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DERIVATION OF BDF COEFFICIENTS FOR EQUIDISTANT TIME STEP*

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Abstract

We present the derivation of the explicit formulae of BDF coefficients for equidistant time step.

1 Introduction

In this paper we deal with the coefficients of *Backward Differential Formulae* (BDF). BDF represent very important scheme for solving stiff ODE's (see [2] and [3]) which can arise from a lot of important practical tasks, see e.g. [1]. For survey on solving stiff problems see [5]. In this paper we present the order conditions for the coefficients of BDF which can be viewed as some linear system of equations, formulate the explicit relations for the BDF coefficients and show that these relations for BDF coefficients represent the solution of this system for arbitrary order. Advantage of our approach is that we use only simple arithmetic means without differentiation. In fact, the differentiation is hidden in derivation of the order conditions, where Taylor expansions are used.

2 BDF and order conditions

We consider $y \in C^1(0,T)$ the solution of ordinary differential equation

$$\begin{aligned} y'(t) &= F(t, y(t))), \quad \forall t \in (0,T), \\ y(0) &= A \in R. \end{aligned} \tag{1}$$

We assume the equidistant partition $t_m = m\tau$, $m = 0, \dots, r$ of interval $[0,T]$ with discretization step $\tau = T/r$. We denote y^m the approximation to the exact solution $y(t_m)$. The difference equation

$$\sum_{v=0}^{k} \alpha_v y^{m+v} = \tau F(t_{m+k}, y^{m+k}), \tag{2}$$

where α_v are some suitable real constants, we call Backward Differential Formula (BDF). We call the method (2) k–step BDF, if $\alpha_k \neq 0$ and $\alpha_0 \neq 0$.

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Now we formulate the order conditions. We say that BDF has order $p \geq 0$, if

$$\sum_{v=0}^{k} \alpha_v v^s = sk^{s-1} \tag{3}$$

for $s = 0, \ldots, p$. The order conditions for general linear multistep method including the proof can be found in e.g. [4].

Theorem 1. *Let $k \geq 1$. Then there exists only one k-step BDF of order k and this method has the coefficients*

$$\alpha_v \equiv (-1)^{k-v} \binom{k}{v} \frac{1}{k-v}, \quad v = 0, \ldots, k-1, \tag{4}$$

$$\alpha_k \equiv \sum_{v=1}^{k} \frac{1}{v}. \tag{5}$$

3 Proof of Theorem

It is simple to see that (3) represents linear system of Vandermonde type (which is obviously nonsingular), if $p = k$.

Lemma 1. *The system of equations (3) is equivalent to the system:*

$$\sum_{v=0}^{k} \alpha_v = 0 \tag{6}$$

$$\sum_{v=0}^{k} \alpha_v (k-v) = -1 \tag{7}$$

$$\sum_{v=0}^{k} \alpha_v (k-v)^s = 0 \tag{8}$$

for $s = 2, \ldots, k$.

Proof. We can see that matrix represented by the system (6)–(8) is nonsingular, because similarly as in the previous case the matrix is of Vandermonde type. At first we will prove that (7) and (8) follows from (3). First equation (6) is one of the equations of (3). Second equation (7) we can divide into two parts and enumerate them by (3):

$$\sum_{v=0}^{k} \alpha_v (k-v) = k \sum_{v=0}^{k} \alpha_v - \sum_{v=0}^{k} \alpha_v v = 0 - 1 = -1. \tag{9}$$

The remaining equations (8) are proved using (3):

$$\sum_{v=0}^{k}\alpha_v(k-v)^s=\sum_{v=0}^{k}\alpha_v\sum_{i=0}^{s}\binom{s}{i}(-1)^i k^{s-i}v^i=\sum_{i=0}^{s}(-1)^i\binom{s}{i}k^{s-i}\sum_{v=0}^{k}\alpha_v v^i \tag{10}$$

$$=\sum_{i=0}^{s}(-1)^i\binom{s}{i}k^{s-i}ik^{i-1}=k^{s-1}\sum_{i=0}^{s}(-1)^i\frac{s!}{i!(s-i)!}i$$

$$=k^{s-1}\sum_{i=1}^{s}(-1)^i\frac{s!}{i!(s-i)!}i=-k^{s-1}\sum_{i=1}^{s}(-1)^{i-1}\frac{s(s-1)!}{(i-1)!(s-1-(i-1))!}$$

$$=-sk^{s-1}\sum_{i=0}^{s-1}\binom{s-1}{i}(-1)^i=-sk^{s-1}(1-1)^{s-1}=0$$

for $s\geq 2$. Now we will prove that (3) follows from (6), (7) and (8). The equation (3) for $s=0$ is exactly (6). The rest we will prove by induction. As first step we will prove that (3) holds for $s=1$.

