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Quadratic RK Shooting solution for a Environmental Parameter Prediction Boundary Value Problem.

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Framework of the talk:

1. The Physical Problem and Information Geometry
2. The Mathematical Problem and its Numerical Solution
3. Numerical solution using Shooting method
4. Numerical Tests and Observations

Environmental Parameter Forecasting and Information Geometry

The need for high quality environmental predictions-simulations is very important due to important applications (Climate change, Renewable energy production,Transportation,Marine pollution,Ship safety)

Weather and wave forecasting models, usually successful in simulating global or intermediate scale environmental conditions, are considered. On local conditions such models may not be successful for various reasons.

In order to study the suitability of the models a "cost function" measuring the bias ("the distance") of the environmental data and the output of the models should be engaged.

The distance/cost-function should be better measured by means of Information Geometry tools instead of of classical Euclidean Geometry tools.

The **minimum distance** between two elements f_1 *and* f_2 of a statistical manifold S is defined by the corresponding ***geodesic*** ω which is the minimum length curve that connects them. Such a curve

$$\omega = (\omega_i) \quad : \quad \mathbb{R} \to S \tag{1}$$

satisfies the following system of $\mathbf{2}^{nd}$ **order differential equations**:

$$\omega_i''(t) + \sum_{j,k=1}^{n} \Gamma_{jk}^{i}(t)\,\omega_j'(t)\,\omega_k'(t) = 0, \quad i = 1,\ 2, \ldots,\ n. \tag{2}$$

under the conditions $\omega(0) = f_1,\ \ \omega(1) = f_2$.

The two parameter Weibull distributions have been proved a good choice for fitting wind and wave data.

These distributions form a 2-dimensional statistical manifold with $\xi=[\alpha,\beta]$, $\Xi = \{[\alpha,\beta];\ \alpha \text{ and } \beta>0\}$ (where α is the shape and β the scale parameter) and

$$p\left(x\right) = \frac{\alpha}{\beta}\left(\frac{x}{\beta}\right)^{\alpha-1} \mathrm{e}^{-\left(\frac{x}{\beta}\right)^{\alpha}}, \qquad \alpha,\ \beta > 0. \tag{3}$$

Let us have $\xi_0 = [\alpha_0, \beta_0]$, $\xi_1 = [\alpha_1, \beta_1]$ two members of the Weibull statistical manifold, then the previous system becomes:

$$
\begin{aligned}
\omega_1''(t) + \frac{6\left(\gamma\alpha_0 - \alpha_0 - \frac{\pi^2}{6}\right)}{\pi^2\beta_0}\left(\omega_1'(t)\right)^2 + \frac{12\left(\gamma^2 - 2\gamma + \frac{\pi^2}{6} + 1\right)}{\pi^2\alpha_0}\omega_1'(t)\,\omega_2'(t) &\; - \\
\frac{6(1-\gamma)\beta_0\left(\gamma^2 - 2\gamma + \frac{\pi^2}{6} + 1\right)}{\pi^2 a^3}\left(\omega_2'(t)\right)^2 &= 0 \\
\omega_2''(t) - \frac{\alpha_0^3}{\pi^2\beta_0^2}\left(\omega_1'(t)\right)^2 + \frac{12\alpha_0(1-\gamma)}{\pi^2\beta_0}\omega_1'(t)\,\omega_2'(t) &\; - \\
\frac{6\left(\gamma^2 - 2\gamma + \frac{\pi^2}{6} + 1\right)}{\pi^2\alpha_0}\left(\omega_2'(t)\right)^2 &= 0
\end{aligned}
$$

under the conditions $\omega(0) = \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix}, \;\; \omega(1) = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix}$

where $\omega(t) = \begin{bmatrix} \omega_1(t) \\ \omega_2(t) \end{bmatrix}$ and is $\gamma =$ the Euler gamma.

