Reduced order models for diffusion systems via collocation methods

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Abstract

Mathematical models for diffusion processes like heat propagation, dispersion of pollutants etc., are normally partial differential equations involving unknown parameters. For practical use, one has to estimate these parameters. In this paper we consider a simple case of heat propagation in a homogeneous wall. The resulting partial differential equation is solved using numerical techniques and tools of system identification are used to estimate the unknown parameters. In particular we examine the effect of model order selection when a Chebyshev collocation method is applied for solving partial differential equations.

Keywords: Diffusion, State-space model, system identification, Collocation method, Chebyshev polynomials.

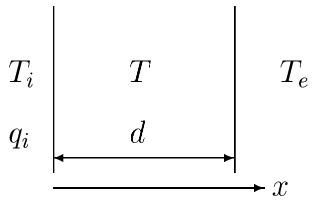

Figure 1: Heat diffusion through a homogeneous wall.

1 Introduction

Diffusion systems have been studied with a lot of interest for a long time [1], [4]. Recently it has thrown a lot of interest among control engineers, as its applications include heat propagation and diffusion of pollutants in the atmosphere. Diffusion is normally modeled by a partial differential equation (PDE), which may involve some unknown parameters. In order to model such a system one has to determine these parameters.

System identification is an experimental approach to model dynamic systems [6]. An experiment is performed by exciting the system with an input signal and recording the corresponding system output. A model is then fitted to the recorded input-output data. A key problem in system identification is to select a model structure, within which a good model has to be found for the given input-output data. Fitting a model within a given structure (parameter estimation) is a simpler problem in most cases. Normally one uses physical insight and prior knowledge about the system when selecting a model structure. If no prior knowledge or physical insight is available, then one selects a model structure which is flexible and have been successful in the past. Models of the former type are called grey box models and models of the latter type are called black box models. Unlike black box models grey box models are strongly application dependent.

In this paper, we consider the simple case of heat propagation in a homogeneous wall. We use this simple case of heat propagation to illustrate the use of system identification to model diffusion systems, by applying an output error method criterion and a collocation method for the numerical solution of the underlying PDE.

2 A case study: the heat diffusion equation

2.1 Statement of the problem

Consider a homogeneous wall of thickness d units. Let x be the coordinate across the wall, T_e the temperature on the exterior side, T_i the temperature on the interior side and q_i the supplied heat on the interior side, cf Figure 1.

Let $T = T(x,t)$ denote the temperature at position x and at time t. Then the heat flow and the temperature are described by

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2} \tag{1}$$

with boundary constraints

$$q_i(t) = -\kappa \frac{\partial T(x,t)}{\partial x} |_{x=0}, \tag{2}$$

$$T_e(t) = T(d,t) \tag{3}$$

For simplicity we consider the intitial condition $T(x,0) = 0$. In the model (1)-(3) the diffusion coefficient α and and the thermal conductivity κ are the unknown parameters.

Needless to say, both the case selected for study and its geometry are simple. While the geometry is chosen for technical ease, the simple case is aimed at getting insight into more difficult systems for future work.

Consider the wall as a dynamic system with input $u(t) = (q_i(t), T_e(t))^T$ and output $y(t) = T_i(t)$.

The estimation problem to be considered is the following.

Given: Discrete-time data $T_e(h), q_i(h), T_i(h), T_e(2h), q_i(2h), \ldots, T_i(Nh)$.

Find: Parameter estimates of α and κ.

It is apparent that the above problem is an example of grey box modeling. Here we consider an output error approach, [6].

We fit a model

$$\mathcal{M}(\theta) : y^m(t) = G(q^{-1}, \theta)u(t) \tag{4}$$

for the given data, where $G(q^{-1}, \theta)$ is a filter, which is asymptotically stable for the system parameter $\theta = (\alpha, \kappa)^T$. In (4) q^{-1} is the backward shift operator, $q^{-1}u(t) = u(t-h)$. An estimate of $\theta = (\alpha, \kappa)^T$ is determined as the minimizer of

$$V(\theta) = \frac{1}{N} \sum_{j=0}^{N-1} [y(jh) - y^m(jh)]^2 \tag{5}$$

As mentioned earlier, the key problem is to determine the model structure $\mathcal{M}(\theta)$. The parameter θ can be determined by any standard non-linear search method.

Any stable numerical scheme which computes the solution of a PDE can be interpreted a dynamical system, which approximates the true system dynamics governed by the PDE. The order of the dynamical system determines the degree of approximation: The higher the order, the better the approximation. Normally one would prefer to have a low model order in order to reduce the computational complexity without compromising too much on the accuracy.

In this paper we use a numerical scheme called Chebyshev collocation method to compute the solution of the PDE. Chebyshev collocation belongs to a class of numerical schemes called collocation methods or pseudo-spectral methods [2], [3]. We first look at the dynamics of the true system before discussing collocation and Chebyshev collocation methods. Finally we will see by some numerical examples how the model order (the number of collocation points) influences the parameter estimates.

2.2 The system dynamics

The defined system is linear and has two inputs, q_i and T_e, and one output, T_i. Interestingly enough, one can rather easily derive the transfer function of the system, which will give an input-output description of the dynamics, [5]. For convenience we repeat the derivation here.

First take the Laplace transform of (1) which gives

$$sT(x,s) = \alpha \frac{d^2}{dx^2} T(x,s) \tag{6}$$

where $T(x,s)$ is the Laplace transform of the temperature $T(x,t)$. Regarding s as a fixed parameter, (6) is a standard ordinary differential equation. It is found that the general solution to (6) can be written as

$$T(x,s) = A(s)\cosh(x\sqrt{\frac{s}{\alpha}}) + B(s)\sinh(x\sqrt{\frac{s}{\alpha}}) \tag{7}$$

Further, taking Laplace transforms on (2),(3) and evaluating the constants $A(s)$ and $B(s)$ gives the following expression for temperature at the interior side.

$$T_i(s) = \underbrace{\frac{\tanh(d\sqrt{\frac{s}{\alpha}})}{\kappa\sqrt{\frac{s}{\alpha}}}}_{G_1(s)} q_i(s) + \underbrace{\frac{1}{\cosh(d\sqrt{\frac{s}{\alpha}})}}_{G_2(s)} T_e(s). \tag{8}$$

Note that both $G_1(s)$ and $G_2(s)$ are transcendental functions. It is also worth noting that $G_1(s)$ and $G_2(s)$ are both of low pass character, see Figures 2 and 3. This property enables us to choose models approximating (8) depending on the frequency contents of the input signals. Since the transfer functions $G_1(s)$ and $G_2(s)$ are of finite magnitude, $T_i(t)$ depends continuously on the input data $q_i(t)$ and $T_e(t)$. Continuous dependence along with the uniqueness of the solution renders the problem well posed in numerical analysis terminology.

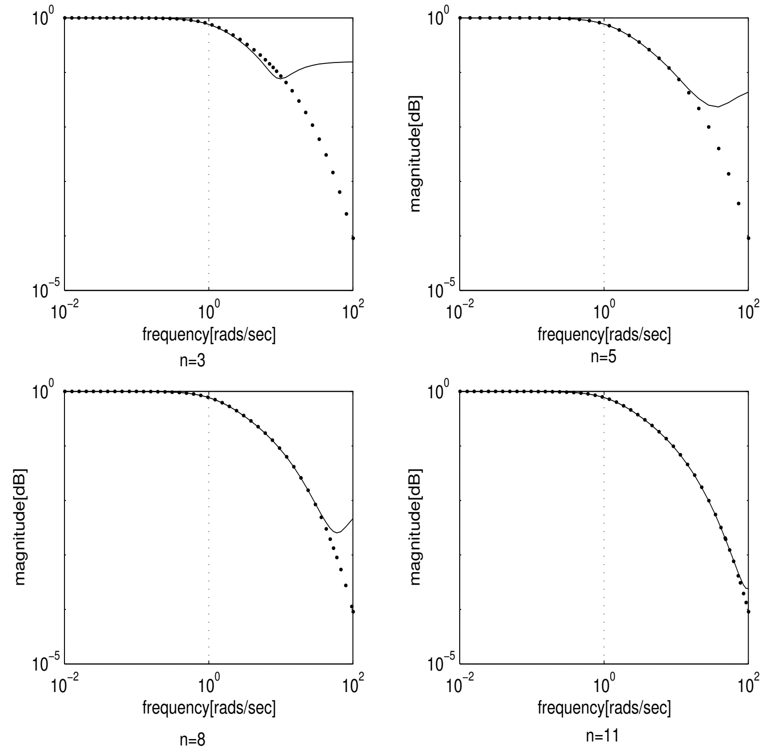

Figure 2: The Chebyshev collocation approximation of $G_1(i\omega)$ for some different model orders($n = 3,\ 5,\ 8,\ 11$) with $\alpha = 2$ m/s^2 and $\kappa = 1$ J/msK . The true transfer function (of infinite order) is plotted with a dotted line and the approximate transfer function (of finite order) is plotted with a solid line.

