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APPLICATION OF DECONVOLUTION TECHNIQUES IN MULTICOMPONENT TRANSIENT SIGNAL ANALYSIS

BY

ZA'IM BIN ISMAIL

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ABSTRACT OF THE THESIS

Though many techniques for analyzing transient exponential signals have been reported in the literature, however, deconvolution based procedures are preferred and often commonly used because the signal parameters of interest are displayed graphically. This thesis discusses three deconvolution techniques for the analysis of transient exponential signals, namely conventional inverse filtering, optimally compensated inverse filtering and homomorphic deconvolution which are implemented by a MATLAB-based algorithm. All the three techniques are based on the Gardner transformation which is needed to convert the exponential signal into a convolution model. Interpolation algorithm is used for the proposed MATLAB algorithm to process data acquired from real physical system. The deconvolved data is generated from either the above techniques. The deconvolved data from either the conventional or optimally compensated inverse filtering is further analyzed using the discrete Fourier transform (DFT) processing via the fast Fourier transform (FFT) algorithm or the singular value decomposition (SVD)-based autoregressive moving average (ARMA) modeling technique. The efficiency of the proposed algorithm in estimating the real-valued decay rate is evaluated by the Cramer-Rao lower bound (CRLB). The proposed algorithm is used to analyze both the simulated data and the data acquired from real physical system. Results from the simulation studies and real-time implementation show that the homomorphic deconvolution is the most computationally efficient but it produces inaccurate estimates of the signal parameters. Indeed, the optimally compensated inverse filtering with ARMA modeling technique is the best technique amongst the three as it produces accurate estimates of the signal parameters even though it involves laborious and complex computations.

ملخص البحث

على الرغم من وجود الكثير من الطرق لتحليل الإشارات المطردة العابرة التي وردت في البحوث ذات الصلة، إلا أنه غالباً ما تفضل طريقة الديكنو فوليتشن على غيرها لأنها تظهر عوامل الإشارات موضوع الاهتمام بتفصيل.تناقش هذه الرسالة ثلاثة طرق ديكنفوليشن لتحليل الإشارة المطردة المعابر وهذه الطرق الثلاثة هي الترشيح العكسي التقليدي الترشيح العكسي ذو التعويض الانسب وهوموموررفيك دكنفوليشن حيث تم تطبيق هذه الطرق باستخدام مخطط خوارزمي على الماتلاب. باعتماد طريقة تحويل جاردنر في تحويل الإشارة المطردة العابرة ولقد تم استخدام مخطط الاقحام كي مايقوم مخطط الخوارزمي ماتلاب المقترح من معالجة البيانات المأخوذة من نظام مادي حقيقي بيانات الديكنفوليشن تم تحليلها أيضاً باستخدام تحويل فوريا المتصلة (DFT) المعالجة إما عبر تحويلات فورية سريعة FFT أو ديكنفوليشن ذي القيمة الأحادية SVD على أساس اتوريجريسف autoregressive ذو المتوسط المتحرك (ARMA).لقد تم تقييم فعالية المخطط الخوارزمي المقترح باستخدام الحد الأدنى لكارمر-رو Cramer-Rao (CRLB). استخدم المخطط الخوارزمي المقترح لكل من بيانات المحاكة وتلك المأخوذة. من نظام مادي حقيقي. إن الطريق الأكثر فاعلية حساباً ــ بحسب نتائج الدراسة ــ هي طريقة هوموموررفك دكنفوليشن غير أنها تؤدى إلى تقدير غير دقيق لعوامل الإشارة. لذا نجد أن طريقة الترشيح العكسي باستخدام التعويض الأنسب هي أفضل هذه الطرق وذلك نسبة لدقة تقديراتها لعوامل الإشارة بالرغم من أنها تحتوي على عمليات حسابية شاقة ومعقدة.

APPROVAL PAGE

I certify that I have supervised and read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Science in Computer and Information Engineering.

Momoh Jimoh E.Salami
Supervisor

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Science in Computer and Information Engineering.

Othman O. Khalifa
Internal Examiner

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Science in Computer and Information Engineering.

Ahmad Zuri Sha'ameri
External Examiner

This thesis was submitted to the Department of Computer Engineering and is acceptable as partial fulfillment of the requirements for the degree of Master of Science in Computer and Information Engineering.

Farhat Anwar
Head, Department of Computer Engineering

This thesis was submitted to the Kulliyah of Engineering and is acceptable as partial fulfillment of the requirements for the degree of Master of Science in Computer and Information Engineering.

