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Identification of the initial function for delay differential equations: Part II: A discrete analogue of the data assimilation problem & computational results.

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Abstract

In this report we consider a difference analogue of the "data assimilation problem" for delay differential equations (DDEs) presented in the first part (Numerical Analysis Report No. 431). The problem consists of finding an initial function that gives rise to a solution of a discretized DDE, which is a close fit to observed data. A rôle for adjoint equations and fundamental solutions in the discrete case is established, and related discrete integral equations (summation equations) are obtained.

Keywords Discrete delay differential equations, initial function, discrete adjoint equations, identification problem, data assimilation, discrete fundamental matrices, regularization parameter.

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1 Introduction

Let us consider an n-dimensional system of linear delay differential equations (DDEs) with *time-dependent* coefficients, of the form

$$\frac{dy(t)}{dt} - A(t)y(t) - B(t)y(t-\tau) = f(t), \quad \text{for } t \in [0,T], \tag{1.1a}$$

subject to

$$y(t) = \varphi(t), \quad \text{for } t \in [-\tau, 0]. \tag{1.1b}$$

Here, τ is a prescribed positive constant (the "lag"), we suppose

$$y(t),\ f(t),\ \varphi(t)\ \in \mathbb{R}^{n\times 1}, \quad A(t),\ B(t)\ \in \mathbb{R}^{n\times n},$$

and these functions will be assumed to be continuous on $[0,T]$. The solution $y(t)$ depends (in particular) upon the initial function $\varphi(t)$; $y(t) \equiv y(\varphi;t)$. The problem that we address is related to the identification of $\varphi(t)$ given τ, $f(t)$, $A(t)$, and $B(t)$, and knowing $y(\varphi;t)$; we shall here study a discrete analogue but we address the continuous problem, briefly, in order to set the scene.

1.1 The continuous data assimilation problem

For the continuous identification problem [8], we introduced the functional

$$S_\alpha^{\beta,\gamma}(\varphi) := \frac{\alpha}{2}\int_{-\tau}^{0} \left\|\varphi(t)-\widehat{\varphi}(t)\right\|^2 dt + \frac{\beta}{2}\left\|\varphi(0)-\widehat{\varphi}(0)\right\|^2 + \frac{\gamma}{2}\left\|y(\varphi;0)-\widehat{y}(0)\right\|^2 + \frac{1}{2}\int_{0}^{T} \left\|y(\varphi;t)-\widehat{y}(t)\right\|^2 dt \tag{1.2}$$

(in which $\alpha, \beta, \gamma \geq 0$ and $y(\varphi;0) = \varphi(0)$) and $\widehat{\varphi} = \widehat{\varphi}(t)$ and $\widehat{y} = \widehat{y}(t)$ are the given functions and where $y(\varphi;t)$ satisfies (1.1). The function $\widehat{\varphi}(t)$ contains information about an expected form of $\varphi(t)$. The function $\widehat{y}(t)$ is based on observations of the solution.

The *data assimilation problem* (as the identification problem is called) can be formulated as follows:

Definition 1.1 *Let $\mathcal{F} \subseteq PC[-\tau,0]$ denote a smoothness class of bounded functions on $[-\tau,0]$. Then the corresponding data assimilation problem for the identification of φ reads as follows.*

> *Define by $y(\varphi;t)$ the solution of (1.1) with initial function φ. Find $\varphi_\star \in \mathcal{F}$, such $y(\varphi_\star;t)$ minimizes $S_\alpha^{\beta,\gamma}(\varphi)$ over $\mathcal{F}$:*
>
> $$\varphi_\star = \arg\min_{\varphi\in\mathcal{F}} S_\alpha^{\beta,\gamma}(\varphi), \tag{1.3}$$
>
> *where $S_\alpha^{\beta,\gamma}(\varphi)$ is defined by (1.2) in terms of $y(\varphi;t)$.*

This formulation embodies parameters $\alpha \geq$ and $\beta \geq 0$, $\gamma \geq 0$, which (when positive) are "regularization parameters" (see [9], for example)[1].

[1] Similar problems have been discussed for ODEs and PDEs, see [1, 2, 3, 11, 14]), in particular for the discrete analogue, see [13]). A functional of the type (1.2) was considered, for example, in [12]. For discussion of related questions for DDEs see [4, 5, 6, 10, 15].

1.2 The scope of this report

This report is related to Numerical Analysis Report No.431 [8], in which we considered the continuous case of the data assimilation problem as posed above. In the present report, we analyze a discrete analogue of the problem presented.

We shall proceed as follows. We first use a stepsize h to introduce a discrete version of the data assimilation problem, along with h-dependent discrete functionals (${}^h\tilde{S}_{\alpha}^{\beta,\gamma}(\tilde{\varphi})$, etc.) that simulate the functional $S_{\alpha}^{\beta,\gamma}(\varphi)$ used in [8]. Conditions for a minimum of ${}^h\tilde{S}_{\alpha}^{\beta,\gamma}(\tilde{\varphi})$ are explored through an analysis of its first variation ${}^h\tilde{P}_{\alpha}^{\beta,\gamma}(\tilde{\varphi})$, and an iterative technique for obtaining the minimum is written down. In order to explore the properties of this iteration, it is convenient to relate it to an iterative algorithm for the solution of a discretized integral equation (a summation equation), for which the properties of the "kernel" can be obtained[2]. It is this analysis that is reflected in the precise choice of ${}^h\tilde{S}_{\alpha}^{\beta,\gamma}(\tilde{\varphi})$. The final half of the report consists of a report of numerical experiments that demonstrate the performance of the algorithm.

2 A discretized data assimilation problem

In practice, one might endeavour to obtain a discretized version of the data assimilation problem in Definition 1.1 through the use of high-order approximate methods that adapt to any possible discontinuities in the derivatives of the solution $y(\varphi; t)$. It proves rather difficult to analyze such adaptive discretizations in a rigorous manner. We therefore adopt a more limited approach, in order to gain insight.

For a stepsize h with $\tau = Nh$ and $T = Kh$, where N, K are both integers, we introduce $t_n = nh$ ($n \in \{-N, 1-N, \dots, -1, 0, 1, \dots, K\}$) and define a *uniform grid* with step size h,

$$-\tau = t_{-N} < t_{1-N} < \dots t_{-1} < 0 = t_0 < t_1 < \dots < t_N < t_{N+1} < \dots < t_K = T.$$

We introduce a discretized equation that results from application of an *Euler formula* to (1.1). Given the grid above, the explicit Euler equations, for the DDE in (1.1), read

$$\widetilde{y}_{n+1} - \widetilde{y}_n - hA_n\widetilde{y}_n - hB_n\widetilde{y}_{n-N} = hf_n, \quad \text{for } n \in \{0, 1, \dots, K-1\}. \tag{2.1a}$$

Here $\widetilde{y}_n \approx y(\varphi; t_n)$, $B_n = B(nh)$, $A_n = A(nh)$, $f_n = f(nh)$, $\tilde{\varphi}_n = \varphi(nh)$. The solution is subject to the initial condition

$$\widetilde{y}_n = \tilde{\varphi}_n, \quad \text{for } -N \le n \le 0. \tag{2.1b}$$

Let us also introduce a discrete analogue of the objective function (1.2). One possibility is the form

$$\frac{\alpha h}{2}\sum_{n=-N}^{-1}\|\tilde{\varphi}_n - \widehat{\varphi}(t_n)\|^2 + \frac{h}{2}\sum_{n=0}^{K-1}\|\tilde{y}_n - \widehat{y}(t_n)\|^2 + \frac{\beta}{2}\left\|\tilde{\varphi}_0 - \widehat{\varphi}(t_0)\right\|^2 + \frac{\gamma}{2}\left\|\tilde{y}_0 - \widehat{y}(t_0)\right\|^2. \tag{2.2}$$

This discretization is associated with the left-hand (explicit) Euler rule applied to the integrals that define (1.2), and at this stage it is not transparent that this is a convenient or appropriate

[2] A linear summation equation is simply a set of linear algebraic equations and the "kernel" is derived from the coefficient matrix.

discretization. At this stage, alternatives possibilities are, perhaps,

$$\frac{\alpha h}{2}\sum_{n=1-N}^{0}\|\tilde{\varphi}_n-\widehat{\varphi}(t_n)\|^2+\frac{h}{2}\sum_{n=1}^{K}\|\tilde{y}_n-\widehat{y}(t_n)\|^2+\frac{\beta}{2}\big\|\tilde{\varphi}_0-\widehat{\varphi}(t_0)\big\|^2+\frac{\gamma}{2}\big\|\tilde{y}_0-\widehat{y}(t_0)\big\|^2, \tag{2.3a}$$

or

$$\frac{\alpha h}{2}\sum_{n=-N}^{-1}\|\tilde{\varphi}_n-\widehat{\varphi}(t_n)\|^2+\frac{h}{2}\sum_{n=1}^{K}\|\tilde{y}_n-\widehat{y}(t_n)\|^2+\frac{\beta}{2}\big\|\tilde{\varphi}_0-\widehat{\varphi}(t_0)\big\|^2+\frac{\gamma}{2}\big\|\tilde{y}_0-\widehat{y}(t_0)\big\|^2. \tag{2.3b}$$

For flexibility of approach, we generalize (2.2) by introducing a suitable set of integers $\{p,q,r,s\}$, and the notation

$$\mathfrak{I}:=\{p,q,r,s\}\cup\{\alpha,\beta,\gamma\} \tag{2.4}$$

and write

$${}^h\tilde{S}_{\mathfrak{I}}(\varphi_n)=\frac{\alpha h}{2}\sum_{n=p}^{q}\|\tilde{\varphi}_n-\widehat{\varphi}(t_n)\|_2^2+\frac{h}{2}\sum_{n=r}^{s}\|\tilde{y}_n-\widehat{y}(t_n)\|_2^2+\frac{\beta}{2}\big\|\tilde{\varphi}_0-\widehat{\varphi}(t_0)\big\|_2^2+\frac{\gamma}{2}\big\|\tilde{y}_0-\widehat{y}(t_0)\big\|_2^2. \tag{2.5}$$

The expression (2.2) arises from ${}^h\tilde{S}_{\mathfrak{I}}(\varphi_n)$ on taking

$$p=-N,\ q=-1,\ r=0,\ \text{and}\ s=K-1, \tag{2.6}$$

but we gain some flexibility if we introduce $\mathfrak{I}$ with more general $\{p,q,r,s\}$. For example, the implicit (right-hand) Euler quadrature (2.3a) corresponds to $p=\ 1-N$, $q=\ 0$, $r=\ 1$ and $s=\ K$. We anticipate the results of our analysis by introducing the notation

$${}^h\tilde{S}_{\alpha}^{\beta,\gamma}:={}^h\tilde{S}_{\mathfrak{I}}(\varphi_n)=\frac{\alpha h}{2}\sum_{n=-N}^{-1}\|\tilde{\varphi}_n-\widehat{\varphi}(t_n)\|_2^2+\frac{h}{2}\sum_{n=0}^{K}\|\tilde{y}_n-\widehat{y}(t_n)\|_2^2+\frac{\beta}{2}\big\|\tilde{\varphi}_0-\widehat{\varphi}(t_0)\big\|_2^2+\frac{\gamma}{2}\big\|\tilde{y}_0-\widehat{y}(t_0)\big\|_2^2 \tag{2.7}$$

which corresponds to the choice $\mathfrak{I}$ in which

$$p=\ -N,\ q=\ -1,\ r=\ 0,\ \text{and}\ s=K. \tag{2.8}$$

Prima facie, this is not the most natural choice but will be suggested by the analysis.

For further analysis we shall need to write down a discrete analogue of the adjoint of (1.1); this we shall regard as an adjoint for (2.1).

Definition 2.1 *(a) Given functions $p^T(t)$ and $\psi^T(t)\in\mathbb{R}^{1\times m}$ (for $t\in[0,T]$ and for $t\in[T,T+\tau]$ respectively, the corresponding* formal adjoint *for (1.1) is*

$$\frac{dx^T(t)}{dt}+x^T(t)A(t)+x^T(t+\tau)B(t+\tau)=p^T(t),\quad \textit{for } t\in[0,T], \tag{2.9a}$$

subject to

$$x^T(t)=\psi^T(t),\quad \textit{for } t\in[T,T+\tau] \tag{2.9b}$$

with a solution $x^T(t)\in\mathbb{R}^{1\times m}$.

(b) A discrete analogue of the adjoint equation (2.9) corresponding to (2.1), is

$$\tilde{x}_n^T=\tilde{x}_{n+1}^T+h\tilde{x}_{n+1}^TA_{n+1}+h\tilde{x}_{n+N+1}^TB_{n+N+1}+hp_{n+1}^T,\quad n=0,1,\ldots,K-1, \tag{2.10a}$$

subject to

$$\tilde{x}_n^T = 0, \quad n = K, \ldots, K+N. \tag{2.10b}$$

We shall refer to (2.9a) as a "formal adjoint equation" for (1.1a) and (2.10a) as a "formal discrete adjoint equation" for (2.1).