The transfer functions of (8) can also be characterized in terms of poles, zeros and static gain. They have the same set of poles, given by

$$p_n = -\frac{\pi^2}{d^2}(n - \frac{1}{2})^2\alpha, \qquad n = 1, 2, \ldots \tag{9}$$

Only $G_1(s)$ has zeros and they are located at

$$z_n = -\frac{\pi^2}{d^2}n^2\alpha \quad n = 1, 2, \ldots \tag{10}$$

Finally, the static gains are

$$G_1(0) = \frac{d}{\kappa}, \qquad G_2(0) = 1. \tag{11}$$

2.3 Collocation method

As mentioned earlier, to construct approximate models for the system, we have to solve the PDE (1)-(3) numerically. In this section we briefly discuss about

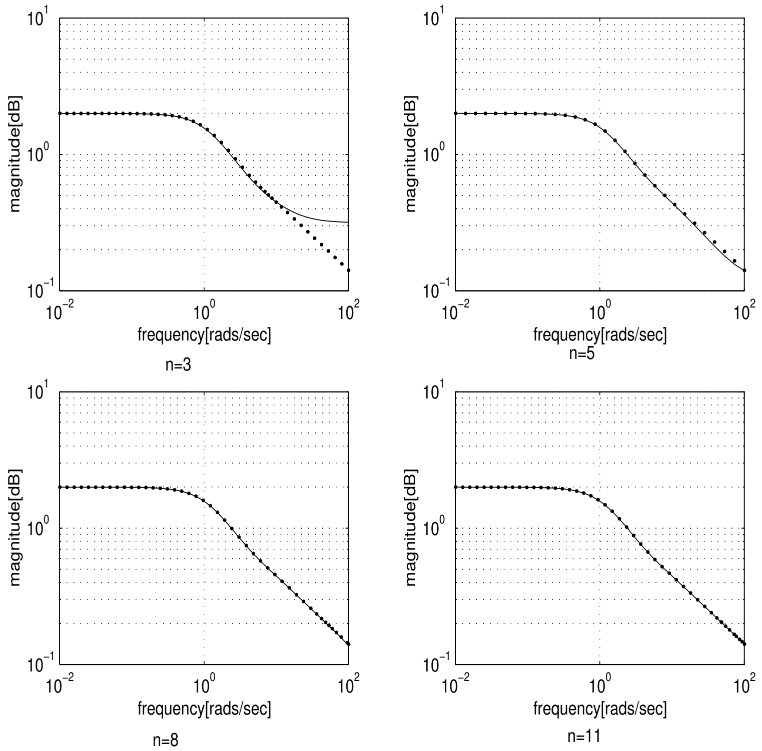

Figure 3: The Chebyshev collocation approximation of $G_2(i\omega)$ for differentmodel orders ($n = 3,\ 5,\ 8,\ 11$) with $\alpha = 2$ m/s^2 and $\kappa = 1$ J/msK. The true transfer function (of infinite order) is plotted with a dotted line and the approximate transfer function (of finite order) is plotted with a solid line.

collocation methods for numerical solution and the advantages of using them.

The underlying idea of collocation methods is that, the solution of the PDE is assumed to be lying in an infinite dimensional function space. One attempts to approximate the solution by a finite linear combination of known functions which span a finite dimensional subspace of the infinite dimensional space.

We illustrate these general ideas by applying them to our problem (1)-(3).

Suppose that we look for an approximate solution of (1)-(2) of the form

$$T_n(x,t) = \sum_{i=0}^{n+1} a_i(t)\phi_i(x) \tag{12}$$

where $\{\phi_i(x)\}_{i=0}^{\infty}$ is a complete orthonormal basis for the infinite dimensional space to which the solution belongs. The basis function $\phi_i(x)$ could typically be a polynomial or a spline or a trigonometric function.

The coefficients $a_i(t)$ are determined by forcing $T_n(x,t)$ to satisfy the PDE exactly at the collocation points $0 < x_1 < ...... < x_n < d$. Further set $x_0 = 0$ and $x_{n+1} = d$. More explicitly,

$$\sum_{i=0}^{n+1} \dot{a}_i(t)\phi_i(x_j) = \alpha \sum_{i=0}^{n+1} a_i(t) \frac{\partial^2 \phi_i(x_j)}{\partial^2 x} \quad j = 1, \ldots, n \tag{13}$$

$$q_i(t) = -\kappa \sum_{i=0}^{n+1} a_i(t) \frac{\partial \phi_i(x_0)}{\partial x} \tag{14}$$

$$T_e(t) = \sum_{i=0}^{n+1} a_i(t)\phi_i(x_{n+1}) \tag{15}$$

$$a_i(0) = 0 \quad i = 0, \ldots, n+1 \tag{16}$$

Note that the approximate temperature at $x = 0$ is given by

$$T_n(x_0, t) = \sum_{i=0}^{n+1} a_i(t)\phi_i(x_0) \tag{17}$$

Setting $a(t) = (a_1(t), \ldots, a_n(t))^T$, equations (13), (14), (15) and (17) can be rewritten in the standard state space form. It is then a dynamical system of order n with $T_n(x_0)$ as the output, $(q_i(t), T_e(t))^T$ as the input and $a(t)$ as the state vector. This dynamical system approximates the true system dynamics and asymptotically converges with respect to n to the true system.

The usage of collocation method gives us a lot of flexibility in choosing lower order models for the true system. The flexibility arises from

1. Position of collocation points ($\{x_i\}$).
2. Choice of basis functions ($\{\phi_i\}$).
3. Number of collocation points (n).

Selections of collocation points and polynomials are interlinked with each other. They determine the accuracy and the computational complexity of the models. A Chebyshev collocation scheme uses Chebyshev polynomials and an associated set of collocation points, which leads to elegant and accurate computational algorithms.

The number of collocation points determine the model order. Naturally one likes to have a model order as small as possible without compromising on accuracy. The primary objective of this paper is to give guidelines on what model order to choose.

2.4 Chebyshev collocation

As mentioned earlier, we use Chebyshev collocation to obtain approximate models. We first briefly discuss about Chebyshev collocation and then construct approximate models.

Let P_{n+1} be the vector space of polynomials of degree less than or equal to $n+1$, with inner product

$$< u, v >= \int_{-1}^{1} \frac{u(x)v(x)}{\sqrt{1-x^2}} dx \tag{18}$$

where $u(x), v(x) \in P_{n+1}$.

Chebyshev polynomials are defined by the recurrence relation

$$C_{i+1}(x) = 2xC_i(x) - C_{i-1}(x) \quad i \geq 1 \tag{19}$$

with $C_0(x) = 1$ and $C_1(x) = x$. Alternatively, one can also define Chebyshev polynomials as

$$C_i(x) = \cos(i \cos^{-1}(x)) \quad i \geq 0 \tag{20}$$

Lemma 1. *The definitions (19) and (20) of the Chebyshev polynomials are equivalent.*

Proof. See appendix.

Lemma 2. *The set $\{C_i(x)\}_{i=0}^{n+1}$ forms an orthogonal basis for the space P_{n+1}.*

Proof. See appendix.

Let

$$x_k = \cos\left(\frac{\pi k}{n+1}\right) \quad k = 0, 1, \ldots, n+1. \tag{21}$$

Note that

$$|C_{n+1}(x_j)| = 1 \quad j = 0, 1, \ldots, n+1. \tag{22}$$

$$C_j(x_k) = C_k(x_j) = \cos(\frac{\pi jk}{n+1}) \quad j, k = 0, 1, \ldots, n+1. \tag{23}$$

In this work, we use a kind of Chebyshev collocation, as proposed by Gottlieb in [2]. In this collocation, we define $n+1$ degree polynomial

$$g_j(x) = \frac{2}{(n+1)c_j} \sum_{k=0}^{n+1} \frac{C_k(x)C_k(x_j)}{c_k} \quad j = 0, \ldots, n+1 \tag{24}$$

where

$$\begin{aligned} c_0 &= c_{n+1} = 2 \\ c_j &= 1 \quad j = 1, 2, \ldots, n \end{aligned} \tag{25}$$

and x_j as defined in (21).

Lemma 3. *The set $\{g_j(x)\}_{j=0}^{n+1}$ forms a basis for the space P_{n+1}.*

Proof. See appendix.

We use $\{g_j(x)\}_{j=0}^{n+1}$ as the basis functions for our collocation procedure, instead of $\{C_j(x)\}_{j=0}^{n+1}$. The reasons for using $g_j(x)$ instead of $C_j(x)$ will become apparent as we proceed.

Lemma 4. *Let $h(x)$ be a polynomial of degree $2n+1$. Then it holds that*

$$\int_{-1}^{1} \frac{h(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{n+1} \sum_{k=0}^{n+1} \frac{h(x_k)}{c_k} \tag{26}$$

where c_k are as given in equation (25) and the points x_k are given by (21).

Proof. See appendix.

Remark: Lemma 3 is normally referred to as **Gauss Lobatoo quadrature formula**, for details refer to [2].

Lemma 5. *For the polynomials $g_j(x)$ as defined in (24), it holds,*

$$g_j(x_k) = \delta_{jk} \quad j, k = 0, \dots, n+1 \tag{27}$$

where x_k is given by (21), and δ_{jk} is the Kronecker delta.

Proof. See appendix.

Since we use $\{g_j(x)\}_{j=0}^{n+1}$ as the basis functions for the collocation procedure, the approximate solution (12) of the PDE is given by

$$T_n(x,t) = \sum_{j=0}^{n+1} a_j(t) g_j(x) \tag{28}$$

Observe that

$$T_n(x_k,t) = \sum_{j=0}^{n+1} a_j(t) g_j(x_k) \tag{29}$$

Since $g_j(x_k) = \delta_{jk}$ from Lemma 4, we can see that

$$T_n(x_k,t) = a_k(t), \tag{30}$$

which gives a natural interpretation of the state $a_k(t)$. Using (30), (28) can be rewritten as

$$T_n(x,t) = \sum_{j=0}^{n+1} T_n(x_j,t) g_j(x). \tag{31}$$

2.5 Chebyshev collocation methods applied to the heat diffusion model

We are now soon ready to apply Chebyshev collocation to our problem. But before that we transform the coordinates from $[0, d]$ to $[-1, 1]$. This is easily achieved by the transformation

$$z = \frac{x - \frac{d}{2}}{\frac{d}{2}} \tag{32}$$

which leads to the following transformation on (1) - (3).

$$\frac{\partial T(z,t)}{\partial t} = \frac{4\alpha}{d^2}\frac{\partial^2 T(z,t)}{\partial z^2} \tag{33}$$

with boundary constraints

$$q_i(t) = -\frac{2\kappa}{d}\frac{\partial T(z,t)}{\partial z}\,|_{z=-1}, \tag{34}$$

$$T_e(t) = T(1,t) \tag{35}$$

and initial condition $T(z,t) = 0$. For the sake of convenience and also to keep up with the earlier notations we refer to z as x from now on.

