

A family of self-starting Extended Backward Differentiation Formulas (BDFs) with two superfuture points for stiff initial value problems

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Outline

1 Motivation

- Solving Stiff IVPs
- The Extended BDF of Cash
- The Modified Extended BDF of Cash
- Inspiration for Hyper-Extended BDF

2 Derivation and Implementation

- Derivation
- Implementation

3 Results and Summary

- Numerical Results
- Summary

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Formal Statement of Problem

- We are interested integrating “Stiff” IVPs
- These problems have the form

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0 \quad (1)$$

- They are defined on the finite interval $[a, b]$
- $y, f \in \mathbb{R}^m$
- $f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$

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Definition of Stiffness

- No agreed definition of “Stiffness”
- We use the definition given by Ramos and Vigo-Aguiar
- They define (1) as stiff if its Jacobian has eigenvalues λ_i with $\text{Re}(\lambda_i) \leq 0$, in addition to eigenvalues of moderate size.

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BDFs solve Stiff problems well

- Gear's Method (Conventional BDF) performed well on stiff IVPs
- Cash's Extended BDF adds a "Superfuture" point
 - ▶ Colocation point beyond x_{n+k}
 - ▶ Enhanced stability properties
- We investigate the effects of a second Superfuture point

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A-stable only for $k = 1$

- Also called “Gear’s Method”
- Takes the form

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k} \quad (2)$$

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A-stable for $k \leq 3$

- Cash introduced a collocation point at x_{n+k+1}
- This “Extended” BDF takes the form

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The Extended BDF of Cash

Notes on Implementation

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- Question: Possible to salvage method with different strategy?

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Repurposing the MEBDF

Using a Self-Starting Predictor/Corrector Strategy

- Replace iterative solving with Predictor/Corrector strategy
 - ▶ Use a $(k + 2)$ -step Adams-Bashforth method as an explicit predictor
- Rederive MEBDF as a continuous scheme (As discussed in Jator, Swindell, and French)
 - ▶ This will allow the method to be self-starting method
- Together, those should overcome the problems encountered by Cash

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Deriving the Continuous Scheme

- Start with an approximation $U(x) = a_0 + a_1x + \cdots + a_{k+2}x^{k+2}$ and $V = (y_0, y_1, \dots, y_{k-1}, f_k, f_{k+1}, f_{k+2})$
- Want to solve for a_i
- Form a matrix M from coefficients of U and U' evaluated at x_i
- Compute $M^{-1} \cdot V$ to find values of a_i
- Discrete methods can be obtained by evaluating $U(x)$ at appropriate points
- Proof of Algorithm given in Jator

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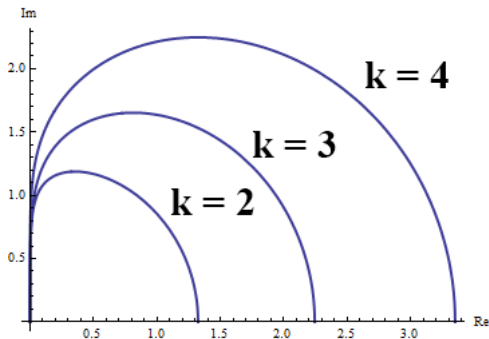
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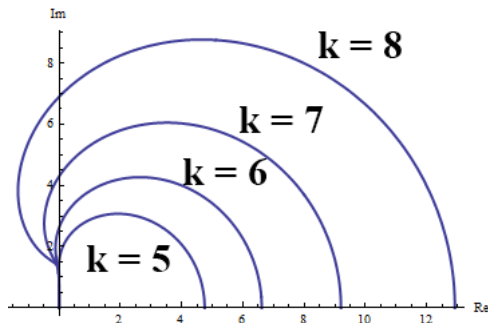
Notes on Stability

A-stable for $k = 2, 3, 4$



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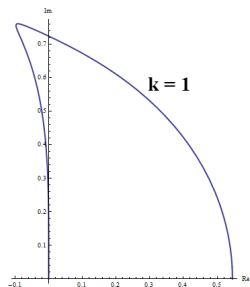
$A(\alpha)$ -stable for $k = 5, 6, 7, 8$



Nearly A -stable for $k = 5$ ($\alpha > 89.9^\circ$)

