ldots, \;)$, satisfying $\mathbf{Hu} = \sigma \bar{\mathbf{u}}$, with positive σ close to the target accuracy . The existence of such vector $\mathbf{u}$ follows from Tagaki's factorization (see [5, p. 22]); the singular value decomposition yields σ as a singular value and $\mathbf{u}$ as a singular vector of $\mathbf{H}$. We label the first $+ 1$ singular values of $\mathbf{H}$ in decreasing order $\sigma_0 \geqslant \sigma_1 \geqslant \cdots \geqslant \sigma$, where σ is chosen so that $\sigma \; / \sigma_0 \approx$. Typically, singular values decay rapidly and, thus, $= \mathcal{O}(\log \;^{-1})$ and $\square$.
- Compute roots γ of the polynomial $(\;) = \sum_{=0}$ whose coe cients are the entries of the singular vector $\mathbf{u}$ computed in the previous step. The weights are obtained solving the least-squares Vandermonde system

$$\sum_{=1} \gamma = \left(\frac{}{2} \right), \quad 0 \leqslant \; \leqslant 2 \; .$$



(a) (b)

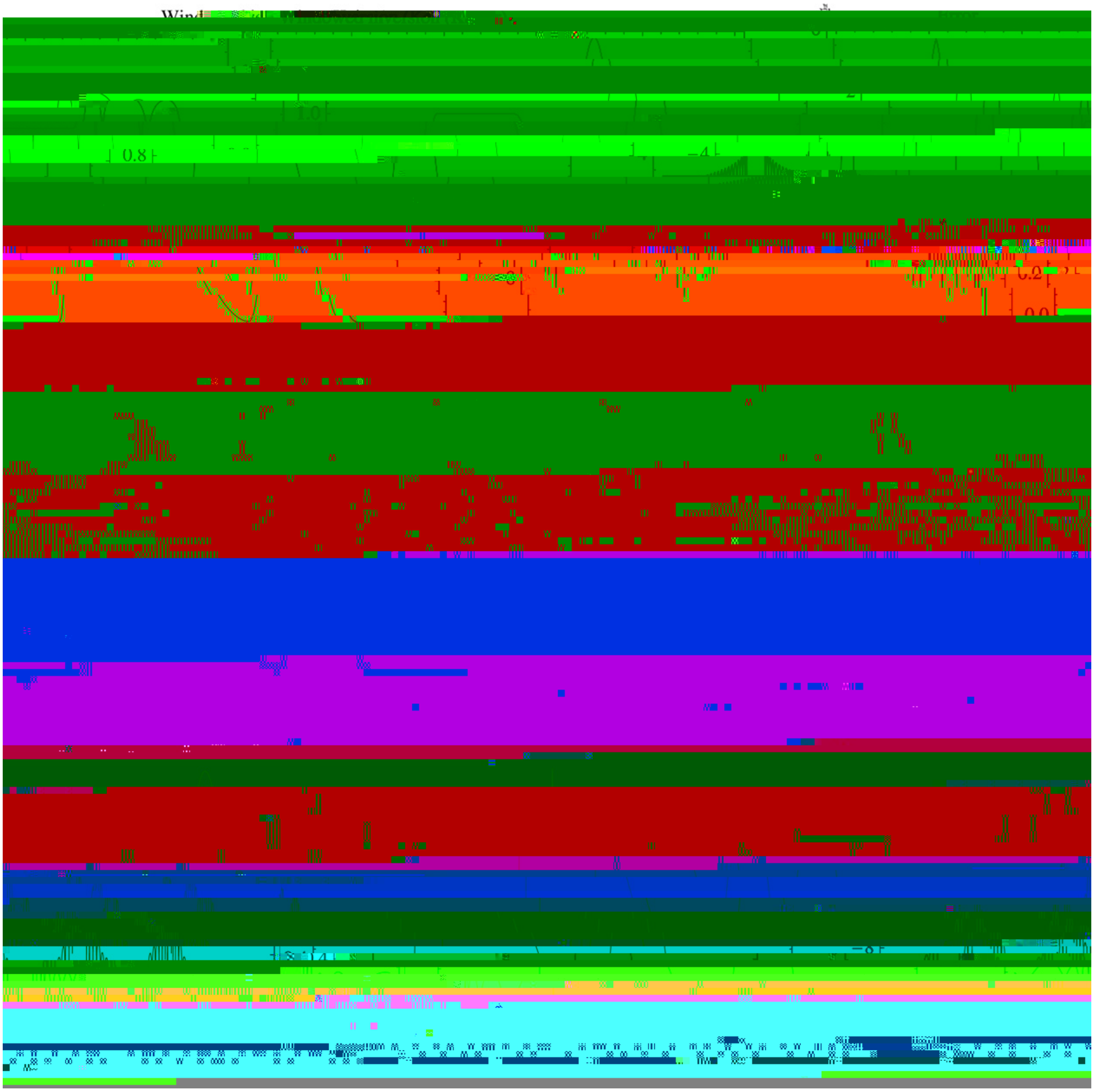


Fig. 4. Comparison of reconstructions with errors displayed using $\log_{10}$ scale on the vertical axis. The horizontal lines indicate the level of $2 \cdot 10^{-5}$ achieved by “flat” window (second from the top). The rational representation with 27 terms is obtained via (5).

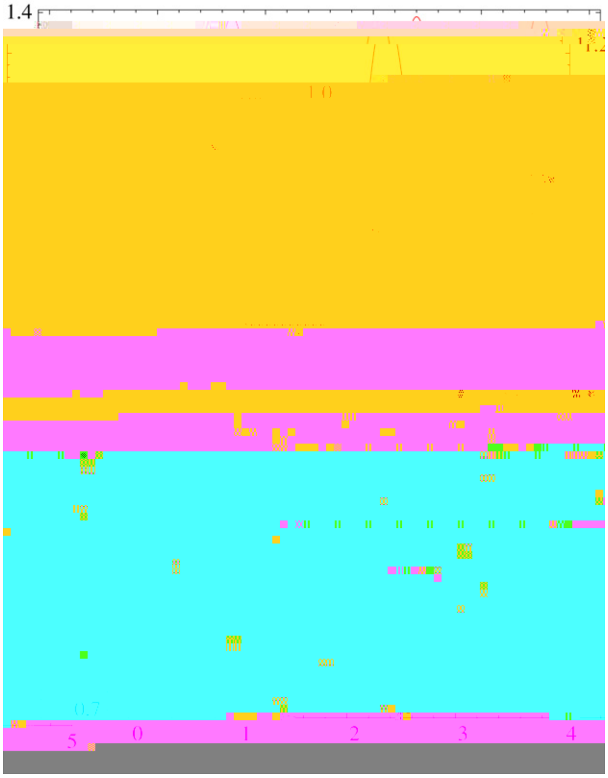


Fig. 5. The top figure displays the piece-wise polynomial function in (8) and, the bottom one, the locations of the 27 poles of its rational representation in (5). We have aligned the horizontal scale of these two figures to illustrate that the positions of the poles in the complex plane arrange themselves in branches as to indicate the location of function singularities (well separated in this case). As poles approach the real axis, their arrangement also corresponds to the type of singularity at that location.