Let $T_n(x,t)$ be the Chebyshev collocation approximation of $T(x,t)$. Thus $T_n(x,t)$ satisfies the PDE (33),(34) and (35) at the collocation points.

$$\frac{\partial T_n(x,t)}{\partial t}\,|_{x=x_j} = \frac{4\alpha}{d^2}\sum_{k=0}^{n+1} T_n(x_k,t)g_k^{''}(x)_{|x=x_j} \quad j = 1,\dots,n \tag{36}$$

$$q_i = -\frac{2\kappa}{d}\sum_{k=0}^{n+1} T_n(x_k,t)g_k^{'}(x_{n+1}) \tag{37}$$

$$T_e(t) = T_n(x_0,t) \tag{38}$$

Equation (37) implies

$$T_n(x_{n+1},t) = \frac{-\frac{q_i d}{2\kappa} - \sum_{k=1}^{n} T_n(x_k,t)g_k^{'}(x_{n+1}) - T_e(t)g_0^{'}(x_{n+1})}{g_{n+1}^{'}(x_{n+1})} \tag{39}$$

Note that $T_i(t) = T_n(x_{n+1},t)$.

Plugging (39) into (36) we have

$$\begin{aligned}\dot{T}_n(x_j,t) = {} & \frac{-2\alpha q_i(t)g_{n+1}^{''}(x_j)}{d\kappa g_{n+1}^{'}(x_{n+1})} + \frac{4\alpha}{d^2}\sum_{k=1}^{n} T_n(x_k,t)(g_k^{''}(x_j) - \frac{g_{n+1}^{''}(x_j)g_k^{'}(x_{n+1})}{g_{n+1}^{'}(x_{n+1})}) \\ & + T_e(t)\frac{4\alpha}{d^2}(g_0^{''}(x_j) - \frac{g_{n+1}^{''}(x_j)g_0^{'}(x_{n+1})}{g_{n+1}^{'}(x_{n+1})})\end{aligned} \tag{40}$$

Setting $x = (T_n(x_1), \dots, T_n(x_n))$ we can write the system of equations (37), (38) and (40) in the standard state space form.

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx + Du \end{aligned} \tag{41}$$

where

$$a_{ij} = \frac{4\alpha}{d^2}\left(g_j''(x_i) - \frac{g_{n+1}''(x_i)g_j'(x_{n+1})}{g_{n+1}'(x_{n+1})}\right) \quad i,j = 1,\dots,n \tag{42}$$

$$b_{j1} = \frac{-2\alpha}{d\kappa}\frac{g_{n+1}''(x_j)}{g_{n+1}'(x_{n+1})} \quad j = 1,\dots,n \tag{43}$$

$$b_{j2} = \frac{4\alpha}{d^2}\left(g_0''(x_j) - \frac{g_{n+1}''(x_j)g_0'(x_{n+1})}{g_{n+1}'(x_{n+1})}\right) \quad j = 1,\dots,n \tag{44}$$

$$C = \left(-\frac{g_1'(x_{n+1})}{g_{n+1}'(x_{n+1})}, \dots, -\frac{g_n'(x_{n+1})}{g_{n+1}'(x_{n+1})}\right) \tag{45}$$

$$D = \left(-\frac{d}{2\kappa g_{n+1}'(x_{n+1})}, -\frac{g_0'(x_{n+1})}{g_{n+1}'(x_{n+1})}\right) \tag{46}$$

Note that, to construct the matrices A, B, C and D, one has to obtain the first and the second derivatives of $g_j(x)$ evaluated at the collocation points.

2.6 Derivatives of $g_j(x)$

One can in fact rather easily compute the derivatives of $g_j(x)$. The following lemma will be useful for that purpose.

Lemma 6. *Introduce*

$$G_j(x) \triangleq \frac{1-x^2}{c_j(n+1)^2}\frac{C_{n+1}'(x)}{x-x_j}(-1)^{j+1} \quad j = 0,\dots,n+1 \tag{47}$$

Then it holds that

$$g_j(x) = G_j(x) \quad j = 0, 1, \dots, n+1$$

Proof. See appendix.

We now proceed to compute the derivatives of $g_j(x)$, but before that, let us fix some notations first. Let

$$T_n \triangleq (T_n(x_0,t), \dots, T_n(x_{n+1},t))^T, \tag{48}$$

then

$$T_n' = (T_n'(x_0,t),\dots,T_n'(x_{n+1},t))^T \tag{49}$$
$$= (\sum_{j=0}^{n+1} T_n(x_j,t)g_j'(x_0),\dots,\sum_{j=0}^{n+1} T_n(x_j,t)g_j'(x_{n+1}))^T \tag{50}$$
$$\triangleq \mathcal{D}T_n \tag{51}$$

where

$$(\mathcal{D})_{kj} = (g_k'(x_j))_{(n+1\times n+1)} \quad j,k=0,\dots n+1 \tag{52}$$

and

$$T_n'' = (T_n''(x_0,t),\dots,T_n''(x_{n+1},t))^T \tag{53}$$
$$= (\sum_{j=0}^{n+1} T_n(x_j,t)g_j''(x_0),\dots,\sum_{j=0}^{n+1} T_n(x_j,t)g_j''(x_{n+1}))^T \tag{54}$$
$$\triangleq \mathcal{A}T_n \tag{55}$$

where

$$(\mathcal{A})_{kj} = (g_k''(x_j))_{(n+1\times n+1)} \quad j,k=0,\dots n+1 \tag{56}$$

Theorem 1. *The elements of the matrix $\mathcal{D}$ are given by*

$$\frac{\partial g_j(x)}{\partial x}\mid_{x=x_k}= \begin{cases} \frac{c_k}{c_j}\frac{(-1)^{j+k}}{x_k-x_j} & j\neq k \\ \frac{-x_j}{2(1-x_j^2)} & 0\neq j=k\neq n+1 \\ \frac{2(n+1)^2+1}{6} & j=k=0 \\ -\frac{2(n+1)^2+1}{6} & j=k=n+1 \end{cases} \tag{57}$$

It also holds that

$$\mathcal{A} = \mathcal{D}^2 \tag{58}$$

Proof. See appendix. (Most of the proof is patterned after [2]).

2.7 Transfer functions of the approximate models

Rewriting (41) in the input-output form we have

$$Y(s) = [G_n^1(s) \;\; G_n^2(s)]\, U(s) \tag{59}$$

where

$$Y(s) = T_i(s) \tag{60}$$

$$G_n^1(s) = D_1 + C(sI - A)^{-1}B_1 \tag{61}$$

$$G_n^2(s) = D_2 + C(sI - A)^{-1}B_2 \tag{62}$$

$$U(s) = [q_i(s), T_e(s)]^T \tag{63}$$

The quantities $q_i(s)$, $T_e(s)$ and $T_i(s)$ are the Laplace transforms of $q_i(t)$, $T_e(t)$ and $T_i(t)$ respectively, and the subscript n in $G_n^1(s)$ and $G_n^2(s)$ denotes the order of approximation. B_1, B_2 are the column vectors of B.

Figures 2 and 3 the true transfer functions G_1 and G_2, respectively, along with their approximations (61) and (62) for different model orders n. The appropriate choice of the model order depends on the frequency contents of the inputs. For example, if the input signals are of low frequency character, then one can use lower order models, otherwise one would have to use higher order models. Also note form Figures 2 and 3, that G_2 is approximated better than G_1 for a given n. In G_1 there is a noticeable frequency leakage which gets damped as the model order is increased.

From (8), one can observe that the effect of α on the true transfer functions $G_1(s)$ and $G_2(s)$ is merely a rescaling of the frequency axis, as $G_1(s)$ and $G_2(s)$ can also be considered as functions of $\frac{s}{\alpha}$. One would expect the effect of α to be same on the approximate transfer functions $G_n^1(s)$ and $G_n^2(s)$ also. It can be noted from (42)-(46) that the way α influences $G_n^1(s)$ and $G_n^2(s)$ is as a multiplicative factor of A and B. Hence we may write the transfer functions as

$$\begin{aligned} G_n^i(s) &= D_i + C[sI - \alpha A_0]^{-1}\alpha B_{i0} \\ &= D_i + C[\frac{s}{\alpha}I - A_0]^{-1}B_{i0} \quad i = 1, 2 \end{aligned} \tag{64}$$

where A_0 and B_{i0} do not depend on α . This calculation shows that the influence of α on G_n^i is merely a rescaling of the frequency axis. One can also see from equations (8), (43) and (46) that, the parameter κ just scales the magnitude of $G_1(s)$ and $G_n^1(s)$ by a factor $\frac{1}{\kappa}$ and has no effect on $G_2(s)$ and $G_n^2(s)$.

3 Parameter estimation

As mentioned earlier we estimate α and κ using the output error method, which is a standard least squares technique [6].

Sticking to the notations used earlier $y^m(t)$ be the model output and $y(t) = T_i(t)$ be the output of the true system. The following criterion function

$$V(\theta) := \frac{\sum_{k=0}^{N-1} [\, T_{n+1}(x_{n+1}, kh) - T_i(kh)]^2}{N} \tag{65}$$

is minimized to obtain the parameter estimate $\hat{\theta} = (\hat{\alpha}, \hat{\kappa})$.

