Solving Stiff Problems Using Generalized Picard Iteration

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Abstract. The main point of the talk is an alternative approach to the construction of numerical methods for stiff problems. It can be interpreted as a generalization of fixed-point iterations for implementation of implicit collocation methods. The algorithms proposed combine easy implementation and low cost of iterations with superior convergence properties on stiff problems compared to conventional Picard iteration.

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INTRODUCTION

Since 1970's in Belarusian State University (Minsk, Belarus) a research group on numerical ODE solution have been working. The specifics of their early results were outlined in [2]. The approach was based on the development of multi-stage methods of sequentially increasing order and traditionally presumed the step size smallness. More detailed reference to these works can be found in the bibliography of [6].

Initial value problem for ODEs is an evolutionary one, therefore during the stepwise process of its numerical solution it is important (especially in case of stiff problem) to provide appropriate qualitative consistency between initial and approximate problems. Some notion about the results of Belarusian mathematicians in this aspect one can get from [5], [3]. These results lie upon various ways of providing spectral level consistency between corresponding evolutionary operators in case of inhomogeneous linear ODE system.

Since the interval of integration for evolutionary problems can be arbitrarily large it is reasonable to construct numerical methods with additional means of approximate solution refining, besides decreasing the step size. This approach has resulted in various processes of sequential solution refinement [7], [4]. The main subject of the further discussion is the numerical methods for stiff problems from [7]. Let us relate it to the current state-of-the-art.

There are two current opinions in numerical solution of stiff ODE systems: i) implicit (Runge–Kutta) methods are needed and ii) Newton iteration should be used for the solution of arising nonlinear equations. The reason for the first item is the fact that implicit methods, compared to explicit ones, have superior stability properties which allow using much larger step sizes during the integration. The necessity of Newton iteration (ii) is commonly justified by the assertion that straightforward fixed-point iteration (so-called Picard iteration) transform implicit method to explicit and thus destroy stability.

The notorious computational complexity of the recipe indicated above has led to various technical enhancements of the computational algorithms (e. g. [10, sect. 5.1]), such as W-transform and simplification of Newton iterations. Another way of increasing the efficiency of implicit RK methods is exploiting parallel computations (e. g. [11] and other related works of van der Houwen).

The numerical methods we are going to talk about emerged as a result of discretization of special analytic iterative processes [7], constructed to improve unsatisfactory properties of Picard iteration on stiff problems. It appears that with certain choice of approximation these discrete iterative processes can be interpreted as alternative (Newton-free) implementation of implicit collocation RK methods and have natural relationship with iterated RK methods [8]. The main advantage of our algorithms is that they combine easy implementation and low cost of iterations with superior convergence properties on stiff problems compared to Picard iteration.

THE STARTING POINT

Consider an IVP for the ODE system of dimension n:

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0. \tag{1}$$

Our goal is to find a continuous approximate solution $u \approx y$, defined on $[x_0, x_0 + h]$. We start with rescaling (1) from $[x_0, x_0 + h]$ to $[0, 1]$ and writing it in the form of integral equation:

$$v(\xi) = \int_0^\xi f(x_0 + h\zeta, y_0 + h\,v(\zeta))d\zeta, \quad \text{or simply} \quad v = \mathscr{S}F(v), \tag{2}$$

where $\mathscr{S}$ is integration operator, $\mathscr{S}v(\xi) = \int_0^\xi v(\zeta)d\zeta$; F is nonlinear operator, $F(v)(\xi) = f(x_0 + h\xi, y_0 + h\,v(\xi))$; v is element of Banach space $\mathbf{V} = \mathbf{C}([0,1], \mathbb{R}^n)$ or $\mathbf{L}_2([0,1], \mathbb{R}^n)$. According to this we clearly have $y(x) = y_0 + h\,v\left(\frac{x - x_0}{h}\right)$. By v^* denote the exact solution of (2).