Remark 2.1 *We obtain (2.10) from (2.9) by using the backward Euler formula ("backward" for increasing t).*

3 The discretized minimization problem

In this section we formulate a discrete analogue of the problem of identifying an optimal initial function. We are concerned to find the minimum of (2.5) over the space $\mathcal{F}^h$ of mesh functions defined on points, say $nh_{n=-N}^0$, where $h = \tau/N$.

In order to find the minimum we need to find its first variation (compare [8]). To write down ${}^h\tilde{S}_{\mathfrak{J}}(\tilde{\varphi}_n + \varepsilon\tilde{\psi}_n)$ we need an expression for $\tilde{y}_n(\tilde{\varphi}_n + \tilde{\varepsilon}\psi_n)$ and we have it in the following lemma.

Lemma 3.1 *Write*

$$L^h y(t) := \frac{\tilde{y}_{n+1} - \tilde{y}_n}{h} - A_n\tilde{y}_n - B_n\tilde{y}_{n-N}$$

and

$$M^h y(t) = \tilde{\varphi}_n \ \ (\textit{for} \ \ n = r-N, \ldots, r).$$

By virtue of the linearity of L^h and M^h,

$$\tilde{y}_n(\tilde{\varphi}_n + \varepsilon\tilde{\psi}_n) = \tilde{y}_n(\tilde{\varphi}_n) + \varepsilon\tilde{z}_n(\tilde{\psi}_n), \tag{3.1}$$

where $\tilde{z}_n(\tilde{\psi}_n)$ satisfies

$$L^h z(t) = 0 \quad (\textit{for } t_n = nh, \ \ n = r, r+1, \ldots, s), \ \ s > r \quad \textit{and} \tag{3.2a}$$

$$M^h z(t) = \tilde{\psi}_n \quad (\textit{for } t_n = nh, \ n = r-N, \ldots, r). \tag{3.2b}$$

Here $A_n = A(nh)$, $B_n = B(nh)$, $\tilde{y}_n = y(nh)$, $\tilde{\varphi}_n = \varphi(nh)$.

The perturbed objective function ${}^h\tilde{S}_{\mathfrak{J}}(\tilde{\varphi} + \varepsilon\tilde{\psi})$ has the form

$${}^h\tilde{S}_{\mathfrak{J}}(\tilde{\varphi} + \varepsilon\tilde{\psi}) = \frac{\alpha h}{2}\sum_{n=p}^{q} \|\tilde{\varphi}_n + \varepsilon\tilde{\psi}_n - \widehat{\varphi}_n\|_2^2 + \frac{h}{2}\sum_{n=r}^{s} \|\tilde{y}_n + \varepsilon\tilde{z}_n - \widehat{y}(t_n)\|_2^2 + {}^h\mathfrak{s}'_0, \tag{3.3a}$$

where

$${}^h\mathfrak{s}'_0 = \frac{\beta}{2}\left\|\tilde{\varphi}_0 + \varepsilon\tilde{\psi}_0 - \widehat{\varphi}(t_0)\right\|_2^2 + \frac{\gamma}{2}\left\|\tilde{y}_0(\tilde{\varphi}_0) + \varepsilon\tilde{z}_0 - \widehat{y}(t_0)\right\|_2^2. \tag{3.3b}$$

We may write (3.3) in the form

$${}^h\tilde{S}_{\mathfrak{J}}(\tilde{\varphi} + \varepsilon\tilde{\psi}) = {}^h\tilde{S}_{\alpha}^{\beta,\gamma}(\tilde{\varphi}) + \varepsilon\left\{{}^h\tilde{P}_{\mathfrak{J}}(\tilde{\varphi}, \tilde{\psi})\right\} + \varepsilon^2\left\{{}^h\tilde{Q}_{\mathfrak{J}}(\tilde{\psi})\right\}, \tag{3.4}$$

where

$${}^h\tilde{P}_{\mathfrak{J}}(\tilde{\varphi}, \tilde{\psi}) = \alpha h\sum_{n=p}^{q}[\tilde{\varphi}_n - \widehat{\varphi}_n]^T\tilde{\psi}_n + h\sum_{n=r}^{s}[\tilde{y}_n - \widehat{y}(t_n)]^T\tilde{z}_n + {}^h\mathfrak{p}_0 \tag{3.5a}$$

with

$$ {}^h\mathfrak{p}_0 = \beta\big[\tilde{\varphi}_0 - \widehat{\varphi}(t_0)\big]^T \tilde{\psi}_0 + \gamma\big[\tilde{y}_0(\tilde{\varphi}_0) - \widehat{y}(t_0)\big]^T \tilde{z}_0. \tag{3.5b} $$

Further,

$$ {}^h\tilde{Q}_{\mathfrak{J}}(\tilde{\psi}) = \frac{\alpha h}{2}\sum_{n=p}^{q}\|\tilde{\psi}_n\|_2^2 + \frac{h}{2}\sum_{n=r}^{s}\|\tilde{z}_n\|_2^2 + \frac{\beta}{2}\|\tilde{\psi}_0\|_2^2 + \frac{\gamma}{2}\|\tilde{z}_0\|_2^2. \tag{3.6} $$

Then, we can state the following result.

Theorem 3.1 *A function $\tilde{\varphi}$ defined on $[-\tau, 0]$ minimizes ${}^h\tilde{S}_{\mathfrak{J}}(\tilde{\varphi})$ for $\tilde{\varphi} \in \mathcal{F}^h$ if and only if ${}^h\tilde{P}_{\mathfrak{J}}(\tilde{\varphi}, \tilde{\psi})$ vanishes for all $\tilde{\psi} \in \mathcal{F}^h$, where $\tilde{z} = \tilde{z}(\tilde{\psi})$ satisfies (3.2).*

3.1 A formula for the first variation

In this section, our objective is to obtain a representation of

$$ {}^h\tilde{P}_{\mathfrak{J}} \equiv {}^h\tilde{P}_{\mathfrak{J}}(\tilde{\varphi}, \tilde{\psi}) $$

in terms of the functions $\tilde{\varphi}$ and $\tilde{\psi}$. We employ a representation of ${}^h\tilde{P}_{\mathfrak{J}}$ obtained using a discrete analogue of the adjoint equation. Let us consider (compare (2.10a))

$$ \tilde{x}_{n-1}^T = \tilde{x}_n^T + h\tilde{x}_n^T A_n + h\tilde{x}_{n+N}^T B_{n+N} + h[\tilde{y}_n(\tilde{\varphi}_n) - \widehat{y}_n], \quad n = r-1, r, \ldots, s, \tag{3.7a} $$

with

$$ \tilde{x}_n^T = 0, \;\; n = s, \ldots, s+N. \tag{3.7b} $$

(If, for example, $r = 0$, (3.7a) defines a value $\tilde{x}_{-1}$.)

For appropriate r and s this is a discrete version of the adjoint equation appearing in [8, p.4], discretized using the implicit Euler formula . We can write (3.5a) in the form

$$ {}^h\tilde{P}_{\mathfrak{J}} = \beta\big[\tilde{\varphi}_0 - \widehat{\varphi}(t_0)\big]^T \tilde{\psi}_0 + \gamma\big[\tilde{y}_0(\tilde{\varphi}_0) - \widehat{y}(t_0)\big]^T \tilde{z}_0 + $$

$$ \alpha h\sum_{n=p}^{q}[\tilde{\varphi}_n - \widehat{\varphi}_n]^T\tilde{\psi}_n + \sum_{n=r}^{s}\Big(\underbrace{(\tilde{x}_{n-1}^T - \tilde{x}_n^T)\tilde{z}_n}_{\mathcal{J}_1} - h\tilde{x}_n^T A_n\tilde{z}_n - \underbrace{h\tilde{x}_{n+N}^T B_{n+N}\tilde{z}_n}_{\mathcal{J}_2}\Big). $$

- Using (A.3) we can write $\mathcal{J}_1$ as

$$ \mathcal{J}_1 \equiv \sum_{n=r}^{s}(\tilde{x}_{n-1}^T - \tilde{x}_n^T)\tilde{z}_n = -\tilde{x}_s^T\tilde{z}_{s+1} + \tilde{x}_{r-1}^T\tilde{z}_r + \sum_{n=r}^{s}\tilde{x}_n^T\big(\tilde{z}_{n+1} - \tilde{z}_n\big). $$

- For the term $\mathcal{J}_2$ we have $\mathcal{J}_2 \equiv h\sum_{n=r}^{s}\tilde{x}_{n+N}^T B_{n+N}\tilde{z}_n =$

$$ h\sum_{n=r}^{s}\tilde{x}_n^T B_n\tilde{z}_{n-N} - \underbrace{h\sum_{n=r}^{r+N-1}\tilde{x}_n^T B_n\tilde{z}_{n-N}}_{\mathcal{J}_3} + h\sum_{n=s+1}^{s+N}\tilde{x}_n^T B_n\tilde{z}_{n-N}. $$

We can write the term $\mathcal{J}_3$ in the form

$$\mathcal{J}_3 = h \sum_{n=r}^{r+N-1} \tilde{x}_n^T B_n \tilde{z}_{n-N} = h \sum_{n=r-N}^{r-1} \tilde{x}_{n+N}^T B_{n+N} \tilde{z}_n.$$

Therefore, (3.5a) has the form

$$^h\tilde{P}_{\mathfrak{J}} = {}^h\mathfrak{p}_0 + h\sum_{n=p}^{q} \Big[\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n)\Big]^T \tilde{\psi}_n + h \sum_{n=r-N}^{r-1} \tilde{x}_{n+N}^T B_{n+N} \tilde{z}_n + \tilde{x}_{r-1}^T \tilde{z}_r - \tilde{x}_s^T \tilde{z}_{s+1} +$$

$$\sum_{n=r}^{s} \tilde{x}_n^T \Big(\tilde{z}_{n+1} - \tilde{z}_n - hA_n\tilde{z}_n - hB_n\tilde{z}_{n-N}\Big) - h\sum_{n=s+1}^{s+N} \tilde{x}_n^T B_n \tilde{z}_{n-N}.$$

Let $\tilde{z}_n$ satisfy

$$\tilde{z}_{n+1} - \tilde{z}_n - hA_n\tilde{z}_n - hB_n\tilde{z}_{n-N} = 0, \quad \text{upon} \;\; n = r, r+1, \ldots, s,$$

with

$$\tilde{z}_n = \tilde{\psi}_n, \quad n = r-N, \ldots, r.$$

(Compare [8, pp.7-8].) Taking into account (3.7), we obtain

$$^h\tilde{P}_{\mathfrak{J}} = {}^h\mathfrak{p}_0 + h\sum_{n=p}^{q} \Big[\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n)\Big]^T \tilde{\psi}_n + h \sum_{n=r-N}^{r-1} \tilde{x}_{n+N}^T B_{n+N} \tilde{\psi}_n + \tilde{x}_{r-1}^T \tilde{\psi}_r$$

which is independent of our choice of s.

Now, from (3.7),

$$\tilde{x}_{r-1}^T = \tilde{x}_r^T + h\tilde{x}_r^T A_r + h\tilde{x}_{r+N}^T B_{r+N} + h[\tilde{y}_r(\tilde{\varphi}_n) - \widehat{y}_r].$$

Therefore,

$$^h\tilde{P}_{\mathfrak{J}} = {}^h\mathfrak{p}_0 + h\sum_{n=p}^{q} \Big\{\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n)\Big\} \tilde{\psi}_n + h \sum_{n=r-N}^{r-1} \tilde{x}_{n+N}^T B_{n+N} \tilde{\psi}_n +$$

$$\Big(\tilde{x}_r^T(1 + hA_r) + h\tilde{x}_{r+N}^T B_{r+N} + h[\tilde{y}_r(\tilde{\varphi}_n) - \widehat{y}_r]\Big)\tilde{\psi}_r.$$

We now set, as in (2.6),

$$p = r - N, \;\; q = r - 1, \tag{3.8}$$

and leave s undefined, and the above applies to $^h\tilde{P}_{\mathfrak{J}}$. Thus, we have

$$^h\tilde{P}_{\mathfrak{J}} = {}^h\mathfrak{p}_0 + h \sum_{n=r-N}^{r-1} \Big(\big[\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n)\big]^T + \tilde{x}_{n+N}^T B_{n+N}\Big)\tilde{\psi}_n +$$

$$\Big(\tilde{x}_r^T(1 + hA_r) + h\tilde{x}_{r+N}^T B_{r+N} + h[\tilde{y}_r(\tilde{\varphi}_n) - \widehat{y}_r]\Big)\tilde{\psi}_r.$$

Since the term $^h\mathfrak{p}_0$ depends on function values at $t = 0$ it is convenient to set $r = 0$. Then, we have

$$^h\tilde{P}_{\mathfrak{J}} = h \sum_{n=-N}^{-1} \Big(\big[\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n)\big]^T + \tilde{x}_{n+N}^T B_{n+N}\Big)\tilde{\psi}_n +$$

$$\Big(\beta\big[\tilde{\varphi}_0 - \widehat{\varphi}(t_0)\big]^T + \gamma\big[\tilde{y}_0(\tilde{\varphi}_n) - \widehat{y}(t_0)\big]^T + \tilde{x}_0^T(1 + hA_0) + h\tilde{x}_N^T B_N + h[\tilde{y}_0(\tilde{\varphi}_n) - \widehat{y}_0]^T\Big)\tilde{\psi}_0. \quad (3.9)$$

The first variation must be zero for all $\tilde{\psi}$ in $\mathcal{F}^h$, therefore we obtain the following result.