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So, we need to study the numerical solution of the following system of differential equations

$$\begin{aligned}\omega_1'' + a_{11}(\omega_1')^2 + a_{12}\omega_1'\omega_2' + a_{22}(\omega_2')^2 &= 0\\ \omega_2'' + b_{11}(\omega_1')^2 + b_{12}\omega_1'\omega_2' + b_{22}(\omega_2')^2 &= 0\end{aligned}$$

under the conditions

$$\omega_1(0) = \omega_1^0, \quad \omega_2(0) = \omega_2^0, \quad \omega_1(1) = \omega_1^{N+1}, \quad \omega_2(1) = \omega_2^{N+1}.$$

This is a **second order Boundary Value Problem** of a form

$$\widetilde{\omega}'' = F(\widetilde{\omega}, \widetilde{\omega}') \text{ where } \widetilde{\omega} = \begin{bmatrix}\omega_1\\ \omega_2\end{bmatrix} \text{ defined on the interval } [0, 1].$$

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It is common to transform this second order system in the form of a first order system of the form:

$$\begin{aligned} y_1' &= y_3 \\ y_2' &= y_4 \\ y_3' &= a_{11}y_3^2 - a_{12}y_3y_4 - a_{22}y_4^2 \\ y_4' &= b_{11}y_3^2 - b_{12}y_3y_4 - b_{22}y_4^2 \end{aligned}$$

under the conditions

$$y_1(0) = \omega_1^0, \quad y_2(0) = \omega_2^0, \quad y_1(1) = \omega_1^{N+1}, \quad y_2(1) = \omega_2^{N+1}.$$

where $y_1 = \omega_1$, $y_2 = \omega_2$, $y_3 = \omega_1'$ and $y_4 = \omega_2'$.

So, this problem can be considered as a problem of the more general class

$$y'(t) = f(t, y(t)), \quad g(y(a), y(b)) = 0 \tag{4}$$

where $t \in [a, b]$, $y : \mathbb{R} \to \mathbb{R}^n$, $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ and $f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$.

In our case $[a, b] = [0, 1]$, $n = 4$ and f is a quadratic function.

Our problem has separable boundary conditions e.g.

$$g(y(a), y(b)) = (g_0(y(a)), g_1(y(b)))^T = (0, 0)^T$$

where $g_0(y(a)) = y(a) - y_a$ and $g_1(y(b)) = y(b) - y_b$.

Numerical Solution of BVPs can be divided into two classes:

- initial value methods e.g. **shooting methods**.
- global methods e.g. **finite difference, collocation and Runge-Kutta schemes**.

In our project we have studied finite difference and collocation methods.

For our problem collocation methods can be included in the class of Runge-Kutta schemes.

Shooting Method

We want to solve the BVP

$$y'(t) = f(t, y(t)), \;\; g(y(a), y(b)) = 0, \quad t \in [a, b]$$

We denote $y_s(t)$ the solution of the IVP problem

$$y^{'}(t) = f(t, y(t)), \;\; y(a) = s, \quad t \in [a, b]$$

and we look for initial condition $s = y_s(a)$ so that
$g(y_s(a), y_s(b)) = 0$

So, the problem is transformed to system of nonlinear algebraic equations

$$g(s, y_s(b)) = 0$$

in each function evaluation of which we have to use the above IVP.

Issues on Shooting Method

- For linear BVPs the shooting method is easier applied. Non-linear BVP case is more complicated.
- Newton's method for the solution of the nonlinear problem needs involves the computation of the Jacobian.
- Jacobian is usually computed using finite differences or as a solution to ODEs.
- The IVP integration can be unstable (to the choice of the initial condition s) even when the BVP is well conditioned.
- The sensitivity of solutions of an initial value problem (IVP) to its initial conditions may influence the accuracy of the derivative values and the (exact) solution $y_s(t)$ of the IVP might exist on an interval shorter than $[a, b]$.
- In our case we have a nonlinear problem where the initial values of $y_3(a) = \omega_1'(0)$ and $y_4(0) = \omega_2'(0)$ are uknown.

Runge Kutta as IVP integrators

The general $s-$stage embedded Runge-Kutta pair of orders $p(p-1)$, advance the problem solution to $t_{n+1} = t_n + h_n$ using two methods which share the same function evaluations :

$$\hat{y}_{n+1} = y_n + h_n \sum_{j=1}^{s} \hat{b}_j f_j \;\text{ and }\; y_{n+1} = y_n + h_n \sum_{j=1}^{s} b_j f_j,$$

where

$$f_i = f(t_n + c_i h_n,\; y_n + h_n \sum_{j=1}^{s} a_{ij} f_j),\;\; i = 1, 2, \cdots, s.$$

and a stepsize control mechanism.

At each step the local error estimate $E_n = \|y_n - \hat{y}_n\|$ of the $(p-1)-$th order Runge-Kutta pair is used for the automatic selection of the step size.