Our research began with the endeavor to improve the analytic Picard iteration

$$v^{(l+1)} = \mathscr{S}F(v^{(l)})$$

which misbehaves when solving stiff problems. The main matter is that this process spoils good initial approximations, i. e. the norm of the error usually grows badly before starting to decay. Therefore we decided to apply a principle which in Russian scientific literature is called "*printsip ustanovleniya*" [1]. This can be translated as "*principle of steadying*"[1]. The essence of this approach is to introduce a fictitious variable t and construct a dissipative differential equation which steady-state solution coincides with the solution of the underlying problem (with v^* in our case). Such differential equation and its operator form are respectively

$$\frac{\partial}{\partial t} w(\xi, t) = -w(\xi, t) + \int_0^\xi f(x_0 + h\zeta, y_0 + h\,w(\zeta, t))d\zeta$$

and

$$W'(t) = -W(t) + \mathscr{S}F(W(t)). \tag{3}$$

Here W is a mapping from $[0, +\infty)$ to $\mathbf{V}$, $W(t)(\xi) = w(\xi, t)$. It is proved that for any Lipschitz continuous f and any step size h equation (3) is dissipative, i. e.

$$\lim_{t \to +\infty} \|W(t) - v^*\|_{\mathbf{V}} = 0$$

for any W satisfying (3).

Applying arbitrary explicit RK method to (3) we obtain an analytic iterative process for approximate solution of (2) (see [7] for details). In particular, explicit Euler method with fictitious time step $\tau = 1$ gives Picard process mentioned above. It is also shown in [7] that varying the value of τ results in processes with nicer behavior on model Dahlquist problem compared to Picard iteration.

METHOD CONSTRUCTION

In order to construct numerical methods corresponding to (3) we choose positive number s and introduce a projection operator

$$\Pi_s : \mathbf{V} \to \mathrm{Span}\{\varphi_i,\, i = 1, \ldots, s\} = \mathbf{U}_s \subset \mathbf{V},$$

where $\varphi_i : [0,1] \to \mathbb{R}$ are certain linearly independent basis functions. Assume that Π_s is determined by the set of s linear functionals $Q_i : \mathbf{V} \to \mathbb{R}^n$:

$$\Pi_s v = \sum_{i=1}^{s} Q_i v\, \varphi_i. \tag{4}$$

Applying Π_s to the mapping F in (2) and (3) we obtain a finite-dimensional version of these equations:

$$v_s = \mathscr{S}\Pi_s F(v_s) \tag{2_s}$$

and

$$W_s'(t) = -W_s(t) + \mathscr{S}\Pi_s F(W_s(t)). \tag{3_s}$$

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[1] In [7] more ambiguous term "stabilization principle" is used instead. Later we found that the word "steadying" is more adequate.

From (4) follows that the solution v_s^* of (2_s) lies in the subspace $\mathscr{S}\mathbf{U}_s \subset V$, i. e. has the form $v_s^* = \sum_{i=1}^s k_i^* \mathscr{S}\varphi_i$, where $k_i^* \in \mathbb{R}^n$ satisfy

$$k_i^* = Q_i F\left(\sum_{j=1}^s k_j^* \mathscr{S}\varphi_i\right), \quad i = 1,\dots,s. \tag{5}$$

Let φ_i be the polynomial Lagrange basis functions with nodes $c_i \in [0,1]$, $\varphi_i(\xi) = \prod_{j\neq i}^s \frac{\xi - c_j}{c_i - c_j}$, and Π_s be interpolation: $Q_i v = v(c_i)$. Then (5), as reader may guess, is nothing but the system solved in implicit RK methods:

$$k_i^* = f(x_0 + c_i h, y_0 + h\sum_{j=1}^s a_{ij} k_j^*(t)), \tag{6}$$

where $a_{ij} = \mathscr{S}\varphi_j(c_i)$, just as it should be for collocation RK method.

As an alternative to direct solution of equations (6) we consider (3_s), assume $W_s(t)(\xi) = \sum_{i=1}^s k_i(t)\mathscr{S}\varphi_i(\xi)$ and obtain an ODE system

$$k_i'(t) = -k_i(t) + f(x_0 + c_i h, y_0 + h\sum_{j=1}^s a_{ij} k_j(t)), \quad i = 1,\dots,s. \tag{7}$$