Lemma 3.2 *A function $\tilde{\varphi}^\star$ defined on $[-\tau, 0]$ which minimizes ${}^h\tilde{S}_{\mathfrak{I}}(\tilde{\varphi})$ for $\tilde{\varphi} \in \mathcal{F}^h$ satisfies the equations*

$$\alpha(\tilde{\varphi}_n^\star - \widehat{\varphi}_n) + \tilde{x}_{n+N}^T B_{n+N} = 0, \quad n = -N, \ldots, -1, \quad (3.10a)$$

$$\tilde{x}_0^T(1 + hA_0) + h\tilde{x}_N^T B_N + \beta\big[\tilde{\varphi}_0 - \widehat{\varphi}(t_0)\big]^T + (\gamma + h)\big[\tilde{y}_0 - \widehat{y}(t_0)\big]^T = 0, \;\; n = 0. \quad (3.10b)$$

4 A discrete integral equation (or summation equation)

In this section we derive a discrete integral equation (a "summation[3] equation") for the initial function that minimizes ${}^h\tilde{S}_{\mathfrak{I}}$ (with choice of $\mathfrak{I}$ in which $p = -N,\ q = -1,\ r = 0$ and $s = K$). The equivalence allows us to analyze the properties of the iterative algorithm.

According to §3 we should introduce a method for determining the optimal initial function. The objective function has the natural form when we set

$$s = K \quad (4.1)$$

in (2.4). Following the discussion in the section §3.1 and from the result of Lemma 3.2 we can consider the system of equations of finding the initial function $\tilde{\varphi}$, which minimizes ${}^h\tilde{S}_{\mathfrak{I}}$. We have

$$\frac{\tilde{y}_{n+1} - \tilde{y}_n}{h} - A_n\tilde{y}_n - B_n\tilde{y}_{n-N} = f_n \quad n = 0, 1, \ldots, K-1, \quad (4.2a)$$

$$\tilde{y}_n = \tilde{\varphi}_n, \;\; n = -N, \ldots, 0, \quad (4.2b)$$

$$-\frac{\tilde{x}_n^T - \tilde{x}_{n-1}^T}{h} - \tilde{x}_n^T A_n - \tilde{x}_{n+N}^T B_{n+N} = h[\tilde{y}_n(\tilde{\varphi}_n) - \widehat{y}_n]^T, \quad (4.2c)$$

$$\tilde{x}_n^T = 0, \;\; n = K, \ldots, K+N, \quad (4.2d)$$

$$\alpha(\tilde{\varphi}_n - \widehat{\varphi}_n) + B_{n+N}^T\tilde{x}_{n+N} = 0, \quad n = -N, \ldots, -1, \quad (4.2e)$$

$$[I + hA_0]^T\tilde{x}_0 + hB_N^T\tilde{x}_N + h[\tilde{y}_0(\tilde{\varphi}_n) - \widehat{y}_0] + {}^h\mathfrak{p}_0 = 0, \;\; n = 0. \quad (4.2f)$$

In the next section we shall establish a discrete integral equation (or "summation equation") for the optimal initial function using formulae for solutions of the equations (4.2a) and (4.2c), and the additional equations (4.2e) and (4.2f) for the initial function.

4.1 The discrete integral equation in terms of fundamental matrices

Let us consider the discrete version of the adjoint equation (4.2c). According to [7, pp.14-15], we may write the solution of the adjoint equation (4.2c) in the form

$$\tilde{x}_k^T = h\sum_{m=k+1}^{s}[\tilde{y}_m - \widehat{y}_m]^T\widetilde{Y}(m, k),$$

[3]The summation equation is an analogue of the integral equation obtained in the continuous case in [8, pp.15-16].

where

$$\tilde{y}_m = \widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l + h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l.$$

(This is a solution of the discrete DDE written in terms of fundamental matrices, see [7, pp.13-14].) Thus, we can write

$$\tilde{x}_k^T = h\sum_{m=k+1}^{s}\Big[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l + h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l\Big]^T\widetilde{Y}(m,k)$$

$$-h\sum_{m=k+1}^{K}[\widehat{y}_m]^T\widetilde{Y}(m,k).$$

Therefore, for $k=0$ we have

$$\begin{aligned}\tilde{x}_0^T &= h\sum_{m=1}^{s}\Big[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l + \\ &+h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l\Big]^T\widetilde{Y}(m,0) - h\sum_{m=1}^{K}[\widehat{y}_m]^T\widetilde{Y}(m,0),\end{aligned} \tag{4.3}$$

for $k=N$,

$$\begin{aligned}\tilde{x}_N^T &= h\sum_{m=N+1}^{s}\Big[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l + \\ &+h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l\Big]^T\widetilde{Y}(m,N) - h\sum_{m=1}^{K}[\widehat{y}_m]^T\widetilde{Y}(m,N),\end{aligned} \tag{4.4}$$

for $k=n+N$,

$$\begin{aligned}\tilde{x}_{n+N}^T &= h\sum_{m=n+N+1}^{s}\Big[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l + \\ &h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l\Big]^T\widetilde{Y}(m,n+N) - h\sum_{m=n+N+1}^{K}[\widehat{y}_m]^T\widetilde{Y}(m,n+N).\end{aligned} \tag{4.5}$$

According to (4.2e), $\tilde{\varphi}_n$ satisfies the discrete equation

$$\alpha\tilde{\varphi}_n + [\tilde{x}_{n+N}^T B_{n+N}]^T = \alpha\widehat{\varphi}_n \quad (\text{for } n=-N,\dots,-1). \tag{4.6}$$

Using (4.5), we can write the latter equation for $\tilde{\varphi}_n$ in the form

$$\alpha\tilde{\varphi}_n + \left[h\sum_{m=n+N+1}^{s}\Big[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l\Big]^T\widetilde{Y}(m,n+N)B_{n+N}\right]^T =$$

$$\alpha\widehat{\varphi}_n - \left[h\sum_{m=n+N+1}^{s}\Big[h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\Big]^T\widetilde{Y}(m,n+N)B_{n+N}\right]^T. \tag{4.7}$$

For $\tilde{\varphi}_0$ we have

$$(\beta+\gamma+h)I\tilde{\varphi}_0 + hB_N^T\tilde{x}_N + [I+hA_0]^T\tilde{x}_0 = (\alpha h+\beta)\widehat{\varphi}_0 + (\gamma+h)\widehat{y}_0. \tag{4.8}$$

Therefore, using (4.3) and (4.4), we obtain from (4.8)

$$(\beta+\gamma+h)\tilde{\varphi}_0 + h\left[\sum_{m=1}^{s}\left[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l\right]^T\widetilde{Y}(m,0)\{I+hA_0\}\right]^T +$$

$$h^2\left[\sum_{m=N+1}^{s}\left[\widetilde{Y}(m,0)\{I+hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l\right]^T\widetilde{Y}(m,N)B_N\right]^T =$$

$$\beta I\widehat{\varphi}_0 + (\gamma+h)I\widehat{y}_0 - h\sum_{m=1}^{s}\left[\left[h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right]^T\widetilde{Y}(m,0)\{I+hA_0\}\right]^T$$

$$- h\sum_{m=N+1}^{s}\left[\left[h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right]^T\widetilde{Y}(m,N)B_N\right]^T.$$

Finally, collecting similar terms, we obtain

$$(\beta+\gamma+h)I\tilde{\varphi}_0 + h\sum_{m=1}^{s}[I+hA_0]^T\widetilde{Y}^T(m,0)\widetilde{Y}(m,0)[I+hA_0]\tilde{\varphi}_0 +$$

$$h^2\sum_{m=1}^{s}[I+hA_0]^T\widetilde{Y}^T(m,0)\widetilde{Y}(m,N)B_N\tilde{\varphi}_0 + h^2\sum_{m=N+1}^{s}B_N^T\widetilde{Y}^T(m,N)\widetilde{Y}(m,0)\left[I+hA_0\right]\tilde{\varphi}_0 +$$

$$h^3\sum_{m=N+1}^{s}B_N^T\widetilde{Y}^T(m,N)\widetilde{Y}(m,N)B_N\tilde{\varphi}_0 + h^2\sum_{m=1}^{s}\sum_{l=-N}^{-1}[I+hA_0]^T\widetilde{Y}^T(m,0)\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l +$$

$$h^3\sum_{m=N+1}^{s}\sum_{l=-N}^{-1}B_N^T\widetilde{Y}^T(m,N)\widetilde{Y}(m,l+N)B_{l+N}\tilde{\varphi}_l =$$

$$\beta I\widehat{\varphi}_0 + (\gamma+h)I\widehat{y}_0 - h\sum_{m=1}^{s}[I+hA_0]^T\widetilde{Y}^T(m,0)\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right) +$$

$$-h^2\sum_{m=N+1}^{s}B_N^T\widetilde{Y}^T(m,N)\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l - \widehat{y}_m\right).$$

Let us define

$$\widetilde{M}_A(m,0) = \widetilde{Y}(m,0)[I+hA_0] \quad \text{and} \quad \widetilde{M}_B(m,N) = h\widetilde{Y}(m,N)B_N. \tag{4.9}$$

Then, taking into account that $\widetilde{Y}(m,N)=0$ when $m \le N$ we can write the formula for $\tilde{\varphi}_0$ in the form

$${}^h\mathcal{D}^{\beta,\gamma}\tilde{\varphi}_0 + h\sum_{m=1}^{s}\sum_{l=-N}^{-1}\left(\ \widetilde{M}_A^T(m,0) + \widetilde{M}_B^T(m,N)\ \right)\widetilde{M}_B(m,l+N)\tilde{\varphi}_l = F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f), \tag{4.10}$$

where

$${}^h\mathcal{D}^{\beta,\gamma} \equiv (\beta+\gamma+h)I + h\sum_{m=1}^{s}\left(\ \widetilde{M}_A^T(m,0) + \widetilde{M}_B^T(m,N)\ \right)\left(\ \widetilde{M}_A(m,0) + \widetilde{M}_B(m,N)\ \right)$$

and

$$F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f)=\beta I\widehat{\varphi}_0+(\gamma+h)I\widehat{y}_0-h\sum_{m=1}^{s}\Big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \Big)\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l-\widehat{y}_m\right).$$

Thus, if we substitute $\tilde{\varphi}_0$ from (4.10) into (4.7) we obtain a "discrete integral equation" for $\tilde{\varphi}$:

$$\alpha\tilde{\varphi}_n+\sum_{m=1}^{s}\sum_{l=-N}^{-1}\widetilde{M}_B^T(m,n+N)\widetilde{M}_B(m,l+N)\tilde{\varphi}_l+$$

$$-h\sum_{m=1}^{s}M_B^T(m,n{+}N)\Big(M_A(m,0){+}M_B(m,N)\Big)[{}^h\mathcal{D}^{\beta,\gamma}]^{-1}\sum_{j=1}^{s}\sum_{l=-N}^{-1}\Big(\widetilde{M}_A^T(j,0){+}\widetilde{M}_B^T(j,N)\Big)\widetilde{M}_B(j,l{+}N)\tilde{\varphi}_l+$$

$$h\sum_{m=1}^{s}M_B^T(m,n+N)\big(\ M_A(m,0)+M_B(m,N)\ \big)[{}^h\mathcal{D}^{\beta,\gamma}]^{-1}F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f)=$$

$$\alpha\widehat{\varphi}_n-h\sum_{m=n+N+1}^{s}\widetilde{M}_B^T(m,n+N)\Big(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l-\widehat{y}_m\Big),\quad n=-N,\dots,-1,$$

and for $\tilde{\varphi}_0$:

$$\tilde{\varphi}_0=-\big[{}^h\mathcal{D}^{\beta,\gamma}\big]^{-1}h\sum_{m=1}^{s}\sum_{l=-N}^{-1}\Big(\ \widetilde{M}_A^T(m,0){+}\widetilde{M}_B^T(m,N)\ \Big)\widetilde{M}_B(m,l{+}N)\tilde{\varphi}_l+\big[{}^h\mathcal{D}^{\beta,\gamma}\big]^{-1}F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f). \tag{4.11}$$

Thus, we can state the following results:

Theorem 4.1 *A function $\tilde{\varphi}$, which minimize ${}^h\tilde{S}_\alpha^{\beta,\gamma}(\tilde{\varphi})$ for $\tilde{\varphi}\in\mathcal{F}^h$ satisfies the summation equation*

$$\alpha\tilde{\varphi}_n+\sum_{l=-N}^{-1}{}^h\mathcal{K}_{nl}^{\beta,\gamma}\tilde{\varphi}_l={}^h\mathcal{G}_\alpha^{\beta,\gamma}(n)\quad\textit{for}\ \ n=-N,-1, \tag{4.12}$$

and

$$\tilde{\varphi}_0=-\big[{}^h\mathcal{D}^{\beta,\gamma}\big]^{-1}h\sum_{m=1}^{s}\sum_{l=-N}^{-1}\Big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \Big)\widetilde{M}_B(m,l+N)\tilde{\varphi}_l+\big[{}^h\mathcal{D}^{\beta,\gamma}\big]^{-1}F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f).$$