$$-\sum_{v=0}^{k}\alpha_v(k-v)=-k\sum_{v=0}^{k}\alpha_v+\sum_{v=0}^{k}\alpha_v v=\sum_{v=0}^{k}\alpha_v v=1=sk^{s-1} \tag{11}$$

Then let us assume that (3) holds for $i=1,\ldots,s-1$. Then

$$0=\sum_{v=0}^{k}\alpha_v(k-v)^s=\sum_{v=0}^{k}\alpha_v\sum_{i=0}^{s}(-1)^i\binom{s}{i}k^{s-i}v^i \tag{12}$$

$$=\sum_{i=0}^{s}(-1)^i\binom{s}{i}k^{s-i}\sum_{v=0}^{k}\alpha_v v^i=(-1)^s\sum_{v=0}^{k}\alpha_v v^s+\sum_{i=0}^{s-1}(-1)^i\binom{s}{i}k^{s-i}\sum_{v=0}^{k}\alpha_v v^i$$

With the induction assumptions we will get from the second term:

$$\sum_{i=0}^{s-1}(-1)^i\binom{s}{i}k^{s-i}\sum_{v=0}^{k}\alpha_v v^i=\sum_{i=0}^{s-1}(-1)^i\binom{s}{i}k^{s-i}ik^{i-1} \tag{13}$$

$$=k^{s-1}\sum_{i=0}^{s-1}(-1)^i\binom{s}{i}i=-(-1)^s sk^{s-1}+k^{s-1}\sum_{i=0}^{s}(-1)^i\binom{s}{i}i$$

Now it is sufficient to show that

$$\sum_{i=0}^{s}(-1)^i\binom{s}{i}i=\sum_{i=1}^{s}(-1)^i\binom{s}{i}i=\sum_{i=1}^{s}(-1)^i\frac{s!}{i!(s-i)!}i \tag{14}$$

$$=-s\sum_{i=1}^{s}(-1)^{i-1}\frac{(s-1)!}{(i-1)!(s-1-(i-1))!}=-s\sum_{i=1}^{s}(-1)^{i-1}\binom{s}{i}$$

$$=-s\sum_{i=0}^{s-1}(-1)^i\binom{s-1}{i}=-s(1-1)^{s-1}=0$$

for $s\geq 2$. From (12), (13) and (14) follows (3). $\square$

Lemma 2. *Let* α_v *are the coefficients of* k*-step BDF of order* $k \geq 2$*. Then*

$$\alpha_v = (-1)^{k-v} \binom{k}{v} \frac{1}{k-v} \tag{15}$$

for $v = 0, \ldots, k-1$*.*

Proof. Because we have shown in Lemma 1 that system of equations (3) is equivalent to system (6), (7) and (8) and since α_k depends only on (6) we can prove our lemma by substituting to (7) and (8). When we substitute to (7) we get by binomial theorem

$$\sum_{v=0}^{k} \alpha_v (k-v) = \sum_{v=0}^{k-1} \alpha_v (k-v) = \sum_{v=0}^{k-1} (-1)^{k-v} \binom{k}{v} \frac{1}{k-v} (k-v) \tag{16}$$

$$= \sum_{v=0}^{k-1} (-1)^{k-v} \binom{k}{v} = \sum_{v=0}^{k} (-1)^{k-v} \binom{k}{v} - 1 = (1-1)^k - 1 = -1,$$

for $k \geq 1$. Now we will prove the rest by induction. We denote α_i^j the coefficient α_i of BDF of order j. As the first step we will prove that our α_v^j satisfies (8) for $s = 2$, $2 \leq j \leq k$:

$$\sum_{v=0}^{j} \alpha_v^j (j-v)^s = \sum_{v=0}^{j-1} \alpha_v^j (j-v)^2 = \sum_{v=0}^{j-1} (-1)^{j-v} \binom{j}{v} \frac{1}{j-v} (j-v)^2 \tag{17}$$