Denoting $k = (k_1,\dots,k_s)^T$, $\mathbf{f}(k) = (f_1(k),\dots,f_s(k))^T$, $f_i(k) = f(x_0 + c_i h, y_0 + h\sum_{j=1}^s a_{ij} k_j)$, represent (7) as

$$k'(t) = -k(t) + \mathbf{f}(k(t)). \tag{8}$$

Now assume that equation (8) is dissipative just like its continuous parent (3) (or at least its steady-state solution is asymptotically stable), choose appropriate initial condition $k(0) = k^{(0)}$ and an explicit σ-stage method with coefficients α_{pq}, β_p, $p = 1,\dots,s$, $q < p$. Applying this method to (8) with step size τ we formally obtain general computation scheme for iterative solution of (5):

$$k^{(l+1)} = k^{(l)} + \tau\sum_{p=1}^{\sigma} \beta_p(\mathbf{f}(K_p^{(l)}) - K_p^{(l)}), \quad l = 0,\dots,N-1; \tag{9a}$$

$$K_p^{(l)} = k^{(l)} + \tau\sum_{q=1}^{p-1} \alpha_{pq}(\mathbf{f}(K_q^{(l)}) - K_q^{(l)}), \quad p = 1,\dots,\sigma. \tag{9b}$$

After N steps of this algorithm we have an approximate values $k_i^{(N)} \approx k_i^*$ and therefore, by definition of (2), (7), can construct approximate collocation polynomial $u \approx y$, $u(x) = y_0 + h\sum_{i=1}^s k_i^{(N)} \mathscr{S}\varphi_i\left(\frac{x-x_0}{h}\right)$ and, of course, conventional approximate value for $y(x_0 + h)$ as final RK stage:

$$y_1 = y_0 + h\sum_{i=1}^s b_i k_i^{(N)} \tag{10}$$

with $b_i = \mathscr{S}\varphi_i(1)$.

DISCUSSION

What we have now is a classic s-stage collocation RK method (10), (6) with alternative scheme of nonlinear system solving. If the solution $k^* = (k_1^*,\dots,k_s^*)^T$ of (6) exists then it is a steady-state solution of (8) and we are searching it out using some explicit σ-stage RK method (9), which we'll refer to as auxiliary method.

As the beginning of justification note that if Euler method with $\tau = 1$ is used then (9) turns into conventional fixed-point iteration, or iterated Runge-Kutta method. Next consider Dahlquist model problem

$$y'(x) = \lambda y(x), \quad y(0) = 1,$$

for which (8) is

$$k'(t) = (\lambda h A - I)k(t) + \lambda e, \tag{11}$$

where A is Butcher matrix, I is identity matrix and and $e = (1, \ldots, 1)^T$. Simple analysis of this linear ODE system reveals the following.

1. For any real $\lambda < 0$ and $h > 0$ steady-state solution of (11) is asymptotically stable whenever all eigenvalues of A have positive real parts.
2. For any $\lambda \in \mathbb{C}$ there exist
   (a) $h_1 > 0$ such that steady-state solution of (11) is asymptotically stable, and
   (b) $h_2 > 0$ such that (11) is contractive, i. e. distance between every solution of (11) decays as $t \to \infty$.

The first of these properties gives us hope that with our method we can use natural step sizes during the integration of stiff problems, as at least Butcher matrices of popular Radau IIA methods do satisfy the imposed requirement. The second one justifies the use of the method for non-stiff problems as well. Another important notice is that Picard iteration is equivalent to solving (8) by explicit Euler formula with constant time step $\tau = 1$. It is clear that in some cases just the reducing of τ can significantly improve convergence properties.

The foregoing analysis lightens the crucial question of choosing auxiliary RK method (9) and the value of the fictitious time step τ. First of all, as the "steadying" problem (8) inherits stiffness of the original problem (1) (unless h is very small), it may seem unreasonable to integrate it with explicit method (9). But we should keep in mind that, in contrast to usual ODE integration, here we are concerned only in detecting the steady state of the process defined by (8). So, any traditional explicit RK method is, surely, not the best choice. One may suggest stabilized explicit methods [9, pp. 43-52], since they are constructed to have largest possible stability region along negative real axis. But we suggest to select a pair "method+step" such that minimizes the absolute value of stability function for given λ. This idea results in several possible strategies of parameters (α_{pq}, b_p and τ) determination which are to be discussed in the talk, as well as the choice of appropriate initial approximation $k^{(0)}$ for (9), various technical details of implementation and the results of experimental code tests.

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