Ahmad Faris Ismail
Dean, Kulliyyah of Engineering

DECLARATION

I hereby declare that this thesis is the result of my own investigations, except where otherwise stated. Other sources are acknowledged by author-date system giving explicit references and a bibliography is appended.

Name: Za'im bin Ismail

Signature:

Date: 23rd March 2004

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LIST OF SYMBOLS

A_k	amplitude
A_0	DC offset
a, b, c, d	constants
$a[k], b[k]$	AR and MA parameters
$A(z), B(z)$	z-transform of $a[k]$ and $b[k]$
$a(m)$	polynomial coefficients
α	weighting factor
Δf	frequency interval
ڤ	rule for combining inputs with each other for generalized principle of superposition
:	rule for combining inputs with scalars for generalized principle of superposition
O	rule for combining system outputs with each other for generalized principle of superposition
ι	rule for combining outputs with scalars for generalized principle of superposition
β_c	convergence parameter
$\beta(k)$	residual error sequences
^	estimate of any function except in homomorphic deconvolution
$*$	convolution operation
*	complex conjugate
c_s	scalar
$c_x[n]$, $c_{xm}[n]$, $c_{xma}[n]$	outputs of the forward homomorphic processing
$c_x[n]$, $\hat{x}[n]$	complex cepstrum
D	characteristic system in homomorphic with no explicit dependence
D[.]	deconvolution technique
$\mathbf{e}$	error vector
e_m	linear prediction approximation error
E	error energy with no explicit dependence
$E[.]$	expectation
ϵ	amplitude equalization parameter
$f(x)$	function of x with no explicit dependence
f, F	type of filter with no explicit dependence
$f(k)$	deconvolved data
$g(\tau)$	certain time-constant distribution
$g(\lambda)$	sum of delta functions
λ_k	real decay rates
$H[.]$	homomorphic system transformation
I	intensity of the fluorescence substances with no explicit dependence
j	complex number where j^2 equals to -1
L	linear system in homomorphic deconvolution
$L_i(x)$	set of Lagrange polynomials

$L(k)$	regularization operator
L	lower rank
M	number of components
mr	value of the power of 2
μ, α_k, β	controlling parameters
N, n	specified number of data points or data samples
N_c	number of cubic polynomials
N_d	number of deconvolved data points
N_{zp}	zero-padded data points
N_0	cepstrum cut-off point
$n(\tau)$	additive, white Gaussian noise
n_{max}, n_{min}	Upper and lower data cut-off points
p, q	AR and MA model orders
p_e, q_e	guess AR and MA model orders
$P_x(t)$	power distribution of $x(t)$
$P(z)$	polynomial function
$p(S;\lambda_k)$	probability density function of $S(\tau)$
$q(y)$	sum of Heaviside step-functions
σ_n^2, σ_v^2	variance of the white Gaussian noise
R	autocorrelation function with no explicit dependence
$S(\tau)$, $f(\lambda,\tau)$	multicomponent decaying transient signal
$S_z(\omega)$	power spectrum of an output signal
$S_n(\omega)$	power spectrum of an input driving sequence
$s(\lambda)$	spectrum in biophysics
$S[n;\lambda_k]$	$S(\tau)$ with negligible noise
$S_f(z)$	power spectral density
$\zeta(\omega)$	power spectra with no explicit dependence
$\delta(\lambda)$	dirac function
^{T}	transpose
$\mathbf{U}$, $\mathbf{\Sigma}$, $\mathbf{V}$	matrices in SVD of the correlation matrix with no explicit dependence
var	variance with no explicit dependence
$\mathbf{X_0}$	gradient matrix
γ	filtering coefficient
y, x, h, v	output function, input function, impulse response function and noise with no explicit dependence
$Y(\omega)$, $X(\omega)$, $H(\omega)$, $V(\omega)$	Fourier transform of y, x, h, v
$Y(k)$, $X(k)$, $H(k)$, $V(k)$	discrete Fourier transform of y, x, h, v

LIST OF ABBREVIATIONS

ADC	Analog-to-Digital conventer
AR	autoregressive
ARMA	autoregressive moving average
CRLB	Cramer-Rao lower bound
CPU	central processing unit
dB	decibels
DC	direct current
DFT	discrete Fourier transform
DLTS	deep-level transient spectroscopy
FFT	fast Fourier transform
LS	least squares
MA	moving average
MATLAB	matrix laboratory
METS	multiexponential transient spectroscopy
NMR	nuclear magnetic resonance
PC	personal computer
SNR	signal-to-noise ratio
SVD	singular value decomposition