Note that this estimate, though conceptually simple, is computationally complex. As $V(\theta)$ depends on θ in a highly nonlinear fashion, a numerical search procedure has to be used to compute $\hat{\theta}$. For each function evaluation, the PDE has to be solved for the current value of θ.

In this study we are primarily interested in the bias of the estimates $(\hat{\alpha}, \hat{\kappa})$ that results due to approximate models. We examine the bias of the estimates by using simulated data to estimate the parameter values for various model orders.

In the numerical study, the input signals q_i and T_e are generated as AR processes with a periodicity of 24 h. The system output T_i is computed from (8) with the true parameters $\alpha = 2$ m/s^2 and $\kappa = 1$ J/msK. The data sequences are of length $N = 16834$ and the sampling interval is 1 h.

Table 1: Model orders and their respective parameter estimates

Model order	$\hat{\alpha}$ m/s^2	$\hat{\kappa}$ J/msK	bias for α m/s^2	bias for κ J/msK
3	1.0306	1.9076	-0.9694	0.9076
5	2.0384	1.0524	0.0384	0.0524
7	2.0313	0.9838	0.0313	-0.0162
9	2.0116	0.9931	0.0116	-0.0069
11	2.0000	1.0003	-0.000309	0.000319

Figure 4 and Table 1 show the bias obtained for different model orders. All the above estimates use a standard nonlinear search with an initial guess of $\alpha = 10$ m/s^2 and $\kappa = 5$ J/msK.

Examination of the criterion function for the simulated data showed the presence of a local maxima at approximately $\alpha = 90$ m/s^2. An initial guess with $\alpha \geq 90$ m/s^2 leads to an estimate $\hat{\alpha}$ which is not meaningful, irrespective the initial guess taken for κ. This is not a big drawback, since in practice α lies between 1 m/s^2 and 3 m/s^2 most building materials.

3.1 Rate of convergence

From Figure 4 and Table 1, one can infer that the bias $|\hat{\theta} - \theta_0|$ converges to zero as n tends to ∞. To find out more about this convergence rate, we assume that

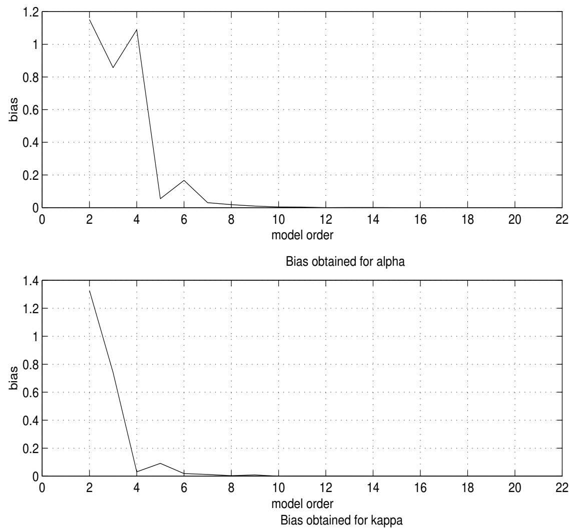

Figure 4: The bias got for α and κ for different model orders ($n = 3, 4, 5, 6, 7, 8, 9$).

$$|\hat{\alpha} - \alpha_0| \approx \frac{C_\alpha}{n^a} \tag{66}$$

$$|\hat{\kappa} - \kappa_0| \approx \frac{C_\kappa}{n^a} \tag{67}$$

where C_α, C_κ and a are constants. Note that if C_α, C_κ and a were known then one can choose a model order depending on the bias, one wishes to tolerate.

From equations (66) and (67) we have

$$\log_{10} |\hat{\alpha} - \alpha_0| = \log_{10} C_\alpha - a \log_{10} n \tag{68}$$

$$\log_{10} |\hat{\kappa} - \kappa_0| = \log_{10} C_\kappa - a \log_{10} n \tag{69}$$

To determine C_α, C_κ and a, one may examine plots of $\log_{10} |\hat{\alpha} - \alpha_0|$ vs $\log_{10} n$ and $\log_{10} |\hat{\kappa} - \kappa_0|$ vs $\log_{10} n$. If the assumptions (66) and (67) were right, the plots would be approximately straight lines with slope $-a$ and intercepts C_α and C_κ respectively. Figure 5 shows that, the plots are approximately straight lines, for large values of n, both for α and κ . For α, a is approximately 5.2 and C_α is approximately 2.63 m/s^2. For κ, a is approximately 6.5 and C_κ is approximately 3.23 J/msK.

Though the assumptions (66) and (67) are heuristic, they are well supported by the simulation results and are not surprising even from a theoretical point of

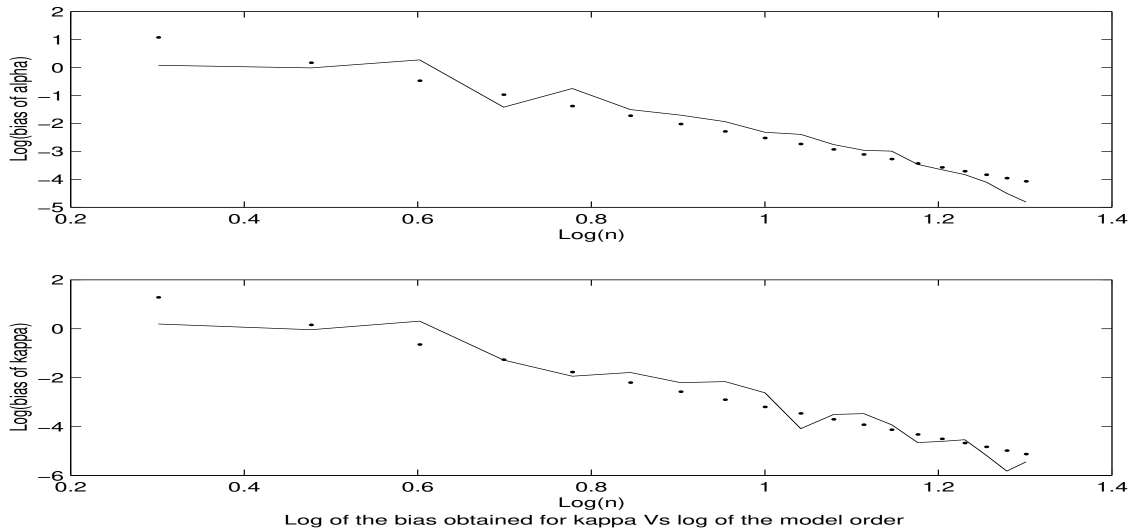

Figure 5: Dotted lines represent the straight lines with slope a and intercept C for α and κ.

view, since the problem is well posed and has a smooth solution. It is known, [2] that the accuracy of numerical solution using Chebyshev collocation converges very quickly with n.

Note that, it is also worthwhile to look into the rate of convergence of the approximate transfer functions G_i^n $i = 1, 2$, to their respective true transfer functions G_i, $i = 1, 2$.

In order to get an idea about the rate of convergence of the transfer functions, we plot the deviation of the transfer functions $\mid G_i^n(i\omega) - G_i(i\omega) \mid$ at different frequency points ω.

Note that, from (8), (43) and (46), parameter κ has no effect on the rate of convergence of the transfer functions, and as for the parameter α, from (8) and (64), we can see that it's effect can be dispensed of by considering $\mid G_i^n(i\frac{\omega}{\alpha}) - G_i(i\frac{\omega}{\alpha}) \mid$ rather than $\mid G_i^n(i\omega) - G_i(i\omega) \mid$, since the effect of the parameter α is merely that of rescaling the frequency axis.

From Figure 6, we can observe that the deviation increases with increase in frequency and flattens out to a constant value at high frequencies. This conclusion is also supported by extensive simulations done at the higher frequencies, see Table 2.

Experiments done in Figure 6 and Table 2 indicate that the rate of convergence is low for higher frequencies, and the deviation ($\mid G_i^n(\frac{i\omega}{\alpha}) - G_i(i\frac{\omega}{\alpha}) \mid$, for $i = 1, 2$) of the transfer functions increases with increase in frequency and has an asymptotic least upper bound, that is, it reaches a maximum at $\omega = \infty$.

Since the convergence of the transfer functions is guaranteed at all frequencies and the deviation being maximum at $\omega = \infty$ for a given model order, one can

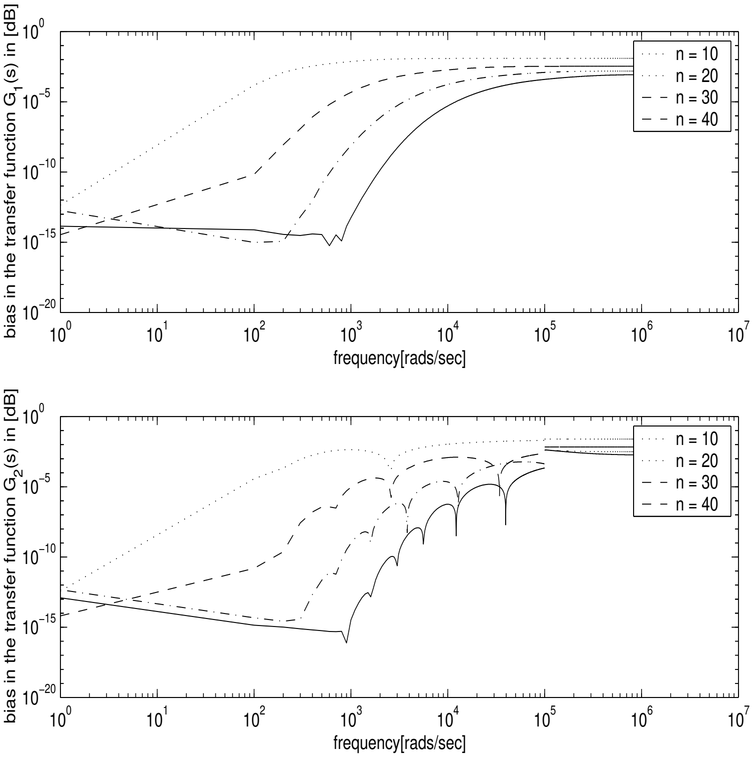

Figure 6: Absolute value of the deviation of the transfer functions $G_1(i\frac{\omega}{\alpha})$ and $G_2(i\frac{\omega}{\alpha})$ from the approximate transfer functions $G_n^1(i\frac{\omega}{\alpha})$ and $G_n^2(i\frac{\omega}{\alpha})$(as defined in (64)) for different model orders ($n = 10,\ 20,\ 30,\ 40$).