Here,

$${}^h\mathcal{K}_{nl}^{\beta,\gamma}=\sum_{m=1}^{s}\widetilde{M}_B^T(m,n+N)\widetilde{M}_B(m,l+N)-h\sum_{m=1}^{s}\sum_{j=1}^{s}\mathcal{M}^T(m,n+N)[{}^h\mathcal{D}^{\beta,\gamma}]^{-1}\mathcal{M}(j,l+N),$$

$${}^h\mathcal{G}_\alpha^{\beta,\gamma}(n)=\alpha\widehat{\varphi}_n-h\sum_{m=1}^{s}\Big\{\widetilde{M}_B^T(m,n{+}N)\Big(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l-\widehat{y}_m\Big)-\mathcal{M}^T(m,n{+}N)[{}^h\mathcal{D}^{\beta,\gamma}]^{-1}F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f)\Big\},$$

$$\mathcal{M}(m,n+N)=\Big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \Big)\widetilde{M}_B(m,l+N),$$

$${}^h\mathcal{D}^{\beta,\gamma}\equiv(\beta+\gamma+h)I+h\sum_{m=1}^{s}\big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \big)\big(\ \widetilde{M}_A(m,0)+\widetilde{M}_B(m,N)\ \big)$$

and

$$F^{\beta,\gamma}(\widehat{\varphi},\widehat{y},f)=\beta I\widehat{\varphi}_0+(\gamma+h)I\widehat{y}_0-h\sum_{m=1}^{s}\Big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \Big)\left(h\sum_{l=0}^{m-1}\widetilde{Y}(m,l)f_l-\widehat{y}_m\right).$$

4.2 Properties of the discrete kernel

We can establish the properties of the of the discrete kernel by adapting the discussion for the continuous case [8].

Let us consider the first variation of the functional (2.5) with the set of limits (3.8). Taking into account (3.9), we can write

$$ {}^h\tilde{P}_\alpha^{\beta,\gamma} = \alpha h \sum_{n=-N}^{-1} (\tilde{\varphi}_n - \widehat{\varphi}_n)\tilde{\psi}_n + h\sum_{n=1}^{s}[\tilde{y}_n(\tilde{\varphi}_n) - \widehat{y}_n]\tilde{z}_n + \widehat{\mathfrak{p}}^h_{\beta,\gamma}, \tag{4.13} $$

where $\widehat{\mathfrak{p}}^h_{\beta,\gamma} = {}^1\widehat{\mathfrak{p}}^h_{\beta,\gamma}(\tilde{\varphi}_0,\tilde{\psi}_0) + {}^2\widehat{\mathfrak{p}}^h_{\beta,\gamma}(\widehat{\varphi}_0,\widehat{y}_0,\tilde{\psi}_0)$. (Observe that we replaced the term $[\tilde{y}_0(\tilde{\varphi}_n) - \widehat{y}_0]\tilde{z}_0$ by the term ${}^2\widehat{\mathfrak{p}}^h_{\beta,\gamma}$.)

We can write (4.13) in the form

$$ {}^h\tilde{P}_\alpha^{\beta,\gamma} = \alpha h \sum_{n=-N}^{-1} \tilde{\varphi}_n\tilde{\psi}_n - \alpha h \sum_{n=-N}^{-1} \widehat{\varphi}_n\tilde{\psi}_n + h\sum_{n=1}^{s}\tilde{y}_n(\tilde{\varphi}_n)\tilde{z}_n - h\sum_{n=1}^{s}\widehat{y}_n\tilde{z}_n + \widehat{\mathfrak{p}}^h_{\beta,\gamma}, $$

or, with an obvious notation,

$$ {}^h\tilde{P}_\alpha^{\beta,\gamma} = \Delta_1^h\tilde{P}_\alpha^{0,0}(\tilde{\varphi},\tilde{\psi}) - \Delta_2^h\tilde{P}_\alpha^{0,0}(\widehat{\varphi},\tilde{\psi}) + \nabla_1^h\tilde{P}_0^{0,0}(\tilde{y},\tilde{z}) - \nabla_2^h\tilde{P}_0^{0,0}(\widehat{y},\tilde{z}) + \widehat{\mathfrak{p}}^h_{\beta,\gamma}. $$

According to [7, pp.13-14] the solution of the discrete DDE can be written in terms of fundamental matrices. Thus we have

$$ \tilde{y}_n = \tilde{Y}(n,0)\{I + hA_0\}\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\tilde{Y}(n,l+N)B_{l+N}\tilde{\varphi}_l + h\sum_{l=0}^{n-1}\tilde{Y}(n,l)f_l, $$

and for the homogeneous equation

$$ \tilde{z}_n = \tilde{Y}(n,0)\{I + hA_0\}\tilde{\psi}_0 + h\sum_{l=-N}^{0}\tilde{Y}(n,l+N)B_{l+N}\tilde{\psi}_l. $$

Using (4.9) we can write the above formulae as

$$ \tilde{y}_n = \tilde{M}_A(n,0)\tilde{\varphi}_0 + h\sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\varphi}_l + h\sum_{l=0}^{n-1}\tilde{Y}(n,l)f_l \tag{4.14} $$

and

$$ \tilde{z}_n = \tilde{M}_A(n,0)\tilde{\psi}_0 + h\sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\psi}_l. \tag{4.15} $$

Thus, using (4.14) and (4.15) we can write $\nabla_1^h\tilde{P}_0^{0,0}(\tilde{y},\tilde{z}) =$

$$ h\sum_{n=1}^{s}\Big\{\tilde{\varphi}_0^T\tilde{M}_A^T(n,0)\tilde{M}_A(n,0)\tilde{\psi}_0 + \sum_{l=-N}^{0}\sum_{m=-N}^{0}\tilde{\varphi}_l^T\tilde{M}_B^T(n,l+N)\tilde{M}_B(n,m+N)\tilde{\psi}_m + $$
$$ h\sum_{l=-N}^{0}\tilde{\varphi}_0^T\tilde{M}_A^T(n,0)\tilde{M}_B(n,l+N)\tilde{\psi}_l + h\sum_{l=-N}^{0}\tilde{\varphi}_l^T\tilde{M}_B^T(n,l+N)\tilde{M}_A(n,0)\tilde{\psi}_0\Big\} + $$
$$ +h^2\sum_{n=1}^{s}\sum_{l=0}^{n-1}\tilde{Y}^T(n,l)f_l^T\Big\{\tilde{M}_A(n,0)\tilde{\psi}_0 + \sum_{m=-N}^{0}\tilde{M}_B^T(n,m+N)\tilde{\psi}_l\Big\}, $$

or, in brief,

$$\nabla_1^h\tilde{P}_0^{0,0}(\tilde{y},\tilde{z}) = {}^1\nabla_1^h\tilde{P}_0^{0,0}(\tilde{\varphi},\tilde{\psi}) + {}^2\nabla_1^h\tilde{P}_0^{0,0}(f,\tilde{\psi}).$$

Let us now consider the discrete bilinear form

$${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi}) = \Delta_1^h\tilde{P}_\alpha^{0,0}(\tilde{\varphi},\tilde{\psi}) + {}^1\nabla_1^h\tilde{P}_0^{0,0}(\tilde{\varphi},\tilde{\psi}) + {}^1\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\tilde{\varphi}_0,\tilde{\psi}_0).$$

Lemma 4.1 *The discrete bilinear form* ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi})$ *is symmetric and positive definite* (${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\varphi}) > 0$ *if* $\{\tilde{\varphi}_n\} \neq 0$) *on* $\mathcal{F}^h$.

Proof. Let us write the term ${}^1\nabla_1^h\tilde{P}_0^{0,0}(\tilde{\varphi},\tilde{\psi})$ in the form

$$h\sum_{n=1}^{s}\Big[\tilde{M}_A(n,0)\tilde{\varphi}_0 + \sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\varphi}_l\Big]^T\Big[\tilde{M}_A(n,0)\tilde{\psi}_0 + \sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\psi}_l\Big],$$

where ${}^1\widehat{\mathfrak{p}}_{\beta,\gamma}^h(\tilde{\varphi}_0,\tilde{\psi}_0) = \tilde{\varphi}_0^T(\beta+\gamma+h)I\tilde{\varphi}_0$. Thus, for ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi})$ we have

$${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi}) = \alpha h\sum_{n=-N}^{-1}\tilde{\varphi}_n\tilde{\psi}_n + h\sum_{n=1}^{s}\Big[\tilde{M}_A(n,0)\tilde{\varphi}_0 + \sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\varphi}_l\Big]^T\times$$

$$\Big[\tilde{M}_A(n,0)\tilde{\psi}_0 + \sum_{l=-N}^{0}\tilde{M}_B(n,l+N)\tilde{\psi}_l\Big] + \tilde{\varphi}_0(\beta+\gamma+h)I\tilde{\psi}_0, \tag{4.16}$$

and it is straightforward from (4.16) that ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi})$ is symmetric and ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\varphi}) \geq 0$. The Lemma is therefore established.

We shall now obtain a result concerning ${}^h\mathcal{K}_{lm}^{\beta,\gamma}$ in Theorem 4.1. Collecting the similar terms in (4.16) we obtain

$${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi}) = h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\sum_{m=-N}^{-1}\tilde{\varphi}_l^T\tilde{M}_B^T(n,l+N)\tilde{M}_B(n,m+N)\tilde{\varphi}_m + \alpha h\sum_{l=-N}^{-1}\tilde{\varphi}_l^T\tilde{\varphi}_l +$$

$$h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\tilde{\varphi}_l^T\tilde{M}_B^T(n,l+N)\left[\tilde{M}_A(n,0)+\tilde{M}_B(n,N)\right]\tilde{\varphi}_0 + \Bigg\{h\sum_{n=1}^{s}\sum_{l=-N}^{-1}\tilde{\varphi}_0^T\left[\tilde{M}_A^T(n,0)+\tilde{M}_B^T(n,N)\right]\times$$

$$\tilde{M}_B^T(n,l+N)\tilde{\varphi}_l + \tilde{\varphi}_0\Big[(\beta+\gamma+h)I + h\sum_{n=1}^{s}\left[\tilde{M}_A^T(n,0)+\tilde{M}_B^T(n,N)\right]\left[\tilde{M}_A(n,0)+\tilde{M}_B(n,N)\right]\Big]\tilde{\varphi}_0\Bigg\}. \tag{4.17}$$

Now we consider the bilinear form ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\varphi})$ with some particular $\tilde{\varphi}_0$, namely

$$\tilde{\tilde{\varphi}}_0 = -h[{}^h\mathcal{D}^{\beta,\gamma}]^{-1}\sum_{n=1}^{s}\sum_{l=-N}^{-1}\Big(\tilde{M}_A^T(n,0)+\tilde{M}_B^T(n,N)\Big)\tilde{M}_B(n,l+N)\tilde{\varphi}_l \tag{4.18a}$$

with

$${}^h\mathcal{D}^{\beta,\gamma} = (\beta+\gamma+h)I + h\sum_{m=1}^{s}\big(\ \widetilde{M}_A^T(m,0)+\widetilde{M}_B^T(m,N)\ \big)\big(\ \widetilde{M}_A(m,0)+\widetilde{M}_B(m,N)\ \big). \tag{4.18b}$$

For $\tilde{\tilde{\varphi}}_0$ defined by (4.18a) the two last terms (within the parenthesis) in (4.17) vanish and we have

$$
{}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi}) = \alpha h \sum_{l=-N}^{-1} \tilde{\varphi}_l^T \tilde{\varphi}_l + h \sum_{n=1}^{s} \sum_{l=-N}^{-1} \sum_{m=-N}^{-1} \tilde{\varphi}_l^T \tilde{M}_B^T(n,l+N) \tilde{M}_B(n,m+N) \tilde{\varphi}_m +
$$

$$
-h^2 \sum_{n=1}^{s} \sum_{k=1}^{s} \sum_{l=-N}^{-1} \sum_{m=-N}^{-1} \tilde{\varphi}_l^T \tilde{M}_B^T(n,l+N) \Big(\tilde{M}_A(n,0) + \tilde{M}_B(n,N)\Big) [\mathcal{D}^h]^{-1} \times
$$

$$
\Big(\widetilde{M}_A^T(k,0) + \widetilde{M}_B^T(k,N)\Big) \widetilde{M}_B(k,m+N) \tilde{\varphi}_m.
$$

The expression for ${}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi})$ can be written in the form

$$
{}^h\mathcal{P}_\alpha^{\beta,\gamma}(\tilde{\varphi},\tilde{\psi}) = \alpha(\tilde{\varphi},\tilde{\varphi}) + ({}^h\mathcal{K}_{lm}^{\beta,\gamma}\tilde{\varphi},\tilde{\varphi}), \tag{4.19}
$$

where $\quad {}^h\mathcal{K}_{lm}^{\beta,\gamma} = \sum_{n=1}^{s} \tilde{M}_B^T(n,l+N)\tilde{M}_B(n,m+N) +$

$$
-h \sum_{n=1}^{s} \sum_{k=1}^{s} \tilde{M}_B^T(n,l+N) \Big(\tilde{M}_A(n,0) + \tilde{M}_B(n,N)\Big) [{}^h\mathcal{D}^{\beta,\gamma}]^{-1} \Big(\widetilde{M}_A^T(k,0) + \widetilde{M}_B^T(k,N)\Big) \widetilde{M}_B(k,m+N). \tag{4.20}
$$

Compare the discrete kernel from Theorem 4.1 and from (4.20) we can establish

Theorem 4.2 *The discrete kernel ${}^h\mathcal{K}_{lm}^{\beta,\gamma} \in \mathbb{R}^{n\times n}$ in Theorem 4.1 is symmetric and positive semidefinite ($\sum\sum {}^h\mathcal{K}_{lm}^{\beta,\gamma}\tilde{\varphi}_l\tilde{\varphi}_m > 0$ if $\{\tilde{\varphi}_l\} \neq 0$) on $\mathcal{F}^h$.*

Proof. Using Lemma 4.1 and taking into account (4.19), Theorem 4.2 is established.