Given a tolerance parameter TOL, if $TOL > E_n$ the algorithm:

$$h_{n+1} = 0.9 \cdot h_n \cdot (\frac{TOL}{E_n})^{\frac{1}{p}},$$

provides the next step length.

In the case $TOL \leq E_n$ we reject the current step and retry by estimating a new stepsize using the same formula replacing in the left side h_{n+1} by h_n.

Usually local extrapolation is applied, hence the integration is advanced using the $p-$th order approximation.

The Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b \\ & \hat{b} \end{array}$$

where $A \in \mathbb{R}^{s \times s}$, b^T, $\hat{b}^T$, $c \in \mathbb{R}^s$ with $c = A \cdot e$ and $e = [1,\ 1, \cdots, 1]^T \in \mathbb{R}^s$. The vectors $\hat{b}$, b define the coefficients of the $(p-1)-$th and $p-$th order approximations respectively.

Implicit Runge Kutta Mehods

If A is not a lower triangular matrix the methods is implicit as f_i is involved in both the right and left part of a nonlinear (generally) equation.

Thus f_i's can not be evaluated explicitly and nonlinear systems of equations have to be solved.

This system shares $(m \times s)$ equations with $(m \times s)$ unknowns. In each step we have to apply a modified Newton's iteration scheme inverting the matrix $I_{m\times s} - hA \otimes \frac{\vartheta f}{\vartheta y}$.

Implicit RK methods can be A-stable and so can be ideal to integrate stiff problems.

Singly Diagonally Implicit Methods

For a method to be called Singly Diagonal Implicit has to satisfy

$$a_{ii} = d,\ i = 1, 2, \cdots, s \text{ and } a_{ij} = 0,\ \text{for } j > i.$$

So now, we have to deal with s systems with m unknowns.

Thus Newton's method involves the inversion of the much easier $I_m - h\, d\frac{\vartheta f}{\vartheta y}$.

So, we treat the stages one after the other and the specific matrix is common for all stages when implementing the Newton's method.

Quadratic Runge Kutta Mehods

The coefficients A, b and c of a conventional Runge–Kutta method have to satisfy certain conditions in order to attain an prescribed order of accuracy.

When dealing with quadratic problems there is no need to satisfy all the equations o attain a specific order. So, we can use the extra parameters to produce methods special constructed for such problems which have the same number of stages (e.g. computational cost) but attain greater order and other characteristics such as stability properties.

24 Test Problems

We choose data from Levantive are (eastern Mediterranean Sea).

For every month of a year we have modeled **wind speed and wave height data** either includes in the simulation the impact of **sea currents** either not.

Second source of data is the available corresponding **satellite data**.

The **data are fitted by a 2-parameter Weibull distribution** to get their Weibull parameters.

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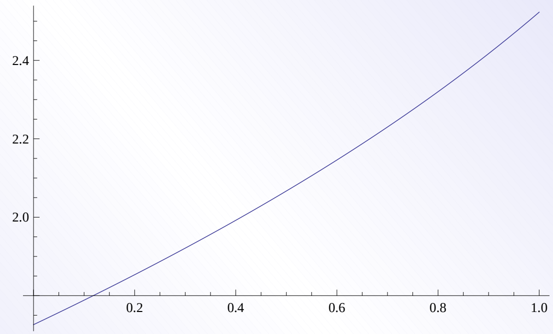
Data for the 24 Test Problems based on Weibull distribution

	model data no current		model data with current		satelite data	
Weibull Parameters	shape α_0	scale β_0	shape α_0	scale β_0	shape α_1	scale β_1
Jan	1.600	1.010	1.726	1.095	2.523	1.441
Feb	1.500	1.400	1.571	1.464	2.450	1.762
Mar	1.462	1.132	1.578	1.225	2.560	1.509
Apr	1.564	0.695	1.719	0.754	2.140	1.012
May	1.533	0.608	1.608	0.661	1.576	0.780
Jun	2.333	0.633	2.542	0.680	3.759	0.759
Jul	2.557	0.837	2.688	0.876	3.515	0.960
Aug	3.099	0.716	3.341	0.759	4.938	0.889
Sep	2.418	0.754	2.580	0.800	3.491	0.968
Oct	1.629	0.551	1.850	0.609	2.204	0.665
Nov	1.446	0.892	1.499	0.919	1.911	1.224
Dec	1.435	1.216	1.512	1.283	2.208	1.442