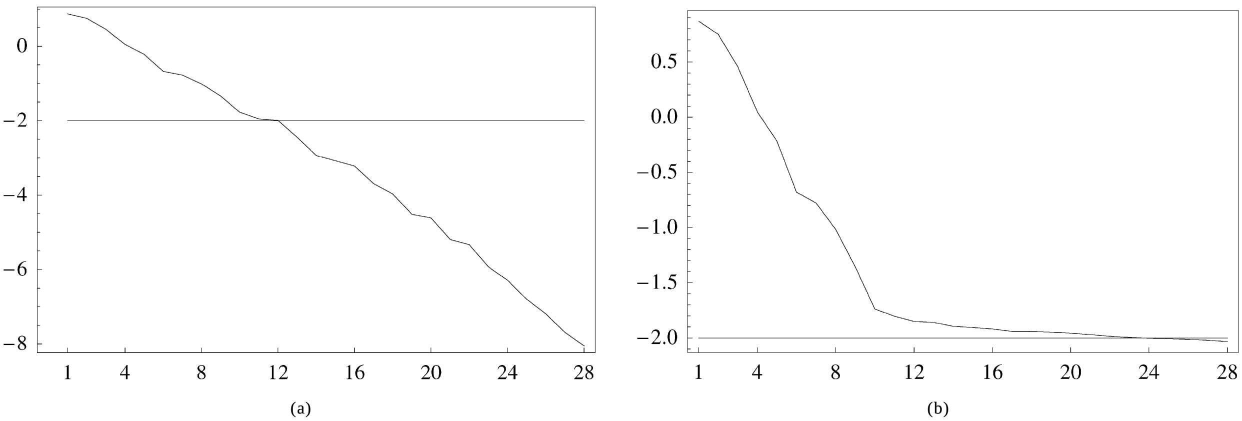


Fig. 6. The first 28 singular values of Hankel matrix with entries in (9) without noise (a) and with Gaussian noise added (b). The singular values are plotted using $\log_{10}$ scale along the verticac [(c [(usi1 170.).)-3pf.5(t)134353.8(w760.8(he)-9-518.8(2)1.7at)1(x)-8.7(v)13(long)-375.7(th2)-518.9(v)15.2hl