Remark 4.1 *Theorem 4.1 and 4.2 are valid for arbitrary s. Earlier in our discussion (see §2) we consider a few possible choices of s, which correspond to different ways of discretization of (1.2). It is convenient at this stage to choose $s = K$ to keep the order in the discretization of the DDEs, even if we have order h error in the quadrature in (2.5).*

5 A discrete iterative technique

To solve the "data assimilation problem" numerically we consider the iterative process associated with (4.2).

$$
\frac{\tilde{y}_{n+1}^{[j]} - \tilde{y}_n^{[j]}}{h} - A_n\tilde{y}_n^{[j]} - B_n\tilde{y}_{n-N}^{[j]} = f_n \quad n = 0,1,\ldots,K-1, \tag{5.1a}
$$

$$
\tilde{y}_n^{[j]} = \tilde{\varphi}_n^{[j]}, \ \ n = -N,\ldots,0, \tag{5.1b}
$$

$$
-\frac{\tilde{x}_n^{T[j]} - \tilde{x}_{n-1}^{T[j]}}{h} - \tilde{x}_n^{T[j]}A_n - \tilde{x}_{n+N}^{T[j]}B_{n+N} = h[\tilde{y}_n^{[j]}(\tilde{\varphi}_n) - \widehat{y}_n]^T, \tag{5.1c}
$$

$$
\tilde{x}_n^{T[j]} = 0, \ \ n = K,\ldots,K+N, \tag{5.1d}
$$

$$
\tilde{\varphi}_n^{[j+1]} = \tilde{\varphi}_n^{[j]} + \delta_n\big(\alpha(\tilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + B_{n+N}^T\tilde{x}_{n+N}^{[j]}\big), \quad n = -N,\ldots,-1, \tag{5.1e}
$$

$$
\tilde{\varphi}_0^{[j+1]} = \tilde{\varphi}_0^{[j]} + \delta_n'\{(\beta+\gamma+h)\tilde{\varphi}_0^{[j]} + (I+hA_0)^T\tilde{x}_0^{[j]} - \beta\widehat{\varphi}_0 - (\gamma+h)\widehat{y}_0\}, \tag{5.1f}
$$

to determine successive approximation to $\tilde{y}$, $\tilde{x}$ and $\tilde{\varphi} \in \mathcal{F}^h$. The function $\tilde{\varphi}$ obtained by the iteration process (5.1) provides the minimum of the functional $S_\alpha^{\beta,\gamma}(\tilde{\varphi})$. Here, j is an iteration index and we use the notation $\tilde{y}_n^{[j]}$, $\tilde{x}_n^{T[j]}$ to emphasize that these are the solutions obtained by some iterative method.

We shall establish the convergence of the iterative process (5.1) by studying the iteration

$$\frac{\tilde{\varphi}_n^{[j+1]} - \tilde{\varphi}_n^{[j]}}{\delta_j} = \mathcal{G}_n^h - \Big(\alpha\tilde{\varphi}_n^{[j]} + \sum_{l=-N}^{-1} {}^hK_{ln}^{\beta,\gamma}\tilde{\varphi}_l^{[j]}\Big), \quad n = \{-N, \ldots, -2, -1\}, \tag{5.2}$$

in which j is the iteration index.

This iteration is based upon the integral equation (4.12). In (5.2), ${}^hK_{ln}^{\beta,\gamma}$ has been shown to be symmetric and positive-definite; the corresponding discrete integral operator on Euclidean space with the norm $\|\psi\|_2^2 = \sum_{l=-N}^{0} \psi_l^2$ is bounded, self-adjoint, and positive-definite. We state the following result.

Lemma 5.1 *The iteration (5.2) is equivalent to the iteration (5.1); for a given $\tilde{\varphi}^{[0]}$, the two sequences $\{\tilde{\varphi}^{[j]}\}$ are identical.*

Proof. From (5.1e), the functions defined by the iteration (5.1) satisfy the relation

$$\frac{\tilde{\varphi}_n^{[j+1]} - \tilde{\varphi}_n^{[j]}}{\delta_j} = \alpha(\tilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + [B_{n+N}]^T x_{n+N}^{[j]}, \quad \text{for } n = \{-N, \ldots, -2, -1\},$$

and we have shown in §4.1 that

$$\alpha(\tilde{\varphi}_n^{[j]} - \widehat{\varphi}_n) + [B_{n+N}]^T x_{n+N}^{[j]} = \alpha\tilde{\varphi}_n^{[j]} + \sum_{l=-N}^{-1} {}^hK_{ln}^{\beta,\gamma}\tilde{\varphi}_l^{[j]} - \mathcal{G}_n,$$

so the result is immediate.

Theorem 5.1 (Convergence) *Suppose $\rho({}^hK^{\beta,\gamma})$ is the spectral radius of the matrix-operator ${}^hK^{\beta,\gamma}$ on $L_2^h[-\tau, 0]$ having the kernel ${}^hK_{ln}^{\beta,\gamma}$. Then, a sufficient condition for the iteration (5.1) to converge in the mean-square norm is*

$$\delta_j \le \frac{2}{\max\left(\alpha, \rho({}^hK^{\beta,\gamma})\right)}, \quad \textit{for all } j. \tag{5.3}$$

Remark 5.1 *All norms on finite-dimensional Euclidean space are equivalent, so the convergence holds in any norms.*

Proof. We shall write ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}\tilde{\varphi}_n = \alpha\tilde{\varphi}_n + \sum_{l=-N}^{-1} {}^hK_{ln}^{\beta,\gamma}\tilde{\varphi}_l$ and the matrix-operator ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$ on Euclidean space with the norm $\|\cdot\|_2$ inherits self-adjointness and (with $\alpha > 0$) positive-definiteness from the corresponding properties of the matrix-operator ${}^hK^{\beta,\gamma}$. For a sequence $\{\delta_j\}$ with $\delta_j > 0$ for all j, we can write the iteration process (5.2) in the form

$$\frac{\tilde{\varphi}_n^{[j+1]} - \tilde{\varphi}_n^{[j]}}{\delta_j} = \mathcal{G}_n - {}^h\mathfrak{L}_\alpha^{\beta,\gamma}\tilde{\varphi}_n^{[j]}. \tag{5.4}$$

Let $\tilde{\varphi}^\star$ be the solution of the equations ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}\tilde{\varphi}_n^\star = \mathcal{G}_n$ and let us define $\varepsilon^{j+1} = \tilde{\varphi}_n^{[j+1]} - \tilde{\varphi}_n^\star$. Then, according to (5.4), we have the relation

$$\varepsilon^{j+1} = (I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\varepsilon^j,$$

and

$$\varepsilon^{j+1} = \prod_{i=0}^{j}(I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\varepsilon^0. \tag{5.5}$$

The iteration (5.4) converges in the mean-square norm if $\|\varepsilon^j\|_2 \to 0$ as $j \to \infty$. From (5.5) we have

$$\|\varepsilon^{j+1}\|_2 \le \left\| \prod_{i=0}^{j}(I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\right\|_2 \|\varepsilon^0\|_2 \le \prod_{i=0}^{j}\left\|(I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma})\right\|_2 \|\varepsilon^0\|_2.$$

Thus, a sufficient condition for convergence of this iteration is

$$\|I - \delta_j {}^h\mathfrak{L}_\alpha^{\beta,\gamma}\|_2 \le \vartheta < 1, \quad \text{for all } j. \tag{5.6}$$

Given the properties of ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$ on chosen space, we have $\|{}^h\mathfrak{L}_\alpha^{\beta,\gamma}\|_2 = \max_r \kappa_r$ (the spectral radius $\rho({}^h\mathfrak{L}_\alpha^{\beta,\gamma})$), where $\{\kappa_r\}_{r\ge 0}$ are the positive eigenvalues of ${}^h\mathfrak{L}_\alpha^{\beta,\gamma}$. Indeed, $\kappa_r = \alpha + \varkappa_r$, where $\{\varkappa_r\}_{r\ge 0}$ are the positive eigenvalues of ${}^hK^{\beta,\gamma}$. Then condition (5.6) becomes

$$\max_r |1 - \delta_j\alpha - \delta_j\varkappa_r| < 1.$$

We have $1-\delta_j\alpha-\delta_j\varkappa_r \in [1-\delta_j\alpha-\delta_j\rho({}^hK^{\beta,\gamma}), 1-\delta_j\alpha) \subseteq (-1,1)$ provided $1-\delta_j\alpha-\delta_j\rho({}^hK^{\beta,\gamma}) > -1$ and Theorem 5.1 is established.

6 Computational results

In this section we present numerical results based upon iterative methods for the linear case (5.1).

We start by applying the results obtained in the above section to the simplest example: the scalar linear delay differential equation with variable coefficients and zero right-hand side,

$$\frac{dy(t)}{dt} - a(t)y(t) - b(t)y(t-\tau) = 0, \quad \text{for } t \in [0,T], \tag{6.1a}$$

subject to

$$y(t) = \tilde{\varphi}(t), \quad \text{for } t \in [-\tau, 0), \quad y(0) = \tilde{\varphi}(0). \tag{6.1b}$$

These equations are (1.1) with $A(t) = a(t) \in \mathbb{R}$ and $B(t) = b(t) \in \mathbb{R}$.

The discrete problem now has the form (4.2) with A_n replaced by $a_n \in \mathbb{R}$ and B_n by $b_n \in \mathbb{R}$.

The criteria we used for the termination of the iterative process (5.1) is the condition

$$\frac{\|\tilde{\varphi}^{[j+1]} - \tilde{\varphi}^{[j]}\|_2}{\|\tilde{\varphi}^{[j]}\|_2} \le \varepsilon, \tag{6.2}$$

where $\varepsilon = 10^{-6}$ and $\|\cdot\|_2$ is the norm

$$\|\psi\|_2 = h\left(\sum_{l=-N}^{0} \psi_l^2\right)^{1/2}. \tag{6.3}$$

The iteration (5.1) terminates when (6.2) is satisfies and we accept the approximation obtained $\tilde{\tilde{\varphi}} \equiv \tilde{\varphi}^{[\mathcal{N}]}$, say, when $\mathcal{N} \equiv \mathcal{N}(\alpha)$. In the presentation of the experiments, together with other information, we plot $\tilde{\tilde{\varphi}}$ and compare it with "true" initial function $\tilde{\varphi}_\star$.

6.1 A remark on the observation data

Before discussing our numerical results in section §6.2, we explore some related question in section §6.1.

According to §1 the "data assimilation problem" for the identification of the initial function required the observation data. In practical application the observation data is given *a priori*.

In order to solve test problems we obtained "pseudo-observation" data by the following procedure: we found the solution of $y(\tilde{\varphi}_\star; t)$ of the original delay differential equation (6.1) with initial function $\tilde{\varphi}_\star$ numerically and took this solution as the "observation data" $\widehat{y}(t)$. At this stage we can also perturb the "observation data" by adding small randomly-generated noise. Then we assumed that the initial function $\varphi(t)$ is unknown and using the iterative method (5.1) with some arbitrary initial guess we determine the approximating mesh-function $\tilde{\varphi}_\star$.

6.2 A solution with minimum norm

In our first set of experiments, we consider the case when $\widehat{\varphi}(t) \equiv 0$. In this case the functional (1.2) has the form

$$S_\alpha^{\beta,\gamma}(\tilde{\varphi}) := \frac{\alpha}{2}\int_{-\tau}^{0} \tilde{\varphi}^2(t)dt + \frac{\gamma}{2}\left|y(\tilde{\varphi};0) - \widehat{y}(0)\right|^2 + \frac{1}{2}\int_{0}^{T} \left|y(\tilde{\varphi};t) - \widehat{y}(t)\right|^2 dt.$$

This is the case where we are seeking the solution with minimum norm in $L_2^h[-\tau, 0]$.