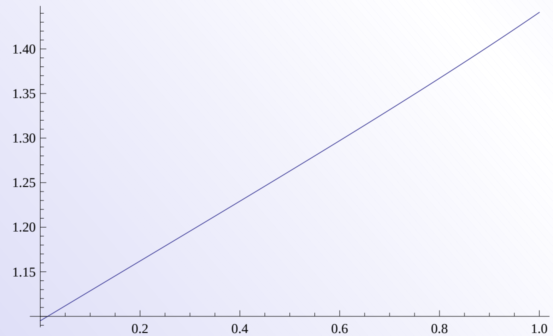
When we consider the**minimum length curve** which connects the each modeled and its corresponding satellite data we **conclude in** 24 **BVP problems**.

A simple case
The solution of problem Jan with current

$$\omega_1(t)$$

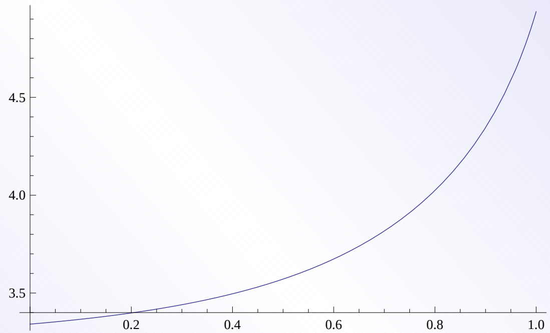


$$\omega_2(t)$$

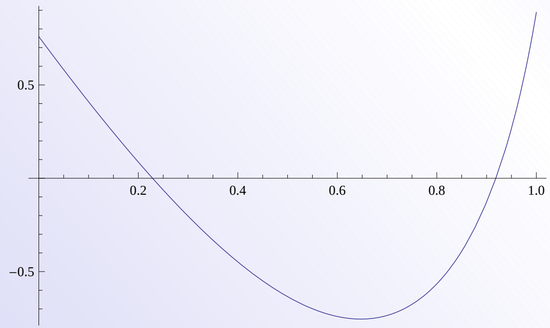


A harder case (stiffness)
The solution of Aug with current

$\omega_1(t)$



$\omega_2(t)$



The two competitors

- As RK integrators we choose pairs of methods.
- **SDIRK4(3)** is a general purpose classical pair of Hairer of orders four and three with five stages.
- **SDIRK5(3)** is a quadratic L-stable pair of Singly Diagonally Implicit methods of Tsitouras and Famelis with orders five and three and the same number of stages.

Numerical tests

- We use the Mathematica and **NDSolve** with **shooting** and variable stepsize providing the one step RK integrator.
- Under the **"NDSolve Method Plug-in Framework"** we provide the NDSolve with **"Step function"** which implements a single step of the diagonally implicit RK pair integrators and returns either the stepsize and the solution in the next timestep or the rejected stepsize in the variable stepsize mode.
- Tolerance parameter os chosen to be $TOL = 1E - 05$.
- NDSolve provides the solution in an **continuous interpolating form** of desired order. So, we can differentiate it and attain approximations of the derivative of the unknown functions too.
- As a measure of the attained accuracy we record the maximum absolute value that the numerical solution fails to satisfy the differential equation e.g. **the defect**.

The **defect** of a differential equation $y'(t) = f(t, y(t))$,

$$\delta(t) = y(t) - f(t, y(t))$$

can be used as an **estimation of the global error** since it arises in the analysis of the mathematical conditioning of the underlying problem where appropriate condition numbers are introduced to quantify the sensitivity of the global error to perturbations of the ODEs.

Three Initial condition choices

- $\mathcal{O}(1)$ approximation of the unknown initial values

$$\omega_1'(0) \approx \frac{\omega_1(1) - \omega_1(0)}{1}\,,\ \omega_2'(0) \approx \frac{\omega_2(1) - \omega_2(0)}{1}$$

- $\mathcal{O}(0.1)$ approximation of the unknown initial values

$$\omega_1'(0) \approx \frac{\tilde{\omega}_1(0.1) - \omega_1(0)}{0.1}\,,\ \omega_2'(0) \approx \frac{\tilde{\omega}_2(0.1) - \omega_2(0)}{0.1}$$

where $\tilde{\omega}_1(0.1) \approx \omega_1(0.1)$ and $\tilde{\omega}_2(0.1) \approx \omega_2(0.1)$