Notes on stability

Poor Stability for $k = 1$



This was unanticipated

Solving the Initial Block

- Discrete methods obtained from $U(x)$ can be solved as a system
- This will yield the first $k + 2$ solution points y_1, y_2, \dots, y_{k+2}
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Employing the Predictor/Corrector Strategy

- Because our method is implicit, we need to predict y_n^*, y_{n+1}^* , and y_{n+2}^* in order to find y_n
- We use $(k + 2)$ -step Adams-Bashforth to predict y_n^*
 - ▶ Then again to predict y_{n+1}^*
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Problem 1

A Chemistry Problem Suggested by Robertson

- We compare our performance to Cash's EBDF on the following problem

$$\begin{aligned}f_1 &= -0.04y_1 + 10000y_2y_3, & y_1(0) &= 1 \\f_2 &= 0.04y_1 - 10000y_2y_3 - 3 * 10^7 y_2^2, & y_2(0) &= 0 \\f_3 &= 3 * 10^7 y_2^2, & y_3(0) &= 0\end{aligned}$$

- Solved on $[0, 40]$ using $h = 0.0002$
- Global error for 3-step EBDF (Cash) was $4 * 10^{-17}$
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A Problem with a Known Solution Suggested by Cash

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- This problem illustrates comparable endpoint error behavior

	HEBDF Error	EBDF Error
t = 20	$y_1 \rightarrow 2.86 * 10^{-11}$ $y_2 \rightarrow 2.77 * 10^{-12}$	$y_1 \rightarrow 3.60 * 10^{-11}$ $y_2 \rightarrow 1.08 * 10^{-11}$
t = 40	$y_1 \rightarrow 9.11 * 10^{-21}$ $y_2 \rightarrow 8.59 * 10^{-20}$	$y_1 \rightarrow 2.55 * 10^{-20}$ $y_2 \rightarrow 8.81 * 10^{-20}$
t = 80	$y_1 \rightarrow 1.30 * 10^{-37}$ $y_2 \rightarrow 2.37 * 10^{-37}$	$y_1 \rightarrow 1.13 * 10^{-37}$ $y_2 \rightarrow 3.12 * 10^{-37}$

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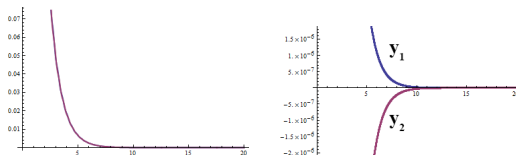
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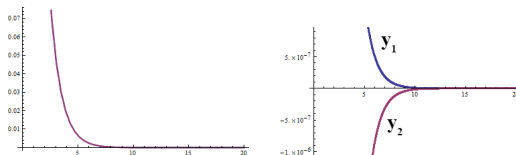
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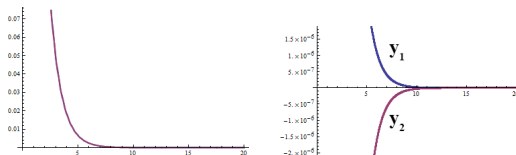
- We also graph the solution and error given by applying our Hyper EBDf:



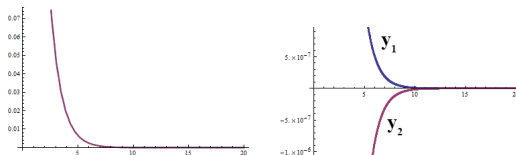
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Self-Starting Hyper Extended BDF

Summary

- Comparable to Cash's Extended BDF for methods of the same order.
- Whereas Extended BDF is A -stable for $k \leq 3$, the Hyper EBDF is A -stable for $k \leq 4$.
- The method is viable if implemented in a self-starting predictor/corrector fashion.
 - ▶ An initial block is generated from a continuous scheme
 - ▶ That block is solved to recover y_1, y_2, \dots, y_{k+2}
 - ▶ Remainder of interval is solved as Predictor/Corrector using a $(k+2)$ -step Adams-Bashforth method together with our own
- Unexpected stability properties for $k = 1$

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Self-Starting Hyper Extended BDF

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Self-Starting Hyper Extended BDF

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- Apply a mesh-refinement algorithm for variable stepsize
- Implement via Newton's method to compare more closely with Cash's implementation
- Apply the problem to PDEs via Method of Lines

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Hyper-Extended BDF

A Self-Starting, Predictor/Corrector BDF with 2 Superfuture Points

Any Questions?