BCLF functions

Work in progress

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Objectives of this study:

- Giving an extensive and up to date review of methods already used for computing BCLF functions.
- Providing algorithms for get exact values of this functions when using arbitrary precision floating point real numbers.
- Providing double precision programs in C to compute BCLF with a limited range for parameters ζ , a and r (possibly using precomputations within a computer algebra system).
- Introducing to further studies using other methods, such as extrapolation methods.
- Numerous formulas are still to check.
- Is it an hard problem to find a stable method to evaluate $A_{\lambda+1/2}^n(1, a, r)$ since this function vanishes on curves in the quarter plane $a, r \ge 0$ when $n \ge 2$ and $\lambda \ge 1$?

Remark.– Some formulas and methods in the following may be original, but litterature should be studied very carefully before any assertion in this matter.

1 Introduction

1.1 Definition of BCLF functions

Let n a nonnegative integer, a and r two real positive numbers, ζ a real positive number. With R defined as

$$R = \sqrt{a^2 + r^2 - 2ar\cos\theta} \tag{1}$$

consider the function $R^{n-1}e^{-\zeta R}$.

Defining $x \in [-1, +1]$ by $x = \cos \theta$, its Lagrange expansion with respect to x on [-1, +1] with respect to x may be expressed as

$$R^{n-1}e^{-\zeta R} = \frac{1}{\sqrt{ar}} \sum_{\lambda=0}^{\infty} (2\lambda+1)A^n_{\lambda+1/2}(\zeta,a,r) P_{\lambda}(x) , -1 \le x \le 1 ,$$
(2)

which defines BCLF functions $A^n_{\lambda+1/2}$. As

$$\int_{-1}^{+1} P_{\lambda}^2(x) dx = \frac{2}{2\lambda + 1}$$
(3)

we immediately deduce from this expression that

$$A_{\lambda+1/2}^{n}(\zeta, a, r) = \frac{\sqrt{ar}}{2} \int_{-1}^{+1} R^{n-1} e^{-\zeta R} P_{\lambda}(x) dx .$$
(4)

A simple expression of BCLF function for n = 0 and $0 < r \le a$ is well known

$$A^{0}_{\lambda+1/2}(\zeta, a, r) = K_{\lambda+1/2}(\zeta a) I_{\lambda+1/2}(\zeta r), \ 0 < r \le a .$$
(5)

From expression (4) it follows that, for $n \ge 0$,

$$A_{\lambda+1/2}^{n+1}(\zeta, a, r) = -\frac{\partial}{\partial \zeta} A_{\lambda+1/2}^n(\zeta, a, r) .$$
(6)

and

$$A^n_{\lambda+1/2}(\zeta, a, r) = -(-1)^n \frac{\partial^n}{\partial \zeta^n} A^0_{\lambda+1/2}(\zeta, a, r) .$$

$$\tag{7}$$

As R is invariant by exchanging a and r

$$A_{\lambda+1/2}^{n}(\zeta, a, r) = A_{\lambda+1/2}^{n}(\zeta, r, a) .$$
(8)

As $A^0_{\lambda+1/2}(\zeta, a, r) = A^0_{\lambda+1/2}(1, \zeta a, \zeta r)$, equation (6) leads by recurrence to

$$A^{n}_{\lambda+1/2}(\zeta, a, r) = \frac{1}{\zeta^{n}} A^{n}_{\lambda+1/2}(1, \zeta a, \zeta r), \ n \ge 0.$$
(9)

Introducing function $\bar{A}^n_{\lambda}(a,r) = A^n_{\lambda+1/2}(1,a,r)$ for $a,r \ge 0$, we get

$$\bar{A}^n_\lambda(a,r) = \zeta^n A^n_{\lambda+1/2}(1,\zeta a,\zeta r), \ n \ge 0, \tag{10}$$

and the equation (6) may be rewritten

$$\bar{A}^{n+1}_{\lambda}(a,r) = n\bar{A}^{n}_{\lambda}(a,r) - \left(a\frac{\partial}{\partial a} + r\frac{\partial}{\partial r}\right)\bar{A}^{n}_{\lambda}(a,r) , n \ge 0.$$
(11)

Equation (9) is called the homogeneity relation for the functions $A_{\lambda+1/2}^n$ and any equation involving these functions should admit a translation into a corresponding equation for functions \bar{A}_{λ}^n .