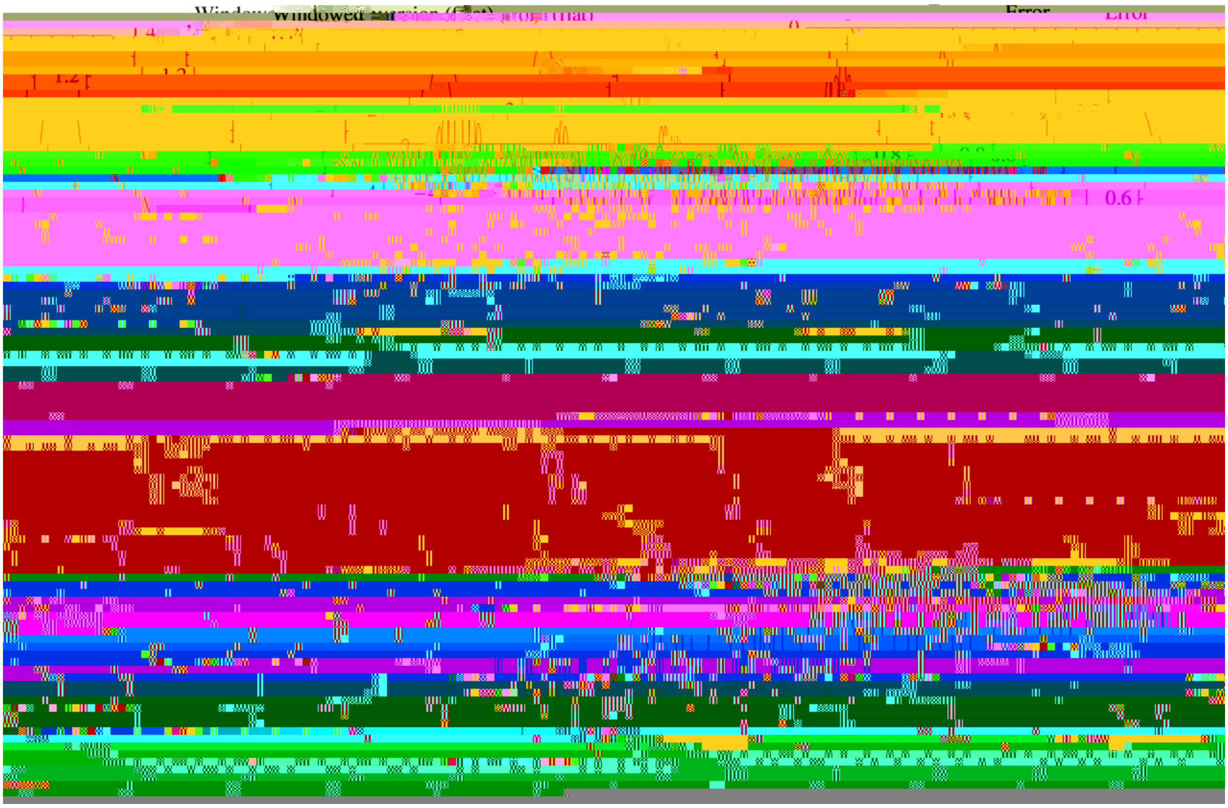


Fig. 7. Comparison of reconstructions in the presence of Gaussian noise with standard deviation $\frac{1}{2} \cdot 10^{-3}$. Absolute errors are displayed on a $\log_{10}$ scale along the vertical axis and the horizontal lines indicate the error level $1.6 \cdot 10^{-3}$. We note that the error using the Kaiser window is already at this level for the noiseless case (see Fig. 4) and is not displayed here for that reason.

where we use $\mathrm{Re} \sum_{=1}$ instead of $\sum_{=1}$ since it approximates the real value $\hat{\ }_0 = \int_0^1 (\ )$.

Again the function in (10) is defined by 2 poles and corresponding residues. Let us consider the rational function $\tilde{\ }(\ )$ such that $\tilde{\ }(\ ^{-2\pi}\ ) = (\ )$. The poles of $\tilde{\ }$ appear in pairs, and $1/\bar{\ }$, $= \ ^{-\eta}$ with residues $^{-\eta}$ and $-\bar{\ }\ \bar{\eta}$ and zero constant term. In illustrating rational representations of the form in (10), we display poles of $(\ )$ to interpret the representation on $[0, 1]$, i.e., we display $\eta\ /2\pi$ rather than the poles of $\tilde{\ }$.

4.1.

For in (8), let us consider $(5\ )$ as a periodic function in $[0, 1]$ and use as input its Fourier coe cients $\frac{1}{5}\hat{\ }(\ /5)$, $= 0, 1, \ldots, 2$, instead of values of the Fourier transform (9) in Section 3. We reconstruct using 63 and 127 of its Fourier coe cients (i.e. $= 31$ and $= 4$

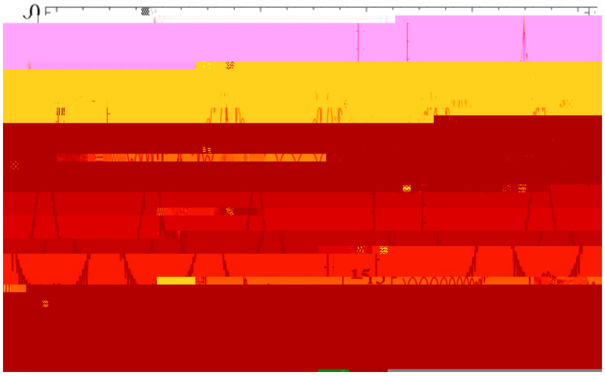


Fig. 8. Reconstruction errors (using $\log_{10}$ scale on vertical axis) for the periodic function $(5\ )$ on $[0, 1]$, where is given in (8). The upper (lower) curve shows the error using as input 63 (127) of its Fourier coe cients.

where we rescaled the interval to $[0, 1]$ to be consistent with our notation. We apply our algorithm to the first 63 and 127 Fourier coe cients of and display the results in Fig. 9. In the case of 63 coe cients, we select $\sigma_{15} \approx 6.2928 \cdot 10^{-9}$ leading to 15 terms in the reconstruction and accuracy away from singularities of the function of about 8 digits. For 127 coe cients, we chose $\sigma_{27} \approx 3.24298 \cdot 10^{-16}$ leading to 27 terms and accuracy away from singularities of about 15 digits. As an improvement over parametric techniques of [10,17,18], we note that, away from singularities of the function, our approach achieves the desirable features of uniform $^{\infty}$-type approximation.