Table 2: Absolute value of the deviation in the transfer functions at higher frequencies

Model order	$\omega[rads/sec]$	bias in $G_1^n(i\omega)$	bias in $G_2^n(i\omega)$
10	2000000	0.0123	0.0247
	4000000	0.0123	0.0247
	6000000	0.0123	0.0247
	8000000	0.0123	0.0247
20	2000000	0.0034	0.0068
	4000000	0.0034	0.0068
	6000000	0.0034	0.0068
	8000000	0.0034	0.0068
30	2000000	0.0016	0.0031
	4000000	0.0016	0.0031
	6000000	0.0016	0.0031
	8000000	0.0016	0.0031
40	2000000	0.0008854	0.00018
	4000000	0.0008904	0.00018
	6000000	0.0008913	0.00018
	8000000	0.0008916	0.00018

obtain a worst case scenario for the rate of convergence of the transfer functions by looking at the rate of convergence at $\omega = \infty$.

For $\omega = \infty$, the response of the true transfer functions are 0, and the response of the approximate transfer functions are D_1 and D_2 respectively, which from (46) is

$$D_1 = \frac{1}{g'_{n+1}(x_{n+1})} \tag{70}$$

$$D_2 = -\frac{g'_0(x_{n+1})}{g'_{n+1}(x_{n+1})}. \tag{71}$$

From Theorem 1, we know that

$$g'_{n+1}(x_{n+1}) = -\frac{2(n+1)^2+1}{6} \tag{72}$$

$$g'_0(x_{n+1}) = \frac{(-1)^n}{2}. \tag{73}$$

Hence

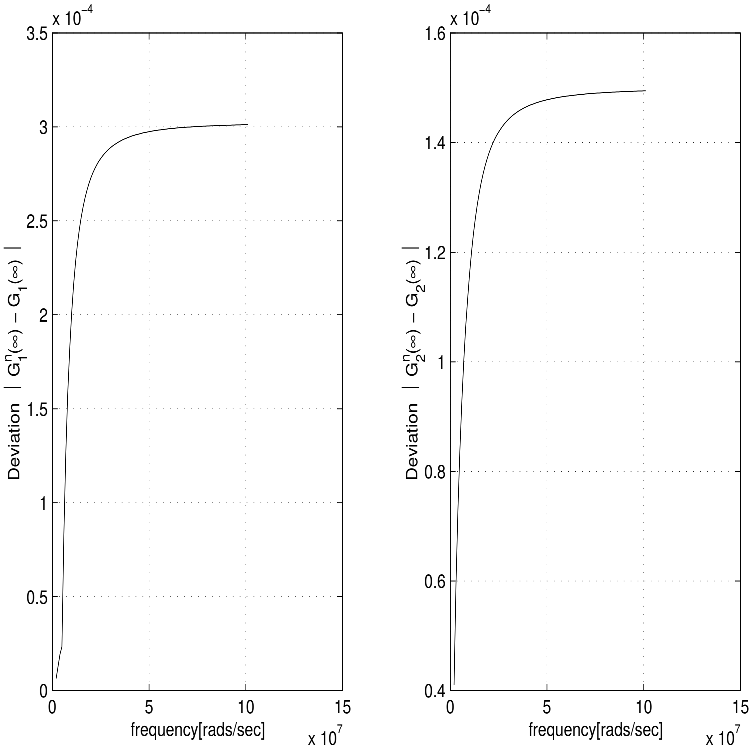

Figure 7: Deviation of the transfer functions at high frequencies for $n = 100$

$$D_1 = \frac{-6}{2(n+1)^2+1} \tag{74}$$

$$D_2 = \frac{3(-1)^{n+1}}{2(n+1)^2+1}, \tag{75}$$

and for large values of n

$$D_1 \approx -\frac{3}{n^2} \tag{76}$$

$$D_2 \approx -\frac{3(-1)^n}{2n^2}, \tag{77}$$

which implies that

$$\mid G_1^n(\infty) - G_1(\infty) \mid \approx \frac{3}{n^2} \tag{78}$$

$$\mid G_2^n(\infty) - G_2(\infty) \mid \approx \frac{3}{2n^2} \tag{79}$$

for large values of n.

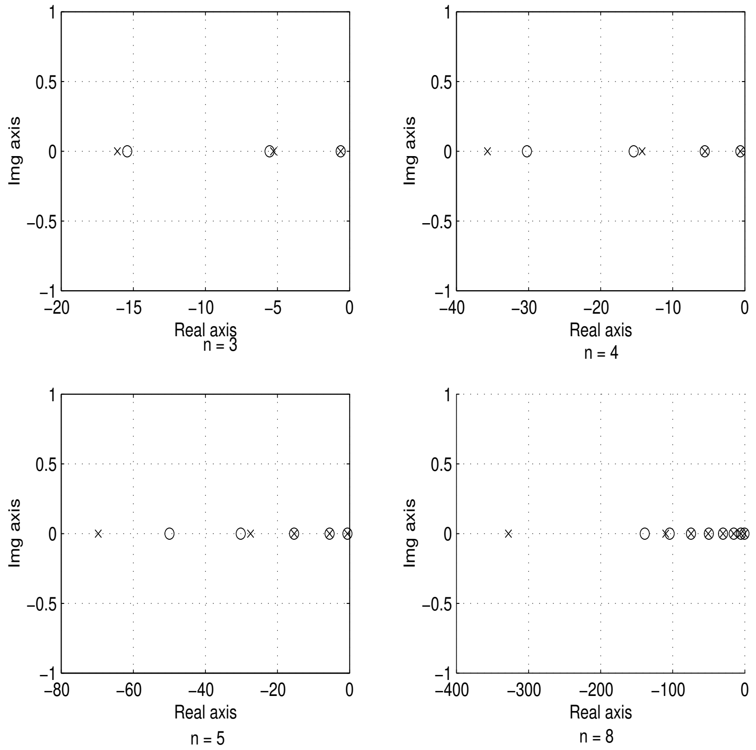

Figure 8: True system poles (marked 'x') and approximate system poles (marked 'o'

Figure 7 shows the deviation $\mid G_i^n(i\frac{\omega}{\alpha}) - G_i(i\frac{\omega}{\alpha}) \mid$ at high frequencies, for $n = 100$. One can see that the curves flatten out close to 3 x 10^{-4} and 1.5 x 10^{-4}, which agrees with our theoretical estimates in (78) and (79), respectively.

Hence, the transfer functions converge at a rate, which is at least as fast as $O(\frac{1}{n^2})$.

3.2 Convergence of Poles

From (9), we know that the true system has poles at

$$\frac{s}{\alpha} = -\frac{(2k-1)^2}{d^2}\frac{\pi^2}{4} \quad k = 1, 2, 3, \ldots\ldots. \tag{80}$$

Since the linear system (41), approximates the true system, the eigenvalues of A_0 in (64) which are the poles of the approximate system should be close to the true system poles (80).

Since the approximate system has only a finite number of poles, as opposed to the true system which has infinite number of poles, it is of interest to know, how close are the approximate system poles to the true system poles and what is the pattern of convergence as $n \to \infty$.

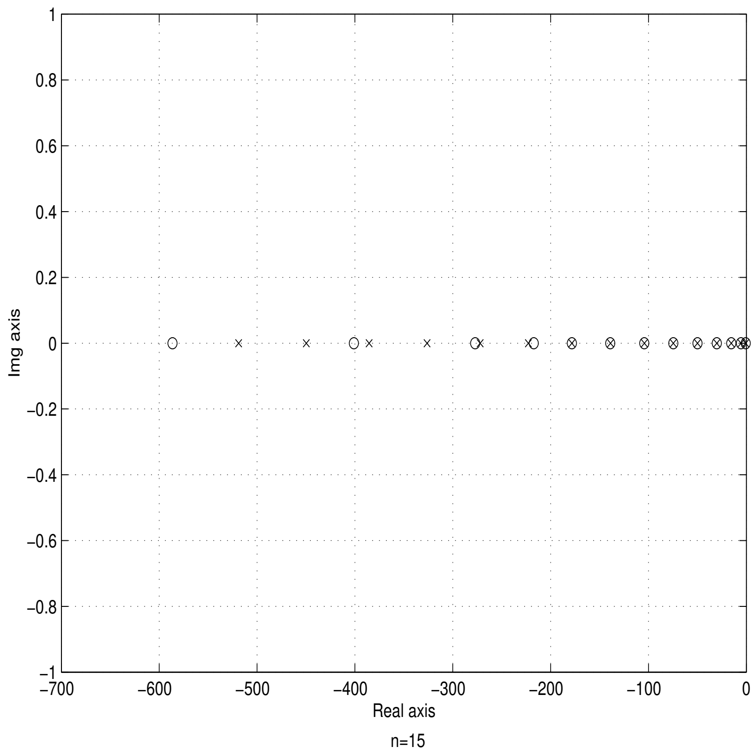

Figure 9: True system poles (marked 'x') and approximate system poles (marked 'o'

For the system (8), which has poles as shown in (80), to be well approximated in the time domain, poles that are close to the origin must be well approximated. Effects of the poles that are far away from the origin (fast poles) become less and less siginificant as $t \to \infty$.