1.2 Recurrence relations

Extending the value of $A_{\lambda+1/2}^{n+1}$ for any integer value of λ by equations (5) and (7) taken as definition relations, one may check the following recurrence relations that are proved in [1].

$$A^{1}_{\lambda+1/2}(\zeta, a, r) = \frac{ar\zeta}{2\lambda+1} [A^{0}_{\lambda-1/2}(\zeta, a, r) - A^{0}_{\lambda+3/2}(\zeta, a, r)].$$
(12)

$$A_{\lambda+1/2}^{n+2}(\zeta, a, r) = (a^2 + r^2) A_{\lambda+1/2}^n(\zeta, a, r) - \frac{2ar}{2\lambda + 1} [\lambda A_{\lambda-1/2}^n(\zeta, a, r) + (\lambda + 1) A_{\lambda+3/2}^n(\zeta, a, r)], \ n \ge 0.$$
(13)

Equations (12) and (7) are equivalent to

$$\bar{A}^{1}_{\lambda}(a,r) = \frac{ar}{2\lambda+1} [\bar{A}^{0}_{\lambda-1}(a,r) - \bar{A}^{0}_{\lambda+1}(a,r)]$$
(14)

$$\bar{A}^{n+2}_{\lambda}(a,r) = (a^2 + r^2)\bar{A}^n_{\lambda}(a,r) - \frac{2ar}{2\lambda+1} [\lambda \bar{A}^n_{\lambda-1}(a,r) + (\lambda+1)\bar{A}^n_{\lambda+1}(a,r)], \ n \ge 0.$$
(15)

Using (14) and (11), it is easily that $\bar{A}^n_{\lambda}(a, r)$ may be expressed as a linear combination of \bar{A}^0_k and coefficients in the set of polynomials in a, r, λ with integer coefficients

$$\bar{A}^n_{\lambda}(a,r) = \sum_{i=-n}^n p_{n,i}(a,r,\lambda) \bar{A}^0_{\lambda+i}(a,r)$$
(16)

For example

Furthermore \bar{A}^0_λ verifies a four term recurrence relation with respect to λ

$$\bar{A}^{0}_{\lambda+4}(a,r) = -\frac{2\lambda+7}{2\lambda+3}\bar{A}^{0}_{\lambda}(a,r) - \frac{(2\lambda+7)(2\lambda+3)}{ar}\bar{A}^{0}_{\lambda+1}(a,r) \\
+ \frac{2\lambda+5}{(2\lambda+3)a^{2}r^{2}} \left[(2\lambda+3)(2\lambda+7)(a^{2}+r^{2}) + 2a^{2}r^{2} \right] \bar{A}^{0}_{\lambda+2}(a,r) \\
- \frac{(2\lambda+7)^{2}}{ar} \bar{A}^{0}_{\lambda+3}(a,r).$$
(17)

Using (16) and (17), it may be deduced that $\bar{A}^n_{\lambda}(a, r)$ may be expressed as

$$\bar{A}^{n}_{\lambda}(a,r) = \sum_{i=0}^{3} Q_{n,i}(a,r,\lambda) \bar{A}^{0}_{\lambda+i}(a,r),$$
(18)

where $Q_{n,i}(a,r,\lambda), i = 0, ..., 3$ are rational functions in a, r, λ .

Denoting by \mathbf{Q}_n the vector of components $Q_{n,i}(a,r,\lambda), i = 0, \ldots, 3$ and by D the linear differential operator $D = a \frac{\partial}{\partial a} + r \frac{\partial}{\partial r}$, it may be proven that

$$\mathbf{Q}_{n+1} = (n\mathbf{I}_4 - \mathbf{M})\mathbf{Q}_n - D\mathbf{Q}_n,\tag{19}$$

where I_4 is the 4 × 4 unit matrix and M is the 4 × 4 matrix

$$\mathbf{M} = \begin{bmatrix} 2\lambda + 1 & -\frac{ar}{2\lambda + 3} & 0 & -\frac{ar}{2\lambda + 3} \\ -\frac{(2\lambda + 3)(2\lambda + 5)(a^2 + r^2) + a^2r^2}{(2\lambda + 5)ar} & 0 & -\frac{ar}{2\lambda + 5} & -(2\lambda + 3) \\ 2\lambda + 5 & \frac{ar}{2\lambda + 3} & 0 & \frac{(2\lambda + 3)(2\lambda + 5)(a^2 + r^2) + a^2r^2}{(2\lambda + 3)ar} \\ \frac{ar}{2\lambda + 5} & 0 & \frac{ar}{2\lambda + 5} & -(2\lambda + 7) \end{bmatrix}$$