5. On rational approximation of functions

So far we constructed our rational representations assuming that we have knowledge of either the values of the Fourier transform of a function on some interval or, alternatively, a limited number of its Fourier coe cients. In this section we consider a related approximation problem, where we control the size of the Fourier interval or the number of the Fourier coe cients. Specifically, given a compactly supported function with integrable singularities, we are interested in constructing a rational approximation and quantifying its properties given its Fourier transform in a bandlimited interval. A theoretical foundation of our approach lies in interpreting results in [5] as an extension of the theory developed by Krein et al. in [1–3]. We plan to address this problem at length elsewhere but, in this section, we present some observations for the purpose of illustration.

Let us show that by an appropriate selection of bandlimit, our approach yields an accurate rational approximation away from singularities. Let be a real, compactly supported, bounded function. We assume that

Table 1

Poles and residues for the rational approximation of cubic B-spline in (19). Additional poles Ms Ms Ms Ms M

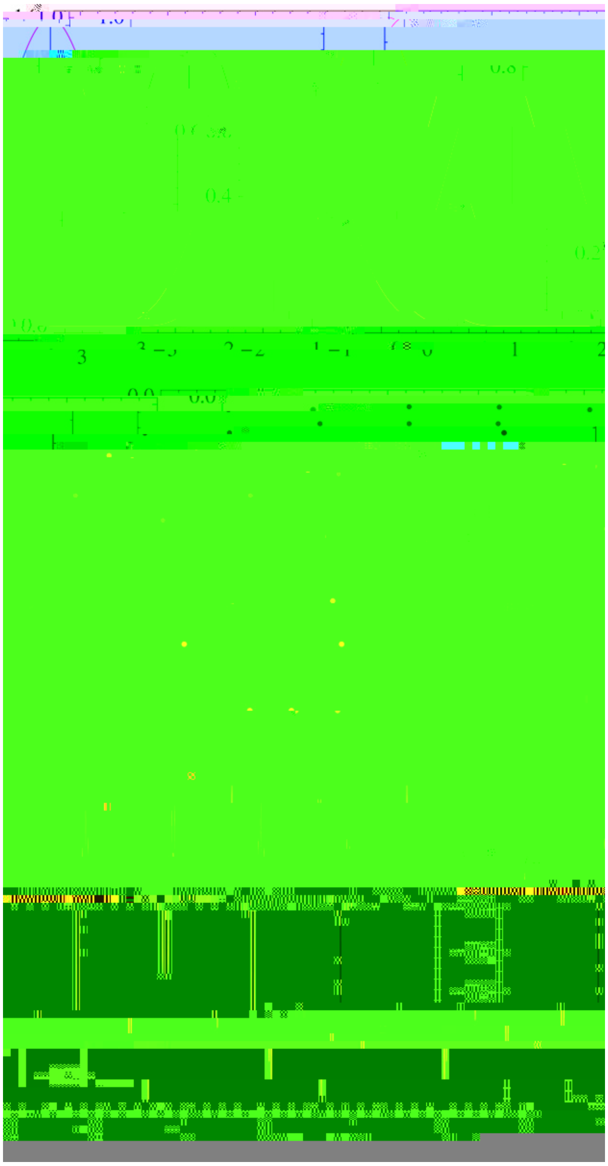


Fig. 10. Cubic B-spline considered in the interval $[-3, 3]$ (top). Locations of the 26 poles (in the lower half-plane) of its rational approximation (middle). Log-error of its reconstruction over the interval $[-3, 3]$ (bottom). We aligned the figures to illustrate the arrangement of the poles in the complex plane vs. singularities of the function being approximated.

where

$$\hat{\beta}(\xi) = \frac{3}{2}\left(\frac{\sin \pi \xi}{\pi \xi}\right)^4,$$

we approximate $\beta(\ )$ by a rational function

$$(\ ) = \mathrm{Re}\left(\sum_{=1} \frac{\ }{-}\right), \tag{19}$$

where, in this example, = 26 and poles and residues are given in Table 1. The positions of the poles and the error of approximation are shown in Fig. 10. In this example, samples were approximated with maximum absolute error ≈ $2.5 \cdot 10^{-8}$ leading to an approximation of $\hat{\beta}$ anywhere in the interval $[0, 25]$ with maximum absolute error 25

.2.