Experiment 1

We start with a constant coefficient case and set $a(t) = -1$ and $b(t) = -1$. We solve the problem on the interval [0,2] ($T = 2\tau$). We found the solution of the problem (6.1) numerically for $\tilde{\varphi}_\star(t) = 2(0.5 + t)^3$, where $t \in [-1, 0]$, and consider this solution as $\widehat{y}(t)$. Then using the iterative method (5.1) we solved the identification problem with initial guess $\tilde{\varphi}^{[0]} = 0$. In the numerical experiments described below, we took 64 points in the interval $[-1, 0]$ ($\tau = 1$).

First we investigate how the convergence of the iteration method depends on the regularization parameter α. The number of iterations and the cpu time needed to obtain the required accuracy $\varepsilon = 10^{-6}$ are given in the Table 1 for different α. The figures for sf cpu time are unreliable because the computer is not a dedicated computer, but this give some indication of the time.

α	1	0.5	0.2	0.1	0.01	0.001	0.0001	0
The number of iterations	432	690	1302	2068	9746	26205	36226	38176
cpu time min:sec	0:0.05	0:0.08	0:0.18	0:0.27	0:1.47	0:11.19	0:26.97	0:30.93

Table 1: The number of iterations versus the regularization parameters α

Introducing the regularization parameter α leads to a solution $\tilde{\varphi} \equiv \tilde{\varphi}^{[\mathcal{N}]}(\alpha)$, differing from the solution $\tilde{\varphi}_\star$. We denote the relative error by the expression

$$\mathcal{R} \equiv \frac{\|\tilde{\varphi}^{[\mathcal{N}]} - \tilde{\varphi}_\star\|_2}{\|\tilde{\varphi}_\star\|_2},$$

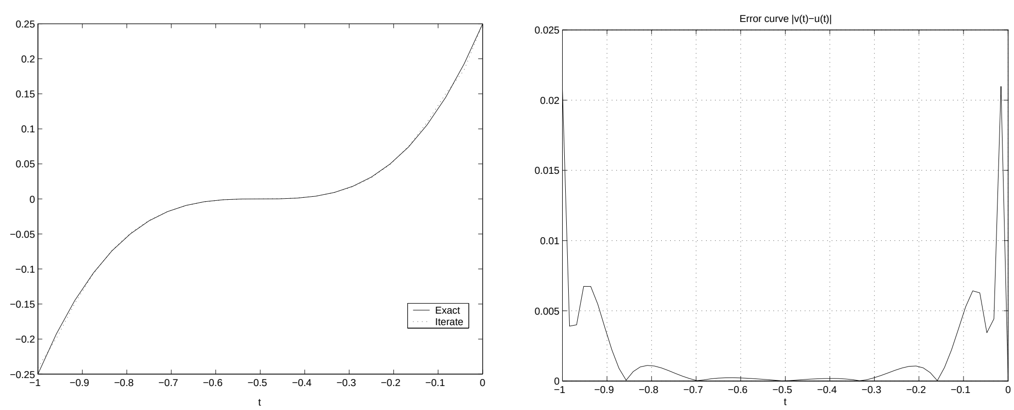
where $\tilde{\varphi}^{[\mathcal{N}]}$ is the iterated solution found by (5.1) and $\|\cdot\|$ is the norm defined in (6.3). Table 2 gives the value of relative error for different α.

α	1	0.5	0.2	0.1	0.01	0.001	0.0001	0
The relative error $\mathcal{R}$	0.894	0.851	0.751	0.646	0.294	0.088	0.043	0.038

Table 2: The value of the relative error versus the regularization parameter α

We see from Tables 1,2 that the introduction of a regularization parameter α speeds up the convergence of the iterative method. This is one of the advantages of introducing the regularizer. The disadvantage, as we can see from Table 2, is that the parameter α leads to an error in the identified solution. (The error decreases with α.)

The result of the above experiments are presented in Figures 1.



(a) The exact function $\tilde{\varphi}_\star(t)$ (solid line) and the iterated function $\tilde{\varphi}^{[\mathcal{N}]}(t)$, $\mathcal{N} = 38176$

(b) The difference curve $|\tilde{\varphi}_\star(t) - \tilde{\varphi}^{[\mathcal{N}]}(t)|$

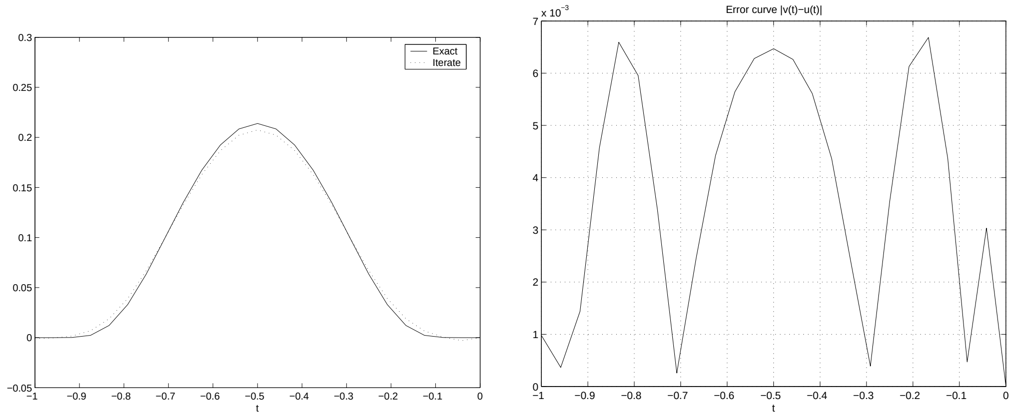
Figure 1: An experiment with the parameter $\alpha = 0$

Remark 6.1 *The qualitative behaviour of $\tilde{\varphi}^{[\mathcal{N}]}(\alpha)$ with respect to the regularization parameter α is typical of that seen with other problems (having differing $\varphi(t)$ and differing $\tilde{\varphi}^{[0]}$).*

Experiment 2

To illustrate the last remark, let us consider a second experiment with "true" initial function $\tilde{\varphi}_\star(t) = 10\exp\left(1/(t(1-t))\right)$. The number of points in the initial interval is 64 and $\tau = 1$.

The results of this experiment are presented in Figure 2 and a summary in Table 3



(a) The exact function $\tilde{\varphi}_{\star}(t)$ (solid line) and the iterated function $\tilde{\varphi}^{[\mathcal{N}]}(t)$

(b) The difference curve $|\tilde{\varphi}_{\star}(t) - \tilde{\varphi}^{[\mathcal{N}]}(t)|$, $\mathcal{N} = 16434$

Figure 2: An experiment with the parameter $\alpha = 0.001$

α	1	0.5	0.2	0.1	0.01	0.001	0.0001	0
$\mathcal{N}$ the number of iterations	327	550	1172	2066	8127	16434	19058	19416
The relative error $\mathcal{R}$	0.862	0.776	0.642	0.543	0.207	0.036	0.012	0.01

Table 3: The number of iterations versus the regularization parameters α. Experiment 2.

The relative error decreases when the parameter α decreases.

Experiment 3

In the next series of experiments, we consider a variable coefficient case. In the experiments 3 the "exact" initial function is $\tilde{\varphi}_{*}(t) = 2(0.5 + t)^3$. The parameters are follows: $\alpha = 0$, $\beta = 0$, $\gamma = 1$. In the experiment presented in Figure 3 the coefficients of the equation (6.1) are

$$a(t) = -1 + \sin(\pi t), \quad b(t) = -2t, \quad \text{where } t \in [0, 4]. \tag{6.4}$$

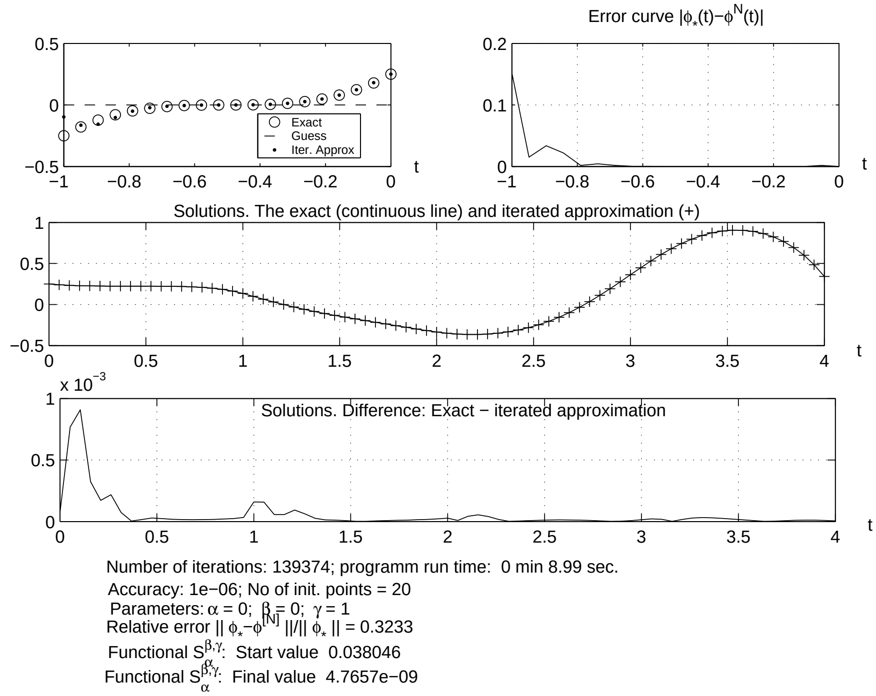


Figure 3: An experiments with $a(t)$ and $b(t)$ defined by (6.4)

Experiment 4

In the next experiments the coefficients are $a(t) = -5t$ and $b(t) = 5t$ and the results are presented in Figure 4. Then initial function is that used in Experiment 3 and $\alpha = \beta = \gamma = 0$.

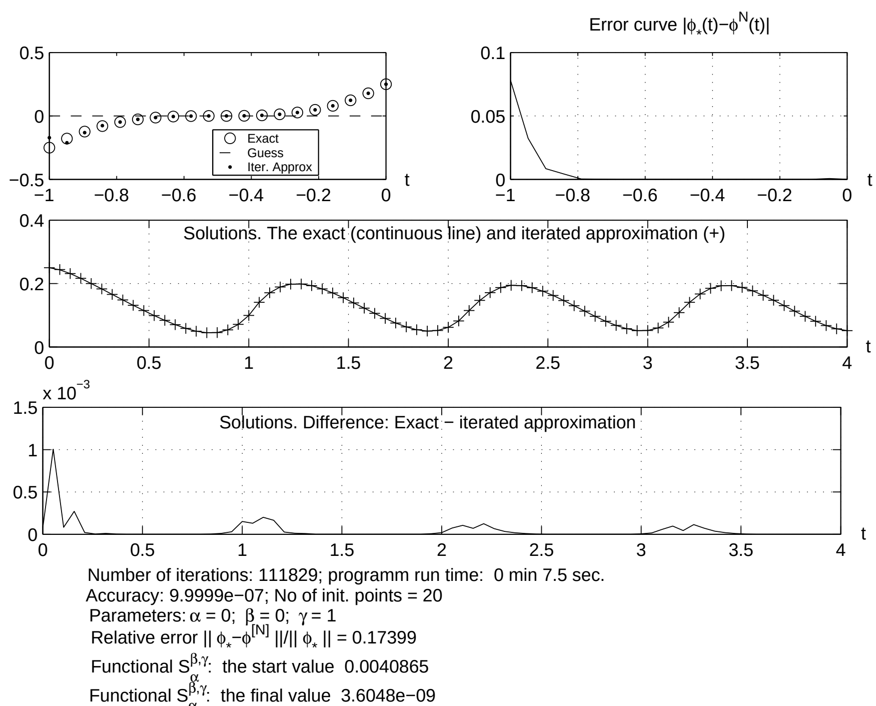


Figure 4: An experiments with $a(t) = -5t$ and $b(t) = 5t$

6.3 A rôle for the function $\widehat{\varphi}$

In this section we discuss the rôle for the function $\widehat{\varphi}(t)$. We shall present results, which may have a practical significance.