Remark.– The following recurrence relation such as printed in [2] is false because it is not coherent with homogeneity equation (9):

$$A_l^{n+1}(\zeta, a, r) = \frac{ar}{2l+1} \left[A_{\lambda-1/2}^n(\zeta, a, r) - A_{\lambda+3/2}^n(\zeta, a, r) - A_{\lambda-1/2}^{n-1}(\zeta, a, r) - A_{\lambda+3/2}^{n-1}(\zeta, a, r) \right],$$

even when replacing $A_l^{n+1}(\zeta, a, r)$ by $A_{l+1/2}^{n+1}(\zeta, a, r)$ in the hand side of the equation because of an obvious misprint.

1.3 Explicit expressions

Equations (5) and (6) together with recurrence and derivative relations on Bessel functions allow to get explicit expressions of $A^n_{\lambda+1/2}(\zeta, a, r)$ in terms of Bessel functions for any n, λ, a and r.

For example

$$A^{1}_{\lambda+1/2}(\zeta, a, r) = \frac{2\lambda + 1}{\zeta} I_{\lambda+1/2}(\zeta r) K_{\lambda+1/2}(\zeta a) - r I_{\lambda-1/2}(\zeta r) K_{\lambda+1/2}(\zeta a) + a I_{\lambda+1/2}(\zeta r) K_{\lambda-1/2}(\zeta a) , 0 \le r \le a ,$$
(20)

or

$$A^{1}_{\lambda+1/2}(\zeta, a, r) = -\frac{2\lambda+1}{\zeta} I_{\lambda+1/2}(\zeta r) K_{\lambda+1/2}(\zeta a) - r I_{\lambda+3/2}(\zeta r) K_{\lambda+1/2}(\zeta a) + a I_{\lambda+1/2}(\zeta r) K_{\lambda+3/2}(\zeta a) , 0 \le r \le a .$$
(21)

The polynomials p_n

Definition.– Polynomials $p_n(x), n \neq 0$ with integer coefficients are defined by the following recurrence

$$p_0(x) = 1,$$
 (22)

$$p_1(x) = x+1,$$
 (23)

$$p_n(x) = (2n-1)p_{n-1}(x) + x^2 p_{n-2}(x), \ n \ge 2.$$
 (24)

For example

$$p_2(x) = x^2 + 3x + 3,$$

 $p_3(x) = x^2 + 6x^2 + 15x + 15.$

Polynomials p_n are encountered in Pade approximants of the function e^{2x} in the following way. $\Pi_{m,n}f(x) = p(x)/q(x)$ is the Pade approximant of order m, n of a function f(x), where p(x), q(x) is the unique pair of polynomials with integer coefficients with respective degrees m an n and relatively primes such that $f(x) - p(x)/q(x) = O(x^{k+l+1})$. Then, when $f(x) = e^{2x}$,

$$\Pi_{m,n}f(x) = \frac{p_n(x)}{p_n(-x)}, \ n \ge 1.$$
(25)

For n nonnegative integer, Bessel functions $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ may be expressed in terms of polynomial $p_n(x)$:

$$I_{n+1/2}(x) = (-1)^n \frac{x^{n+1/2}}{\sqrt{2\pi}} \left[\frac{p_n(-x)e^x - p_n(x)e^{-x}}{x^{2n+1}} \right]$$
(26)

the term into brackets beeing a regular function at x = 0 with even parity,

$$K_{n+1/2}(x) = \frac{\sqrt{\pi}e^{-x}}{\sqrt{2}x^{n+1/2}}p_n(x) .$$
(27)

Theorem.– The functions $\bar{A}^n_{\lambda}(a,r)$ has the following explicit representation

$$\bar{A}^{n}_{\lambda}(a,r) = \frac{e^{-a}}{2a^{\lambda+1/2}r^{\lambda+1/2}} \left[p^{(n)}_{\lambda}(a,r)e^{r} + q^{(n)}_{\lambda}(a,r)e^{-r} \right],$$
(28)

where $p_{\lambda}^{(n)}(a,r)$ and $q_{\lambda}^{(n)}(a,r)$ are polynomials in a and r with integer coefficients, with degree $n + \lambda$ with respect to each variable a, r and with total degree $n + 2\lambda$ with respect to a and r.