- $\mathcal{O}(0.01)$ approximation of the unknown initial values

$$\omega_1'(0) \approx \frac{-\tilde{\omega}_1(0.2) + 4\tilde{\omega}_1(0.1) - 3\tilde{\omega}_1(0)}{2 \cdot 0.1}\,,\ \omega_2'(0) \approx \frac{-\tilde{\omega}_2(0.2) + 4\tilde{\omega}_2(0.1) - 3\tilde{\omega}_2(0)}{2 \cdot 0.1}$$

where $\tilde{\omega}_1(0.1) \approx \omega_1(0.1)$, $\tilde{\omega}_2(0.1) \approx \omega_2(0.1)$ and $\tilde{\omega}_2(0.2) \approx \tilde{\omega}_2(0.2)$

	Defect for the 24 problems (* means not succeeded)					
	DIRK43			DIRK53		
	initial conditions estimation			initial conditions estimation		
	$\mathcal{O}(1)$	$\mathcal{O}(0.1)$	$\mathcal{O}(0.01)$	$\mathcal{O}(1)$	$\mathcal{O}(0.1)$	$\mathcal{O}(0.01)$
Jan no c.	2.27773E-07	2.27773E-07	2.27773E-07	4.06234E-09	4.06470E-09	4.06232E-09
Jan wi c.	6.08631E-08	6.08628E-08	6.08628E-08	8.20685E-10	8.20686E-10	8.20712E-10
Feb no c.	2.33444E-08	2.33444E-08	2.33440E-08	2.40410E-10	2.41323E-10	2.40410E-10
Feb wi c.	1.54921E-08	1.55180E-08	1.54923E-08	1.47390E-10	1.49771E-10	1.47440E-10
Mar no c.	1.74658E-07	4.50210E-07	4.50210E-07	9.03559E-09	9.03552E-09	9.03619E-09
Mar wi c.	1.74684E-07	4.50210E-07	1.74658E-07	1.47390E-10	2.86132E-09	2.86124E-09
Apr no c.	1.06854E-07	1.06855E-07	1.06854E-07	2.85923E-09	1.77438E-09	1.77447E-09
Apr wi c.	7.27396E-09	7.27390E-09	7.27394E-09	7.32224E-11	7.27160E-11	7.01154E-11
May no c.	1.15521E-11	1.24961E-11	1.20954E-11	1.25582E-11	1.11290E-11	1.11668E-11
May wi c.	1.28693E-11	1.18670E-11	1.18482E-11	1.22677E-11	1.21850E-11	1.20289E-11
Jun no c.	*	*	*	*	2.51851E-03	6.37770E-03
Jun wi c.	*	*	*	*	9.33820E-05	9.33820E-05
Jul no c.	*	9.02619E-06	9.02619E-06	*	3.45436E-07	3.45436E-07
Jul wi c.	*	1.86711E-06	1.86708E-06	*	5.10881E-08	5.10882E-08
Aug no c.	*	*	*	*	*	9.46509E-02
Aug wi c.	*	*	*	*	2.11818E-03	2.11818E-03
Sep no c.	*	7.19628E-05	7.19514E-06	*	3.31465E-06	3.31465E-06
Sep wi c.	*	7.54889E-06	7.54889E-06	*	2.81104E-07	2.81104E-07
Oct no c.	*	7.54889E-06	1.81217E-06	*	5.57580E-08	5.57580E-08
Oct wi c.	2.73956E-08	2.73962E-08	2.73962E-08	3.52567E-10	3.52567E-10	3.55544E-10
Nov no c.	5.08204E-10	5.09301E-10	5.09429E-10	1.29120E-11	1.28251E-11	1.27783E-11
Nov wi c.	3.09348E-10	3.09794E-10	3.09922E-10	1.15062E-11	1.23028E-11	1.15062E-11
Dec no c.	2.66150E-08	2.66403E-08	2.66150E-08	2.97735E-10	2.97613E-10	2.97640E-10
Dec wi c.	1.45463E-08	1.45463E-08	1.45463E-08	1.42820E-10	1.42872E-10	1.52062E-10

Remarks

- Both DIRK pairs have similar computational cost.
- DIRK 5(3) attains in (almost) all problems better approximations (up to two digits).
- The sensitivity of shooting method in the accuracy of the initial choices of $\omega_1'(0), \omega_2'(0)$ is very high.
- DIRK 5(3) proves to be less sensitive as it succeeds in cases where DIRK 4(3) fails.