Although we have considered piecewise polynomials, our approach is not limited to constructing rational approximations of such functions. In fact, by interpreting one of our examples in [5], we obtain a rational approximation of

$$(\ ) = \begin{cases} \dfrac{\ ^2}{\sqrt{1-\ ^2}}, & |\ | < 1, \\ 0, & \end{cases}$$

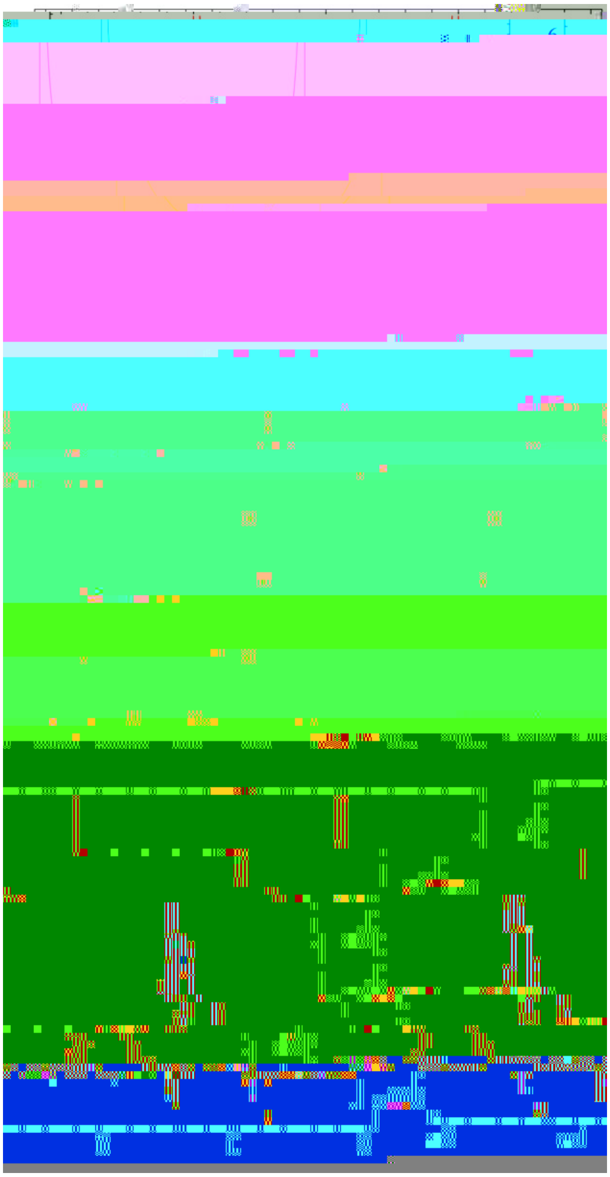


Fig. 11. The function $\frac{\sqrt{2}}{1-\ ^{2}} 1_{[-1,1]}(\ )$

we not only obtain an accurate approximation of ( ) but also an a posteriori estimate of the noise level that we read off the change in the rate of decay of the singular values of the corresponding Hankel matrix.

7. Conclusions

The nonlinear inversion of the bandlimited Fourier transform of this paper avoids Gibbs phenomenon without resorting to traditional windowing or more sophisticated filtering techniques. We show how to apply our method when the measured or computed data are either values of the Fourier transform or coe cients of the Fourier series. The nonlinear approximation of the Fourier data by a sum of exponentials is near optimal, i.e. requires a near minimal number of terms, and, hence, yields an e cient rational representation. The poles of the rational representation arrange themselves in patterns indicating