Looking at the system in the frequency domain, for low frequencies, poles close to the origin contribute more to the magnitude of the transfer functions, as compared to the poles far away from the origin, which have almost negligible contribution. As the frequency ω increases more and more poles start playing a role in the magnitude of the transfer functions, with many of them having effects that are almost equal to the effects produced by the poles close to the origin. In fact as $\omega \to \infty$ almost all the poles have nearly equal effect on the magnitude of the the transfer functions. Hence from a frequency point of view it is important to know study the convergence of the poles, including the ones that are far away from the origin.

From the Figures 8 and 9, we can see that for a given model order n, the $n \times n$ matrix A_0 has n distinct eigenvalues (n distinct poles) and all of them are negative. A closer look at the figures would reveal that the poles close to origin are better approximated than the poles far away from the origin. In fact one can conclude that, given a model of order $n \geq 4$, at least the first $\frac{n}{2}$ poles (the poles (80) with $k = 1, \dots, \frac{n}{2}$) are well approximated.

Figure 10 shows the deviation of the eigenvalues of the approximate system from the true system poles, for the first five poles, that is for $k = 1, 2, \dots, 5$ in (80). Figure 10 suggests that poles close to the origin converge much faster than the poles away form the origin.

4 Conclusions

A grey box modeling of a diffusion process was considered. The use of a nonlinear search in the estimation part makes it computationally complex, as each iteration in the search procedure requires the PDE to be solved for the current value of parameter estimate. The primary concern in our study has been the effect of approximating the dynamics, which is of infinite order, by a finite order model. A large model order approximates the system dynamics very well, thus improving the estimates but it also increases the computational load. A low model order leads to a large bias. Simulation studies indicate that the choice of model order can be linked with the spectral content of the input signals.

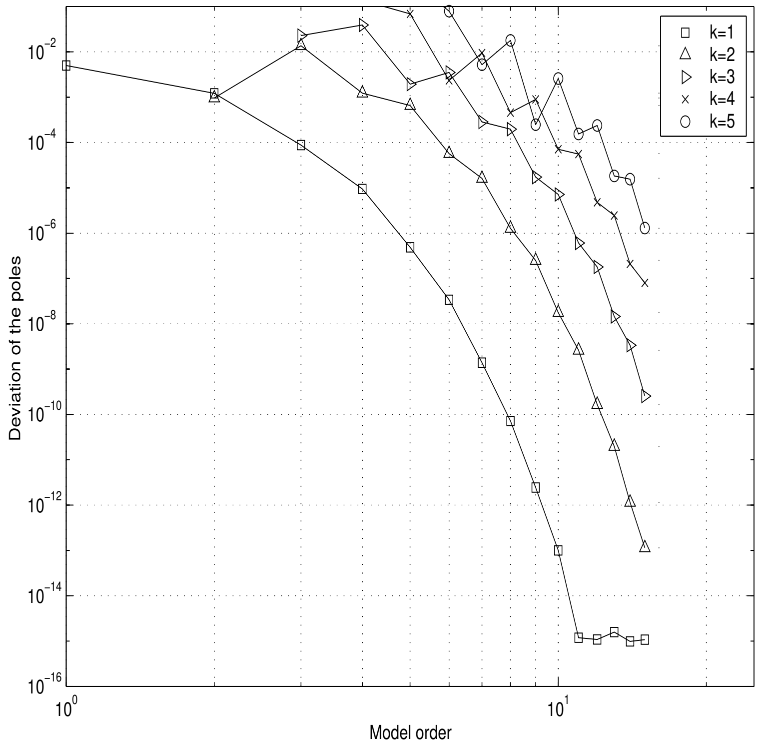

Figure 10: Deviation of the eigen values of the approximate system from the true system poles, for the first five poles close to the origin

5 Appendix

Derivatives of Chebyshev polynomials:

The following results will be used while proving some of the lemmas. First recall (20)

$$C_m(x) = \cos(m\cos^{-1}(x))$$

Straightforward differentiation of $C_m(x)$ leads to

$$C'_m(x) = \frac{m\sin(m\cos^{-1}(x))}{\sqrt{1-x^2}}, \quad x^2 \neq 1 \tag{81}$$

Hence

$$C'_{n+1}(x_k) \quad = \quad 0 \quad k = 1, 2, \dots, n \tag{82}$$

where x_k are as defined in (21). Applying L'Hospitals rule for the cases $k = 0$ and $n + 1$, we have

$$C'_{n+1}(x_{n+1}) = (-1)^n(n+1)^2, \tag{83}$$

$$C'_{n+1}(x_0) = (n+1)^2. \tag{84}$$

Also note that, for $m = 1, 2, \dots, n$, we have

$$C'_m(x_{n+1}) = (-1)^{m-1}m^2 \tag{85}$$

$$m = 1, \dots, n$$

$$C'_m(x_0) = m^2 \tag{86}$$

Straightforward differentiation of (81) leads to

$$C''_m(x) = \frac{-m^2\cos(m\cos^{-1}(x)) + m\sin(m\cos^{-1}(x))\frac{x}{\sqrt{1-x^2}}}{1-x^2} \quad x^2 \neq 1 \tag{87}$$

Proof of Lemma 1:

Recall the trigonometric identity

$$\cos m\theta \cos n\theta = \frac{1}{2}[\cos(m+n)\theta + \cos(m-n)\theta]. \tag{88}$$

With the change of variable $x = \cos\theta$ and use of (20), (88) becomes

$$C_m(x)C_n(x) = \frac{1}{2}[C_{m+n}(x) + C_{m-n}(x)].$$

Setting $m = 1$, and noting that $C_1(x) = x$, we have

$$xC_n(x) = \frac{1}{2}[C_{n+1}(x) + C_{n-1}(x)]$$

which can easily be rewritten as (19). ■

Proof of Lemma 2:

Recall the trigonometric integral (use (88), for example)

$$\int_0^\pi \cos n\theta \cos m\theta \, d\theta = d_n \delta_{mn} \tag{89}$$

where

$$d_0 = \pi, \quad d_n = \frac{\pi}{2} \ \ (n \neq 0) \tag{90}$$

and δ_{mn} is the Kronecker delta.

With the usual change of variable, $x = \cos\theta$ and use of (20), (89) becomes

$$\int_{-1}^{1} \cos\left(n\cos^{-1}(x)\right) \cos\left(m\cos^{-1}(x)\right) \frac{dx}{\sqrt{1-x^2}} = d_n \delta_{mn}.$$

which can be rewritten using (20) as

$$\int_{-1}^{1} \frac{C_n(x)C_m(x)}{\sqrt{1-x^2}} dx = d_m \delta_{mn}. \tag{91}$$

Hence the set $\{C_i(x)\}_{i=0}^{n+1}$, is a set of $n+1$ orthogonal polynomials, and therefore orthogonal basis for the space P_{n+1}. ■

Proof of Lemma 3:

A necessary and sufficient condition for the set $\{g_j(x)\}_{j=0}^{n+1}$ to be linearly independent is that the expression

$$\sum_{j=0}^{n+1} \alpha_j g_j(x) = 0 \quad \text{for all } x \tag{92}$$

implies that

$$\alpha_j = 0 \quad j = 0, 1, \ldots, n+1 \tag{93}$$

Let us assume that the expression (92) is true and prove that it implies (93).

Since from (24) we know that

$$g_j(x) = \frac{2}{(n+1)c_j} \sum_{k=0}^{n+1} \frac{C_k(x)C_k(x_j)}{c_k} \quad j = 0, \ldots, n+1,$$

(92) implies that

$$\sum_{j=0}^{n+1} \alpha_j g_j(x) = \sum_{k=0}^{n+1} \frac{2}{(n+1)c_k} \left(\sum_{j=0}^{n+1} \alpha_j \frac{C_k(x_j)}{c_j} \right) C_k(x) = 0. \tag{94}$$

Using (23) the above equation can be rewritten as

$$\sum_{k=0}^{n+1} \frac{2}{(n+1)c_k} \left(\sum_{j=0}^{n+1} \alpha_j \frac{C_j(x_k)}{c_j} \right) C_k(x) = 0. \tag{95}$$

Since $\{C_k(x)\}_{j=0}^{n+1}$ forms an orthogonal basis for P_{n+1}, from (95) we have

$$\sum_{j=0}^{n+1} \alpha_j \frac{C_j(x_k)}{c_j} = 0 \quad k = 0, 1, \ldots, n+1. \tag{96}$$

Rewriting (96) in matrix form gives

$$\begin{bmatrix} C_0(x_0) & C_1(x_0) & \ldots C_{n+1}(x_0) \\ C_0(x_1) & C_1(x_1) & \ldots C_{n+1}(x_1) \\ \vdots & \vdots & \vdots \\ C_0(x_{n+1}) & C_1(x_{n+1}) & \ldots C_{n+1}(x_{n+1}) \end{bmatrix} \begin{bmatrix} \alpha_0/c_0 \\ \alpha_1/c_1 \\ \alpha_2/c_2 \\ \vdots \\ \alpha_{n+1}/c_{n+1} \end{bmatrix} = 0 \tag{97}$$

To prove that (97) implies $\alpha_k = 0, \; k = 0, \ldots, n+1$, we adopt the following procedure. Let

$$Q(x) \triangleq \sum_{k=0}^{n+1} \alpha_k C_k(x), \tag{98}$$

where α_k are as defined in (92).