CHAPTER 1: INTRODUCTION

1.0 Introduction

According to Karrakchou et al. (1992), basic solution to a large variety of problems that arises in many engineering disciplines can be written as a sum of exponentials. This type of solution arises from many mathematical equations such as linear differential equations, linear differential-difference equations, systems of linear differential equations and systems of differential-difference equations. Amongst these solutions is the analysis of multicomponent decaying transient signals with real exponential constants. This analysis was first introduced by Gardner et al. (1959) in the study of first order chemical kinetics and some order-disorder transitions in solid state physics.

The analysis of multicomponent decaying transient signals is very important in many areas of scientific disciplines such as the study of nuclear magnetic resonance (NMR) in medical diagnosis (Cohn-Sfetcu et al. 1975), relaxation kinetics of cooperative conformational changes in biopolymers (Provencher 1976), solving system identification problems in control and communication engineering (Prost and Goutte 1976), fluorescence decay of proteins (Karrakchou et al. 1992), kinetics of isotropic exchange (Karrakchou et al. 1992), analysis of reaction rates (Sohie et al. 1990) and electromagnetic problems (Yu 1990). Recently, the multicomponent transient signal analysis has found its applications in deep-level transient spectroscopy (DLTS) for characterization of semiconductor materials (Sohie et al. 1990) and in the estimation of the pulmonary capillary pressure (Karrakchou et al. 1992) and the list of problems could continue.

1.1 Thesis objectives

The main objectives of this thesis are:

a) to test the performance of the proposed algorithm in estimating the number of components and the real-valued decay rate either from the simulation studies or from the real-time implementation,

b) to compare the efficiency of the proposed algorithm in estimating the real-valued decay rate by using the Cramer-Rao lower bound, and

c) to see the effect of interpolation algorithm on the performance of the proposed algorithm.

1.2 Problem statement

The multicomponent exponential signal can be represented by a linear combination of exponentials of the form

$$S(\tau) = \sum_{k=1}^{M} A_k \exp(-\lambda_k \tau) + n(\tau), \tag{1.1}$$

where M is the number of components, A_k and λ_k respectively correspond to the amplitude and real-valued decay rate constants of the kth component and $n(\tau)$ is the additive white Gaussian noise with variance σ_n^2. It is insufficient according to Gardner et al. (1959) for a function to merely approximate the measured data, $S(\tau)$ closely but these signal parameters need to be accurately estimated by the function. The exponentials in equation (1.1) are assumed to be separated and unrelated. That is none of the components is produced from the decay of another component. Therefore, it is desirable to obtain the signal parameters, M, A_k and λ_k from equation (1.1). The estimation of signal parameters is a difficult problem due to the nonorthogonal nature of the exponential signals. This leads to an ill-posed problem, making it difficult to accurately estimate the signal parameters. Nevertheless, the analysis of multiexponential signals is very important because these signals arise in many scientific areas as mentioned above.

1.3 Significance of the problem

The above problem arises in many scientific areas. The significance of the problem is illustrated by the following examples taken from many disciplines of science and engineering.

a) Analysis of biological NMR relaxation data

The early experiments on the analysis of NMR data according to Kroeker and Henkelman (1986) were the measurements of the relaxation time in water and other homogeneous liquids. These early experiments showed that the regrowth and decay of magnetization in homogeneous samples are exponential. Calculation of data in these experiments was not difficult because the sample under study and the conditions affecting the samples were well understood. In contrast, the measurements of complex biological samples are very difficult due mainly to the lack of understanding of the conditions that affect the decay time.

Several techniques are introduced for the analysis of NMR data according to Kroeker and Henkelman (1986) such as one-component exponential model, two-component exponential model and continuum technique.

b) Analysis of multiexponential transient spectroscopy (METS) signals

The general formula for a set of samples generated from a certain time-constant distribution, $g(\tau)$ which is given by Marco et al. (2001) as

$$s(t) = \int_0^\infty g(\tau) e^{-\left(\frac{t}{\tau}\right)} d\tau. \tag{1.2}$$

The underlying $g(\tau)$ is going to be determined from this equation. The inverse Laplace transform of the signal is taken for solving the problem of any exponential analysis. This operation is possible if the analytical expression of $s(t)$ is known. Unfortunately, this is not the case with multiexponential transient spectroscopy (METS) signals. Therefore, another approach termed an improved spectroscopic technique is applied to the analysis of METS signals.