Experiment 5

We start with the case when in (6.1) $a(t) = -1$ and $b(t) = -1$ and $T = 2$ ($T = 2\tau$, $\tau = 1$). In the first numerical experiments the "true" initial function is $\tilde{\varphi}_\star(t) = 1 - 16(t + 0.5)^4$ and $\widehat{\varphi}(t) = \widehat{\varphi} = 1.1$. The number of points on the initial interval is 20 and the initial guess is $\tilde{\varphi}^{[0]} = 0$. The result of this experiment is shown in Figure 5

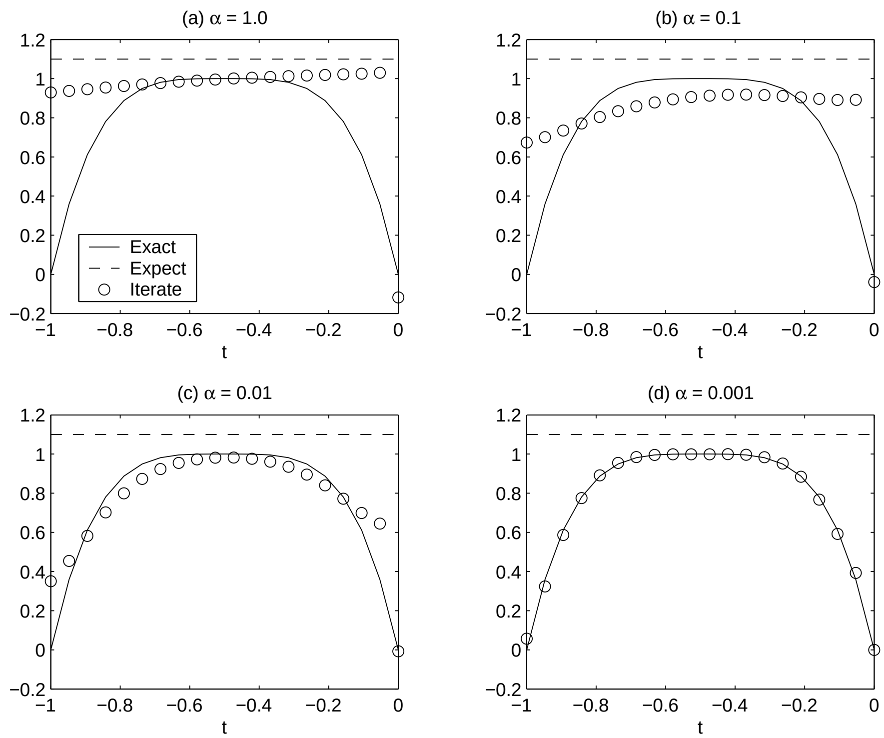


Figure 5: The rôle of $\widehat{\varphi}$ for different α. (Experiment 5)

Experiment 6

In the next experiment suppose that we have some information about the initial function (its general form, some coefficients, etc.) and want to improve this information. For example, we know the general form of the initial function, but we need to correct some coefficients.

As an example, we consider the function

$$\tilde{\varphi}(t) = \sigma_1 \exp\left(\frac{\sigma_2}{(t+1)t}\right);$$

here, the structure is assumed but we suppose σ_1 and σ_2 unknown. Observe that we do not estimate σ_1, σ_2 but compute the mesh values of on approximation $\tilde{\varphi}$ to $\tilde{\varphi}_\star$. The equation is that considered in Experiment 5.

For the "true" initial function we take the following sets of the coefficients: $\sigma_1 = 500$, $\sigma_2 = 1.8$ and for the function $\widehat{\varphi}$ $\sigma_1 = 10$, $\sigma_2 = 1$. The number of initial points is 50 and $\tau = 1$. In the

Table 4 we give a summary of the experiments. The exact initial function, the function $\widehat{\varphi}$ and the

The parameter α	1	0.1	0.01	0.001
The number of iterations	372	2415	10499	21598
cpu time (min:sec)	0:1.65	0:10.98	0:49.49	1:53.7
The relative error	0.471	0.365	0.006	0.002

Table 4: A summary of the experiment 6

iterated solution, which we accept as on approximation to $\tilde{\varphi}$, are shown in the Figure 6.

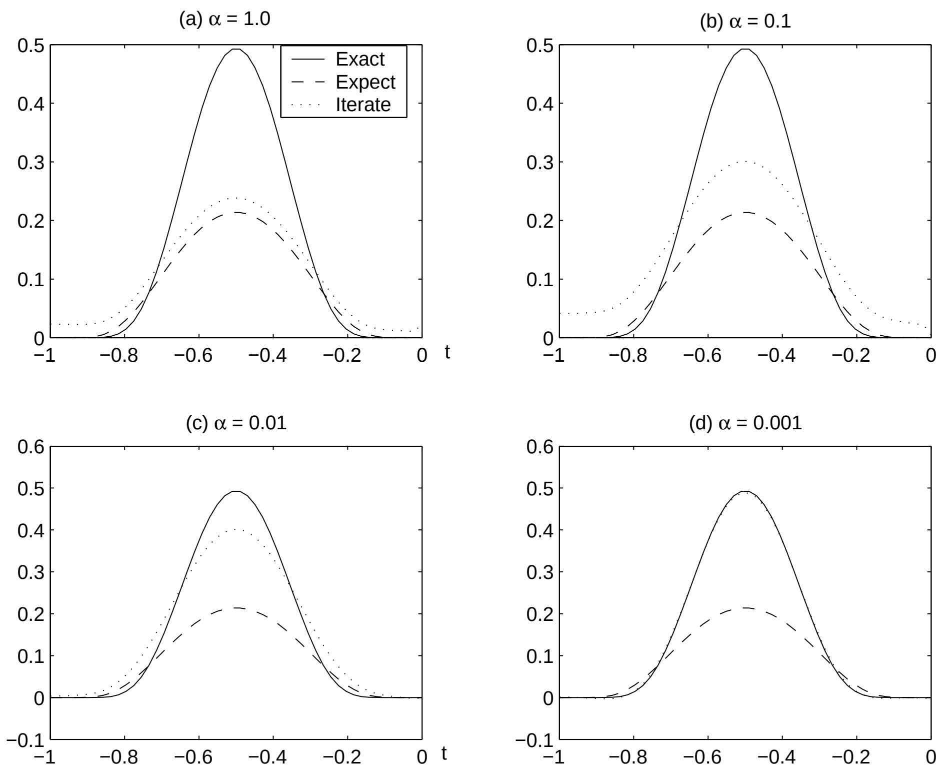


Figure 6: The rôle of $\widehat{\varphi}$ for different α. (Experiment 6)

As we see from these experiments the behaviour of the accepted iterate function depends on the regularization parameter α. When $\alpha \approx 1$ the approximate solution is relatively close to the function $\widehat{\varphi}$; when $\alpha \to 0$ the accepted function becomes closer to the "true" initial function.

It can be shown, that in the case when the integral equation of the first kind ($\alpha = 0$) has a unique solution, the resulting approximate solution is independent of the function $\widehat{\varphi}$. When there is not a unique solution, the choice of $\widehat{\varphi}$ influences $\tilde{\varphi}_\star$ as $\alpha \to 0$.

6.4 A "coarse grid" strategy

In this section, we discuss a strategy that we can use to recover the initial function when the function $\widehat{\varphi}$ is not stated (the case $\alpha = 0$, $\beta = 0$) or alternatively the case where we set $\widehat{\varphi} \equiv 0$ for the want of something better. This is the case when the shape of the initial function cannot be predicted from real observation or an understanding of the process itself.

To illustrate, we solve the identification problem for a problem with "true" initial function $\tilde{\varphi}_\star(t) = 2(t + 0.5)^4$ on the interval $t \in [-1, 0]$ with 100 points. The coefficients of the delay differential equation (6.1) are $a(t) = 1$, $b(t) = 1$. The results of the experiment (in which $\alpha = \beta = 0$) is shown in Figure 7. As we see in Figure 7, the error near both boundaries of the initial interval ($t = -1$ and $t = 0$) is significantly large than in the rest of interval for stepsize $h = 0.01$ ($h = \tau/N$, where N is a number of points on the initial interval $[-1, 0]$).

Here we suggest a possible way to "improve" the behaviour of the algorithm near the boundary points by analyzing the discrete version of the identification problem. It is quite simple: we try to use a coarser mesh on the initial interval (that is, a larger step h). However, too coarse a mesh is also inappropriate.

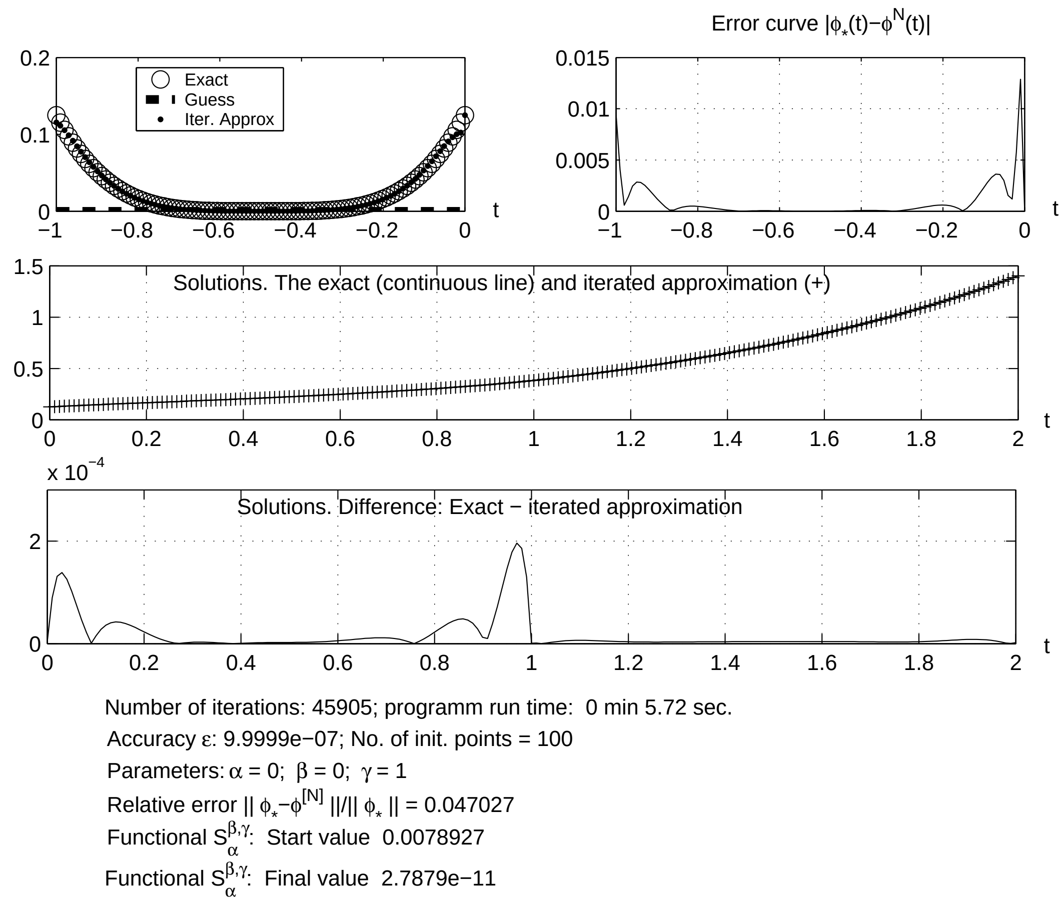


Figure 7: An experiment with 100 points on the initial interval and parameter $\alpha = 0$

Remark 6.2 *We offer some insight. As we know (see §4) the optimal control problem for recovery of the initial function is equivalent to an integral equation of the second kind when $\alpha \neq 0$, but if the parameter α vanishes our problem is equivalent to an integral equation of the first kind. Earlier in our discussion (see Lemma 3.2 and §4) we obtain an equivalent condition for a minimum in the form (3.10). The formula (3.10b) depends on the step h, and the solution obtained is* *equivalent to that obtained by discretizing the integral equation. In the case of a first-kind integral equation, there is a trade-off between improving the discretization error by selecting a small h and the increased ill-conditioning (in the equations discretizing the integral equation) associated with this small h. Roughly speaking, as h is reduced, the order of the system of discrete equations increases, the number of singular values (the absolute values of the eigenvalues in the case the kernel is symmetric) of the coefficient matrix increases, and their ratio (which reflects the ill-conditioning) grows larger*[4] *This does not of itself explain why the approximation is worse at the interval end-points. To explain this requires an investigation of the singular vectors of the kernel (of the eigenvectors where the kernel is symmetric), and there is a link here with the properties of the kernel; further, the introduction of* $\alpha \neq 0$ *again alleviates the problem. Non of this is obvious because we do not compute* ${}^h\mathcal{K}_{nl}^{\beta;\gamma}$ *explicitly in our computation of* $\tilde{\varphi}$.