Note that $Q(x)$ is a polynomial of degree $n+1$. From (97) we can see that

$$Q(x_j) = 0 \quad j = 0, 1, \ldots, n+1. \tag{99}$$

Hence $Q(x) = 0$ at $n+2$ distinct points. Since $Q(x)$ is a polynomial of degree $n+1$, it must be identically zero:

$$Q(x) = \sum_{k=0}^{n+1} \alpha_k C_k(x) \quad \equiv \quad 0 \quad \text{for all } x \tag{100}$$

Since $\{C_k(x)\}_{k=0}^{n+1}$ forms a basis, α_k must be equal to 0 for all $k = 0, 1, \dots, n+1$. ■

Proof of Lemma 4:

Since any polynomial of degree n, defined on $[-1, 1]$, can be written as a linear combination of Chebyshev polynomials up to degree n, it is enough to check the validity of (26) for $C_k(x)$, $0 \le k \le 2n+1$.

We start by checking (26) for $C_0(x) = 1$. In this case the right hand side of (26) is

$$\frac{\pi}{n+1} \sum_{j=0}^{n+1} \frac{1}{c_j} = \pi$$

and the left hand side is

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} dx = \sin^{-1}(x) \mid_{-1}^{1} = \pi$$

Let, now $k > 0$, and consider (26) for $h(x) = C_k(x)$. The left hand side is clearly zero, since due to Lemma 2, $C_k(x)$ is orthogonal to the function $C_0(x) = 1$. The right hand side in this case is

$$\frac{\pi}{n+1} \sum_{j=0}^{n+1} \cos\left(\frac{k\pi j}{n+1}\right) \frac{1}{c_j}. \tag{101}$$

To prove that (101) is equal to zero, consider the two cases.

Case 1: Let k be odd.

Observe that

$$\begin{aligned} c_j &= c_{n+1-j} \\ \cos\left(\frac{\pi j k}{n+1}\right) &= -\cos\left(\frac{\pi(n+1-j)k}{n+1}\right). \end{aligned}$$

Using this in (101) gives

$$
\begin{aligned}
\frac{\pi}{n+1}\sum_{j=0}^{n+1}\cos\left(\frac{k\pi j}{n+1}\right)\frac{1}{c_j} &= \frac{\pi}{2(n+1)}\sum_{j=0}^{n+1}\left\{\cos\left(\frac{\pi jk}{n+1}\right)\frac{1}{c_j}+\cos\left(\frac{\pi(n+1-j)k}{n+1}\right)\frac{1}{c_{n+1-j}}\right\} \\
&= \frac{\pi}{2(n+1)}\sum_{j=0}^{n+1}\frac{1}{c_j}\left\{\cos\left(\frac{\pi jk}{n+1}\right)+\cos\left(\frac{\pi(n+1-j)k}{n+1}\right)\right\} \\
&= 0.
\end{aligned}
$$

Case 2: Let k be even.

Consider

$$
\sum_{j=0}^{n}\cos\left(\frac{k\pi j}{n+1}\right) = \mathrm{Re}\left(\sum_{j=0}^{n}\exp(i\frac{kj\pi}{n+1})\right).
$$

But, one can easily see that

$$
\left(\sum_{j=0}^{n}\exp(i\frac{kj\pi}{n+1})\right) = 0
$$

for k even. Hence

$$
\begin{aligned}
\sum_{j=0}^{n+1}\cos\left(\frac{k\pi j}{n+1}\right)\frac{1}{c_j} &= -\frac{1}{2}+\frac{(-1)^k}{2}+\mathrm{Re}\left(\sum_{j=0}^{n}\exp(i\frac{kj\pi}{n+1})\right) \\
&= 0 \qquad (102)
\end{aligned}
$$

and hence we have completed the proof of Lemma 4. ■

Proof of Lemma 5:

From (24), we can see that

$$
g_j(x_k) = \frac{2}{(n+1)c_j}\sum_{m=0}^{n+1}\frac{C_m(x_k)C_m(x_j)}{c_m} \qquad (103)
$$

Consider first the case, where either j or k is not equal to $n+1$. Using (23), we have

$$
g_j(x_k) = \frac{2}{(n+1)c_j}\sum_{m=0}^{n+1}\frac{C_k(x_m)C_j(x_m)}{c_m} \qquad (104)
$$

By using Gauss Lobatoo formula (26), we have

$$g_j(x_k) = \frac{2}{\pi c_j} \int_{-1}^{1} \frac{C_k(x) C_j(x)}{\sqrt{1-x^2}} dx \tag{105}$$

Since, from Lemma 2 we have

$$g_j(x_k) = 0 \quad j \neq k$$

and from (90), (91) and (105) we have

$$g_j(x_j) = 1 \quad .$$

Hence we have

$$g_j(x_k) = \delta_{jk} \quad j, k \neq n+1. \tag{106}$$

Finally consider the case, where both i and j are equal to $n+1$. Then

$$g_{n+1}(x_{n+1}) = \frac{2}{(n+1)c_{n+1}} \sum_{m=0}^{n+1} \frac{C_m(x_{n+1}) C_m(x_{n+1})}{c_m}. \tag{107}$$

Since $c_{n+1} = 2$ and $C_m(x_{n+1}) = (-1)^m$, compare (23), (107) becomes

$$g_{n+1}(x_{n+1}) = \frac{1}{(n+1)} \sum_{m=0}^{n+1} \frac{1}{c_m} = 1$$

Hence the lemma is proved. ■

Proof of Lemma 6: Note that the numerator

$$(1-x^2) C'_{n+1}(x), \tag{108}$$

of $G_j(x)$ is a polynomial of degree $n+2$.

From (82) and also from the fact $x_{n+1}^2 = x_0^2 = 1$, we can see that

$$x_k, \quad k = 0, 1, \ldots n+1,$$

are the roots of the polynomial (108). Hence the denominator $(x - x_j)$ is a factor of the numerator, which implies that $G_j(x)$ is a polynomial of degree $n+1$ for all $j = 0, 1, \ldots, n+1$.

Since both $G_j(x)$ and $g_j(x)$ are polynomials of degree $n+1$, it is enough to prove that both $G_j(x)$ and $g_j(x)$ agree at $n+2$ points.

We know that

$$g_j(x_k) = \delta_{jk} \quad j,k = 0,\ldots,n+1 \tag{109}$$

and it is hence sufficient to prove $G_j(x_k) = \delta_{jk}$.

To prove $G_j(x_k) = \delta_{jk}$, consider the following cases.

Case 1: $j \neq k$.

Note that $(1-x_k^2)C'_{n+1}(x_k) = 0$ for $k = 0,\ldots,n+1$, and hence

$$G_j(x_k) = 0 \quad j \neq k \tag{110}$$

Case 2: $j = k$.

We use L'Hospitals rule for this case. Applying L'Hospitals rule to (47), we get

$$G_j(x_j) = \frac{(-1)^{j+1}}{c_j(n+1)^2}\left(-2xC'_{n+1}(x) + (1-x^2)C''_{n+1}(x)\right)|_{x=x_j} \tag{111}$$

Note that from (81) and (87), we have

$$C''_{n+1}(x) = \frac{-(n+1)^2 C_{n+1}(x) + xC'_{n+1}(x)}{(1-x^2)} \tag{112}$$

Using (112) in (111) we get

$$G_j(x_j) = \frac{(-1)^{j+1}}{c_j(n+1)^2}\{-x_jC'_{n+1}(x_j) - (n+1)^2C_{n+1}(x_j)\} \tag{113}$$

Remember that $C_{n+1}(x_j) = (-1)^j$, see (23), and now consider the following subcases

When $0 \neq j \neq n+1$, $C'_{n+1}(x_j) = 0$ and (113) becomes

$$G_j(x_j) = \frac{1}{c_j} = 1. \tag{114}$$

When $j = 0$, $C'_{n+1}(x_0) = (n+1)^2$, see (84), and (113) becomes

$$G_0(x_0) = \frac{(-1)^1}{c_0(n+1)^2}\{-2(n+1)^2\} = 1. \tag{115}$$

When $j = n+1$, $C'_{n+1}(x_{n+1}) = (-1)^n(n+1)^2$, see (83), and (113) becomes

$$G_{n+1}(x_{n+1}) = \frac{(-1)^{n+2}}{c_{n+1}(n+1)^2}\{2(-1)^{n+2}(n+1)^2\} = 1. \tag{116}$$

From (110), (114), (115) and (116), we can see that

$$G_j(x_k) = \delta_{jk}$$

and hence the lemma is proved. ∎

Proof of Theorem 1: Since $g_j(x) = G_j(x)$ for any x and $j = 0, \ldots, n+1$, the derivatives of $g_j(x)$ must be equal to the derivatives of $G_j(x)$ for all x.