$$= \sum_{v=0}^{j-1} -(-1)^{j-1-v} \frac{j(j-1)!}{v!(j-1-v)!}$$

$$= -j \sum_{v=0}^{j-1} (-1)^{j-1-v} \binom{j-1}{v} = -j(1-1)^{j-1} = 0$$

Now let us assume that α_v^j satisfies (8) for $j = 2, \ldots, k-1$. Now we want to prove that α_v^k satisfies (8) for $2 \leq s \leq k$. We know that it holds for $s = 2$. We will assume that it holds for $s - 1$. From this follows

$$\sum_{v=0}^{k} \alpha_v^k (k-v)^s = k \sum_{v=0}^{k} \alpha_v^k (k-v)^{s-1} - \sum_{v=0}^{k} \alpha_v^k (k-v)^{s-1} v \tag{18}$$

$$= 0 - \sum_{v=1}^{k-1} \alpha_v^k (k-v)^{s-1} v = - \sum_{v=1}^{k-1} (-1)^{k-v} \binom{k}{v} (k-v)^{s-2} v$$

$$= - \sum_{v=1}^{k-1} (-1)^{k-1-(v-1)} \frac{k(k-1)!}{(v-1)!(k-1-(v-1))!} (k-1-(v-1))^{s-2}$$

$$= -k \sum_{v=0}^{k-2} (-1)^{k-1-v} \frac{(k-1)!}{v!(k-1-v)!} (k-1-v)^{s-2}$$

$$= -k \sum_{v=0}^{k-2} \alpha_v^{k-1} (k-1-v)^{s-1} = 0$$

□

Lemma 3. *Let α_v are the coefficients of k-step BDF of order $k \geq 2$. Then*

$$\alpha_k = \sum_{v=1}^{k} \frac{1}{v} \tag{19}$$

Proof. We will use the notation α_v^j for α_v of the BDF of order j. It is easy to compute that α_1^1 and α_2^2 satisfy our lemma. Now we want to show that $\alpha_{k+1}^{k+1} - \alpha_k^k = \frac{1}{k+1}$, which proves our lemma. From (6) follows

$$\begin{aligned}
\alpha_{k+1}^{k+1} &= -\sum_{v=0}^{k} \alpha_v^{k+1} = -\sum_{v=0}^{k} (-1)^{k+1-v} \binom{k+1}{v} \frac{1}{k+1-v} \qquad (20)\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=1}^{k} (-1)^{k+1-v} \binom{k+1}{v} \frac{1}{k+1-v}\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=1}^{k} (-1)^{k-(v-1)} \frac{1}{v} \frac{(k+1)k!}{(v-1)!(k-(v-1))!} \frac{1}{k-(v-1)}\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=0}^{k-1} (-1)^{k-v} \binom{k}{v} \frac{1}{k-v} \frac{k+1}{v+1}\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=0}^{k-1} \alpha_v^k \frac{k+1}{v+1}
\end{aligned}$$

Now we can compute $\alpha_{k+1}^{k+1} - \alpha_k^k$. From (20) and $\alpha_k^k = -\sum_{v=0}^{k-1} \alpha_v^k$ we get

$$\begin{aligned}
\alpha_{k+1}^{k+1} - \alpha_k^k &= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=0}^{k-1} \alpha_v^k \left(\frac{k-v}{v+1} \right) \qquad (21)\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=0}^{k-1} (-1)^{k-v} \binom{k}{v} \frac{1}{k-v} \left(\frac{k-v}{v+1} \right)\\
&= -(-1)^{k+1} \frac{1}{k+1} - \sum_{v=0}^{k-1} (-1)^{k-v} \frac{k!}{(v+1)!(k-v)!}\\
&= -\frac{1}{k+1} \left((-1)^{k+1} + \sum_{v=0}^{k-1} (-1)^{k+1-(v+1)} \frac{(k+1)!}{(v+1)!(k+1-(v+1))!} \right)\\
&= -\frac{1}{k+1} \left((-1)^{k+1} + \sum_{v=1}^{k} (-1)^{k+1-v} \binom{k+1}{v} \right)\\
&= -\frac{1}{k+1} \sum_{v=0}^{k} (-1)^{k+1-v} \binom{k+1}{v} = \frac{1}{k+1} - \frac{1}{k+1} \sum_{v=0}^{k+1} (-1)^{k+1-v} \binom{k+1}{v}\\
&= \frac{1}{k+1} - \frac{1}{k+1} (-1+1)^{k+1} = \frac{1}{k+1}
\end{aligned}$$

□

We can verify by simple calculation that Lemma 2 and Lemma 3 hold for $k = 1$, too.

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