Figure 7 demonstrates the behaviour of the solution obtained from (5.1) near boundary points $t = -\tau$ and $t = 0$. To investigate this phenomenon, we decrease the number of points on the initial interval to 5 and (using the same initial function) we obtain the following result:

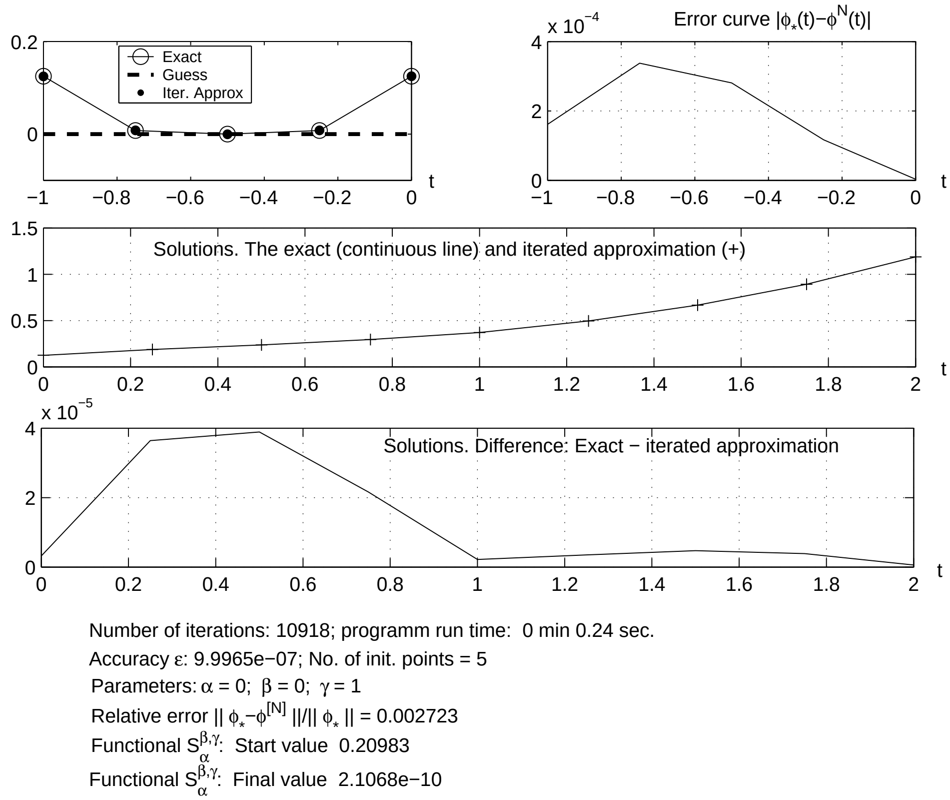


Figure 8: An experiment with 5 points on the initial interval and parameter $\alpha = 0$

In Table 5 we give summarize the results of our experiments with differing numbers of points (equally distributed) in the initial interval, including the cases shown on Figures 7 and 8. Here $\alpha = 0$, $\beta = 0$, $\gamma = 1$.

[4]This problem is alleviated if $\alpha \neq 0$.

The number of points	5	10	25	50	100
The number of iterations	10913	24751	40201	44272	111040
cpu time min:sec	0:7.91	0:39.88	2:21.71	4:33.26	10:20.87
The relative error	0.0027	0.0099	0.0309	0.0425	0.0470

Table 5: A summary of the experiment with different number of initial points

Compare this results we see that we obtain more accurate iterate solution for less number of initial points. This leads us to the following method for solving the optimal control problem (when the general form of the initial function is unknown):

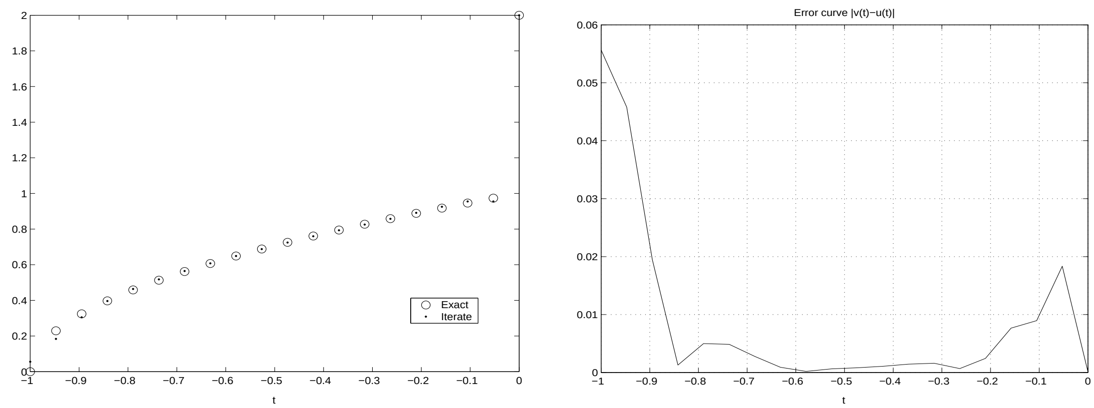
1. Solve the optimal control problem with a few points and with the parameter $\alpha = 0$ (the number of points have to be sufficient to use an interpolation method).
2. Using an interpolation method and the points from step 1, construct a function $\widehat{\varphi}$ to approximate the "true" initial function.
3. Increase the number of points in the initial interval and solve the optimal control problem using non-zero parameter α and the function from step 2 as a function $\widehat{\varphi}$.

6.5 A jump at the initial point

Another problem, which arises for delay differential equation is the possibility of a jump in the initial function at the initial point t_1 (in our case $t_1 = 0$). In section 4 we write the equivalent formulation for the fist variation of the functional (1.2) and obtain two equations for the initial function (4.2e) and (4.2f). Therefore, it is easy to see that we can extend the identification problem to the case where the initial function has a jump. Let us consider the numerical experiment with the "true" initial function in the form

$$\tilde{\varphi}_\star(t) = \begin{cases} \sqrt{1+t}, & t \in [-1, 0),\ \tau = 1 \\ 2, & t = 0. \end{cases} \tag{6.5}$$

The parameters in this experiment are taken to be $\alpha = 0$, $\beta = 0$, $\gamma = 1$, the coefficients are $a(t) = -1$ and $b(t) = -1$. The number of points on the initial interval is 20 and $T = 4$. The results are shown in Figures 9.



(a) The exact function $\tilde{\varphi}_\star(t)$ (solid line) and the iterated function $\tilde{\varphi}^{[\mathcal{N}]}(t)$, $\mathcal{N} = 38420$

(b) The difference curve $|\tilde{\varphi}_\star(t) - \tilde{\varphi}^{[\mathcal{N}]}(t)|$

Figure 9: An experiment with the jump at the initial point when the exact initial function defined by (6.5)

From the above figures we see, that results obtained for initial function with jump is similar to that obtained for a continuous initial function.

In Figure 10 the "true" initial function is

$$\tilde{\varphi}_\star(t) = \begin{cases} 1 - 16(t+0.5)^4, & t \in [-1, 0),\ \tau = 1 \\ 1.5, & t = 0. \end{cases} \tag{6.6}$$

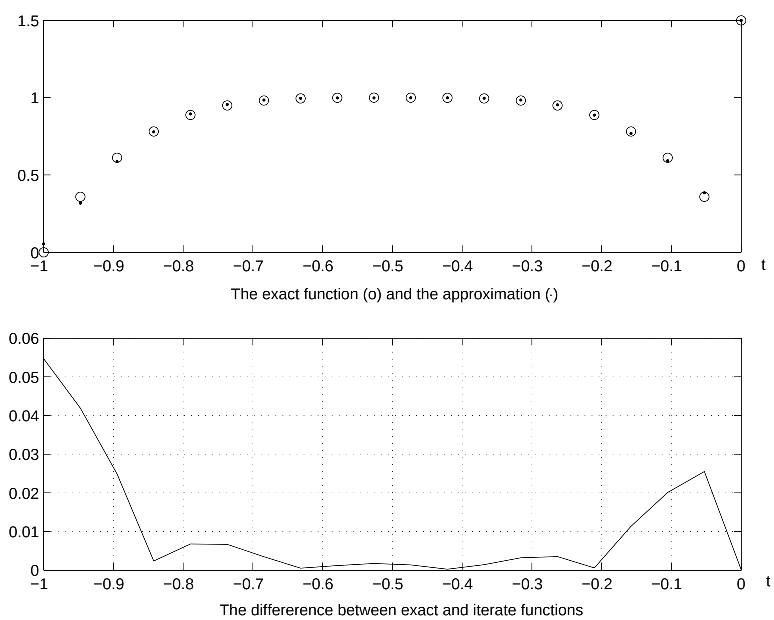


Figure 10: An experiment with a jump at the initial point when the exact initial function defined by (6.6)

6.6 An experiment with perturbed data

In practice, data observed from physical experiments always has some noise. Therefore, to justify our approach we need some numerical experiments where a perturbation is added to the "observation data". To investigate the behaviour of the iterative method we add to our "observation data" $\widehat{y}(t)$ a noise $\sigma\eta(t_i)$, where $\eta(t_i) \in N[0,1]$, $t_i = ih$. Then we solve the identification problem of finding the initial function with "new observation data" $\widehat{y}(t_i) + \sigma\eta(t_i)$. Here we use a scalar factor $\sigma \in \mathbb{R}$ to obtain a sufficiently small noise (approximately 5% of the "observation data").

One of the experiments with perturbed "observation data" is shown in Figure 11. In this experiments the "true" initial function is $\tilde{\varphi}_*(s) = 50 \exp 1/(s(1-s))$, where $s \in [-1, 0]$. The coefficients of the equation (6.1) are $a(t) = -2t$ and $b = t$, where $t \in [0, 4]$.

Thus, we can conclude that, in the current experiment and run on for sufficiently small noise, the method allows us to recover an initial function with reasonable accuracy.

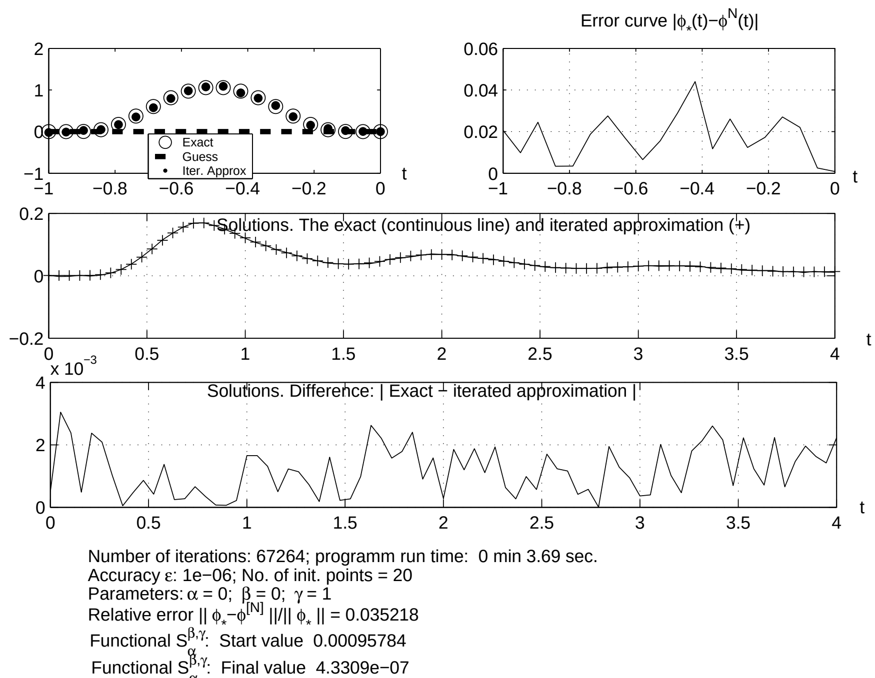


Figure 11: An experiment with perturbed "observation data"

6.7 Concluding remarks

Here we considered the identification problem through the example of a simple linear delay differential equations. The main experimental results are as follows.

If the regularization parameter α is equal to zero, the convergence rate of the method presented (the Picard iteration) is very slow and the result quite inaccurate. This is supported by the theoretical analysis provided in Chapter 3, where we stated that in the case $\alpha = 0$ we have to solve an integral equation of the first kind.

The introduction of a regularization parameter α speeds up the convergence. This is the case then we have to solve the integral equation of second kind with symmetric and positive-definite kernel. A disadvantage of introducing a regularization parameter lies in fact that an error, which depend on α, is introduced to the solution. The error decreases with α, but, at the same time, the number of iteration increases. The dependence on β and γ is not so strong, compared with the dependence upon α. In fact, when $\alpha = 0$ and β and γ are non-negative, we still have to solve an integral equation of the first kind.

Numerical experiments also show that the iterative method proposed can be used to solve the problem, when the initial function has a jump at the initial point. The behaviour of the algorithms in this case is similar to that we have for continuous initial function.

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A Appendix

A.1 Summation by parts formula

In order to obtain the equivalent form for the first variation of the objective function we need, at some stage, the summation by parts formula. In the continuous case we have

$$\frac{d}{dt}(uv) = u'v + uv'.$$

A corresponding discrete version has the form

$$u_{n+1}v_{n+1} - u_n v_n = \big(u_{n+1} - u_n\big)v_n + u_{n+1}\big(v_{n+1} - v_n\big). \tag{A.1}$$

This leads us to

$$\sum_{n=k}^{s} \big(u_{n+1} - u_n\big)v_n = u_{s+1}v_{s+1} - u_k v_k - \sum_{n=k}^{s} u_{n+1}\big(v_{n+1} - v_n\big). \tag{A.2}$$

If we now take $u_n = x_n$ and $v_n = \tilde{z}_{n+1}$ we obtain

$$\sum_{n=k}^{s} \big(x_{n+1} - x_n\big)\tilde{z}_{n+1} = x_{s+1}\tilde{z}_{s+2} - x_k\tilde{z}_{k+1} - \sum_{n=k}^{s} x_{n+1}\big(\tilde{z}_{n+2} - \tilde{z}_{n+1}\big). \tag{A.3}$$