Straightforward differentiation of $G_j(x)$, (47), gives

$$\begin{aligned} G'_j(x) &= \frac{(-1)^{j+1}C''_{n+1}(x)(1-x^2)}{c_j(n+1)^2(x-x_j)} - \frac{(-1)^{j+1}2xC'_{n+1}(x)}{c_j(n+1)^2(x-x_j)} \\ &\quad - \frac{(-1)^{j+1}C'_{n+1}(x)(1-x^2)}{c_j(n+1)^2(x-x_j)^2}. \end{aligned} \tag{117}$$

Using (87), we can rewrite (117) as

$$\begin{aligned} G'_j(x) &= \frac{(-1)^{j}C_{n+1}(x)}{c_j(x-x_j)} + \frac{(-1)^{j}xC'_{n+1}(x)}{c_j(n+1)^2(x-x_j)} \\ &\quad + \frac{(-1)^{j}C'_{n+1}(x)(1-x^2)}{c_j(n+1)^2(x-x_j)^2}. \end{aligned} \tag{118}$$

Let

$$G'_j(x) = T_1(x) + T_2(x) + T_3(x), \tag{119}$$

where

$$T_1(x) = \frac{(-1)^{j}C_{n+1}(x)}{c_j(x-x_j)} \tag{120}$$

$$T_2(x) = \frac{(-1)^{j}xC'_{n+1}(x)}{c_j(n+1)^2(x-x_j)} \tag{121}$$

$$T_3(x) = \frac{(-1)^{j}C'_{n+1}(x)(1-x^2)}{c_j(n+1)^2(x-x_j)^2}. \tag{122}$$

To find the derivatives $G'_j(x_k)$, let us inspect the following cases

Case 1: $j \neq k$.

Consider $T_1(x_k)$. Since $C_{n+1}(x_k) = (-1)^k$, see (23),

$$T_1(x_k) = \frac{(-1)^{j+k}}{c_j(x_k - x_j)}. \tag{123}$$

For $T_2(x_k)$, since $C'_{n+1}(x_k) = 0$ for $k = 1, \ldots, n$, see (82),

$$T_2(x_k) = 0 \quad k = 1, \ldots, n. \tag{124}$$

If $x = x_0$, from (84) we know that $C'_{n+1}(x_0) = (n+1)^2$, and hence

$$T_2(x_0) = \frac{(-1)^j}{c_j(x_0 - x_j)}. \tag{125}$$

If $x = x_{n+1}$, from (83) we know that $C'_{n+1}(x_{n+1}) = (-1)^n(n+1)^2$, and hence

$$T_2(x_{n+1}) = \frac{(-1)^{j+n+1}}{c_j(x_{n+1} - x_j)}. \tag{126}$$

Note that, since $(1-x^2)C'_{n+1}(x_k) = 0$ for $k = 0, 1, \ldots, n+1$, see (82),

$$T_3(x_k) = 0 \quad k = 0, 1, \ldots, n+1. \tag{127}$$

Using (119) and (123) - (127) we get

$$\begin{aligned} G'_j(x_k) &= T_1(x_k) \\ &= \frac{(-1)^{j+k}}{c_j(x_k - x_j)} \\ &= \frac{c_k}{c_j}\frac{(-1)^{j+k}}{(x_k - x_j)}, \end{aligned} \tag{128}$$

For $k = 0$ it holds that

$$\begin{aligned} G'_j(x_0) &= T_1(x_0) + T_2(x_0) \\ &= \frac{(-1)^j}{c_j(x_0 - x_j)} + \frac{(-1)^j}{c_j(x_0 - x_j)} \\ &= \frac{c_0}{c_j}\frac{(-1)^j}{(x_0 - x_j)}, \end{aligned} \tag{129}$$

Similarly for $k = n+1$ we get

$$\begin{aligned} G'_j(x_{n+1}) &= T_1(x_{n+1}) + T_2(x_{n+1}) \\ &= \frac{(-1)^{j+n+1}}{c_j(x_{n+1} - x_j)} + \frac{(-1)^{j+n+1}}{c_j(x_{n+1} - x_j)} \\ &= \frac{c_{n+1}}{c_j}\frac{(-1)^{j+n+1}}{(x_{n+1} - x_j)}. \end{aligned} \tag{130}$$

Combining (128) - (130) we get

$$G_j'(x_k) = \frac{c_k}{c_j}\frac{(-1)^{j+k}}{(x_k - x_j)}. \tag{131}$$

Case 2: $j = k \neq 0$, $j = k \neq n+1$.

We use L'Hospital's rule for evaluating the derivative. Applying L'Hospital's rule to $T_1(x)$ at $x = x_j$ and using (82), we get

$$T_1(x)_{|x=x_j} = \frac{(-1)^j C_{n+1}'(x)}{c_j} \,|_{x=x_j} = (-1)^j C_{n+1}'(x_j) = 0 \tag{132}$$

Applying L'Hospitals rule to $T_2(x)$ at $x = x_j$ and using (82) and (87), we get

$$\begin{aligned} T_2(x)_{|x=x_j} &= \frac{(-1)^j}{c_j(n+1)^2}[xC_{n+1}''(x) + C_{n+1}'(x)] \,|_{x=x_j} \\ &= \frac{(-1)^j x_j C_{n+1}''(x_j)}{(n+1)^2} \\ &= (-1)^j x_j \frac{-(n+1)^2 C_{n+1}(x_j) + x_j C_{n+1}'(x_j)}{(n+1)^2(1-x_j^2)} \\ &= -\frac{x_j}{(1-x_j^2)}. \end{aligned} \tag{133}$$

For $T_3(x)$ we use L'Hospital's rule twice. Applying L'Hospital's rule for the first time, $T_3(x)$ becomes

$$T_3(x)_{|x=x_k} = \frac{(-1)^j}{2(n+1)^2} \lim_{x \to x_k} \frac{(1-x^2)C_{n+1}''(x) - 2xC_{n+1}'(x)}{(x - x_j)}.$$

Using (81) and (87) to replace $C_{n+1}''(x)$, as we did in Lemma 5, we get

$$\begin{aligned} T_3(x)_{|x=x_k} &= \frac{(-1)^j}{2(n+1)^2} \lim_{x \to x_k} \frac{-(n+1)^2 C_{n+1}(x) - xC_{n+1}'(x)}{(x - x_j)} \\ &= \frac{(-1)^j}{2(n+1)^2} \left(\lim_{x \to x_k} [\frac{-(n+1)^2 C_{n+1}(x)}{(x - x_j)}] - \lim_{x \to x_k} [\frac{xC_{n+1}'(x)}{(x - x_j)}] \right) \end{aligned}$$

From (120), (121) and (122) we have

$$T_3(x)_{|x=x_k} = -\frac{1}{2} \lim_{x \to x_k} [T_1(x) + T_2(x_k)].$$

Applying L'Hospital's for the second time we get

$$T_3(x)_{|x=x_k} = \frac{x_j}{2(1-x_j^2)} \tag{134}$$

Hence combining (132) - (134) we get

$$G_j(x_j) = -\frac{x_j}{2(1-x_j^2)} \tag{135}$$

Case 3: $j = k = 0$
In this case, it is easier to use the definition of $g_j(x)$ in (24) rather than $G_j(x)$. This gives

$$g_0^{'}(x_0) = \frac{1}{n+1}\sum_{m=0}^{n+1}\frac{C_m(x_0)C_m^{'}(x_0)}{c_m} \tag{136}$$

From (86) and (20), we know that $C_m^{'}(x_0) = m^2$ and $C_m(x_0) = 1$. Hence (136) becomes

$$\begin{aligned}
g_0^{'}(x_0) &= \frac{1}{n+1}\sum_{m=0}^{n+1}\frac{m^2}{c_m} \\
&= \frac{1}{n+1}\left[\sum_{m=0}^{n} m^2 + \frac{(n+1)^2}{2}\right] \\
&= \frac{1}{n+1}\frac{n(n+1)(2n+1)}{6} + \frac{(n+1)}{2} \\
&= \frac{2(n+1)^2+1}{6} \qquad (137)
\end{aligned}$$

Case 4: $j = k = n+1$
In this case, differentiating (24) and plugging in x_{n+1} gives

$$g_{n+1}^{'}(x_{n+1}) = \frac{1}{n+1}\sum_{m=0}^{n+1}\frac{C_m(x_{n+1})C_m^{'}(x_{n+1})}{c_m} \tag{138}$$

From (85) and (20), we know that $C_m^{'}(x_{n+1}) = (-1)^{m-1}m^2$ and $C_m(x_{n+1}) = (-1)^m$, hence (138) becomes

$$\begin{aligned}
g_{n+1}^{'}(x_{n+1}) &= \frac{1}{n+1}\sum_{m=0}^{n+1}\frac{-m^2}{c_m} \\
&= -\frac{2(n+1)^2+1}{6}. \qquad (139)
\end{aligned}$$

From (131),(135), (137) and (139) we have proved the first part of the theorem.

To prove (58), recall that $T_n(x,t)$ is a polynomial of degree $n+1$, which implies that $T_n^{'}(x,t)$, the derivative of $T_n(x,t)$ with respect to the variable x, is a polynomial of degree less than or equal to n. It can hence be written as a linear combination of the basis $\{g_j(x)\}_{j=0}^{n+1}$, i.e.

$$T_n^{'}(x,t) = \sum_{j=0}^{n+1} a_j(t) g_j(x)$$

From Lemma 5 we can deduce that

$$T_n^{'}(x,t) = \sum_{j=0}^{n+1} T_n^{'}(x_j,t) g_j(x). \tag{140}$$

By differentiating (140) with respect to the variable x, we get

$$T_n^{''}(x,t) = \sum_{j=0}^{n+1} T_n^{'}(x_j,t) g_j^{'}(x). \tag{141}$$

Recalling the expressions for $T_n^{'}$ and $T_n^{''}$ from (49) and (53) and using the expression (141) for $x = x_k$, where $k = 0, \dots, n+1$ we have

$$T_n^{''} = \mathcal{D} T_n^{'} \tag{142}$$

Using (51) in (142) we can see that

$$T_n^{''} = \mathcal{D}^2 T_n$$

Hence

$$\mathcal{A} = \mathcal{D}^2$$

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