c) Analysis of "discrete spectra" problem in biophysics

Signals from a variety of experiments are represented by an integral over an exponential kernel (Provencher 1976), that is

$$S(\tau) = \int_0^\infty e^{-\lambda\tau} s(\lambda) d\lambda. \tag{1.3}$$

It is desirable to determine the spectrum, $s(\lambda)$ as accurately as possible from equation (1.3). The most common form of this problem in biophysics involves "discrete spectra". This problem is still difficult in biophysics because of the unknown mechanism or appropriate model that will be determined. Therefore, a technique that produces good estimates of the signal parameters is needed to obtain good results.

d) Other types of analysis

Recently, the analysis of multiexponential signals has found its application in deep-level transient spectroscopy (DLTS) and characterization of semiconductor materials according to Sohie et al. (1990).

1.4 Previous techniques of analysis

Several techniques have been proposed for solving the above mentioned problem and these techniques are divided into two categories, namely time-domain and frequency-domain methods.

During 1950s, the most common time-domain technique for solving a decay curve into its components was the graphical or peeling approach according to Gardner et al. (1959). This technique is the easiest to perform but it often gives inaccurate estimate of the signal parameters; also this procedure can be painstakingly laborious and only a skilled person can perform it successfully.

Prony suggested a time-domain technique for modeling data of equally samples by a linear combination of exponentials (Kay and Marple 1981). This technique is called Prony's method or linear least squares technique (Osborne and Smyth 1995). Unfortunately, this technique performs poorly even for a slightly contaminated signal. A modified Prony technique was described by Osborne and Smyth (1995) to overcome this difficulty. This modified technique provides improved performance but still gives inaccurate estimates of λ_k especially when λ_k is closely related to each other. Apart from that, these two techniques require a priori information about M.

A nonlinear least squares technique is used in the iterative technique for computing the signal parameters according to Marquardt (1963). The solution of this iterative technique will converge if the starting values of the unknown parameters are appropriately determined. This technique is less attractive to many researchers due to the problems of multiple convergence as well as being computationally inefficient.

The discussed time-domain techniques have the disadvantage of producing incorrect results either when the data is noisy or the number of components, M is unspecified. The main reason for the poor performance of the time-domain techniques is the nonorthogonal nature of the transient signals as mentioned before.

The drawbacks of the time-domain techniques can be alleviated by using the frequency-domain methods. One of the earliest frequency-domain techniques is the Gardner transformation by Gardner et al. (1959). This technique is suitable for analyzing signal with low noise since signal with large noise will result in performance degradation. It is possible to obtain a high resolution without any a priori knowledge of the signal parameters and the number of components, M.

The main disadvantage of the Gardner transformation at that time was due to the difficulty in performing fast numerical integration by Fourier transform. Apart from that, results of the analysis are affected by error ripples. These error ripples are caused by a variety of factors such as integration error, data error, data perturbation and truncation error.

The numerical integrals encountered in using the Gardner transformation can be replaced by the discrete Fourier transform according to Schlesinger (1973). This discrete Fourier transform can be easily calculated using the FFT algorithm, which is available during early 1970s. Therefore, the original Gardner transformation is improved by the FFT algorithm. Unfortunately, the implementation of this FFT algorithm fails to solve the problems of error ripples and poor resolution display in frequency-domain.

Another improvement over Schlesinger (1973) technique is given by Cohn-Sfetcu et al. (1975). This improvement is based on the introduction of the Gaussian filtering. The high frequency noise is reduced by this filter so that the signal-to-noise ratio (SNR) of the deconvolved data is improved. This improved technique is sensitive to noise because deconvolution and nonlinear change of variable enhance the noisiest part of the data. Therefore, this technique needs data with high accuracy, which is rarely possible in real-time implementation. This technique also suffers from longer computational time due to the increased number of points in the FFT computation in order to improve the resolution. A need for highly accurate data is eliminated by Provencher (1976) with the introduction of a convergence parameter as well as an amplitude equalization parameter into the existing FFT technique.

Swingler (1977) improved this FFT technique using a simple first-order difference procedure by introducing an alternative starting point instead of forming the usual product of $e^x S(e^x)$. The alternative starting point is done by the formation of the x-derivative, $S'(e^x)$. The advantages of this improved FFT technique are that it

a) yields outputs whose peaks are proportional to the amplitude, A_k directly,