To do:

Another explicit representation for $A^1_{\lambda+1/2}(\zeta, a, r)$

$$A^{1}_{\lambda+1/2}(\zeta, a, r) = aI_{\lambda+1/2}(\zeta r)K_{\lambda-1/2}(\zeta a) - rI_{\lambda+3/2}(\zeta r)K_{\lambda+1/2}(\zeta a)$$
(29)

Another explicit expression for $A_{\lambda}^{(2)}(a,r)$ is

$$A_{\lambda}^{(2)}(a,r) = (a^{2} + r^{2} + 2\lambda(2\lambda + 1))I_{\lambda+1/2}(r)K_{\lambda+1/2}(a) + 2rI_{\lambda+3/2}(r)K_{\lambda+1/2}(a) -2a(rI_{\lambda+3/2}(r)K_{\lambda+3/2}(a) + \lambda I_{\lambda+1/2}(r)K_{\lambda+3/2}(a))$$
(30)

1.4 Integral representations

As in [3] using the integral representation of the product of two modified Bessel function (equation 6.541 page 703 in [4])

$$K_{\nu}(\zeta a)I_{\nu}(\zeta r) = \int_{0}^{+\infty} \frac{t}{t^{2} + \zeta^{2}} J_{\nu}(at)J_{\nu}(rt) dt , 0 \le r \le a .$$
(31)

equations (5) and (7) provide

$$A^{n}_{\lambda+1/2}(\zeta, a, r) = \int_{0}^{+\infty} (-1)^{n} \frac{\partial^{n}}{\partial \zeta^{n}} \left(\frac{t}{t^{2}+\zeta^{2}}\right) J_{\lambda+1/2}(at) J_{\lambda+1/2}(rt) dt .$$

$$(32)$$

This is equivalent to equation (29) in [3].

The following integral representations are used in [2]

$$A^{0}_{\lambda+1/2}(\zeta, a, r) = \frac{1}{2} \int_{0}^{+\infty} I_{\lambda+1/2}\left(\frac{ar}{2u}\right) e^{-\zeta^{2}u - \frac{a^{2} + r^{2}}{4u}} \frac{du}{u},$$
(33)

$$A_{\lambda+1/2}^{n}(\zeta, a, r) = \frac{1}{2} \int_{0}^{+\infty} u^{n/2} H_{n}(\zeta\sqrt{u}) I_{\lambda+1/2}\left(\frac{ar}{2u}\right) e^{-\zeta^{2}u - \frac{a^{2} + r^{2}}{4u}} \frac{du}{u}.$$
(34)

where H_n is the Hermite polynomial of degree n.

1.5 BCLF functions for r = a

This paragraph is devoted to the study of BCLF function on the diagonal r = a. For integers $n \ge 1$ and $\lambda \ge 0$, function $g_{\lambda}^{(n)}$ are defined by

$$g_{\lambda}^{(n)} = A_{\lambda+1/2}^{(n)}(1,a,a) = \bar{A}_{\lambda}^{(n)}(a,a).$$
(35)

It is straightforward to verify the following relations

$$g_{\lambda}^{(1)}(a) = \frac{a^2}{2\lambda+1} [g_{\lambda-1}^{(0)}(a) - g_{\lambda+1}^{(0)}(a)], \qquad (36)$$

$$g_{\lambda}^{(n+2)}(a) = 2a^2 \left[g_{\lambda}^{(n)}(a) - \frac{1}{2\lambda+1} (\lambda g_{\lambda-1}^{(n)}(a) + (\lambda+1)g_{\lambda+1}^{(n)}(a)) \right], \ n \ge 0.$$
(37)

$$g_{\lambda}^{(n+1)}(a) = ng_{\lambda}^{(n)}(a) - a\frac{d}{da}g_{\lambda}^{(n)}(a), \ n \ge 0.$$
(38)

The three term recurrence relation on λ is verified

$$g_{\lambda+3}^{(n)}(a) = \frac{2\lambda+5}{2\lambda+3}g_{\lambda}^{(n)}(a) + \left[\frac{(2\lambda+3)(2\lambda+5)}{a^2} + 1\right]g_{\lambda+1}^{(n)}(a) \\ -\frac{2\lambda+5}{a^2}\left[\frac{2\lambda+3}{a^2} + \frac{a^2}{2\lambda+3}\right]g_{\lambda+2}^{(n)}(a) \ n \ge 0.$$
(39)

Theorem.– For $n \ge 0$, $\lambda \ge 0$, the function $g_{\lambda}^{(n)}$ has the following Taylor series expansion

$$g_{\lambda}^{(n)}(a) = \sum_{k=0}^{+\infty} c_{n,\lambda,k} a^{k} \quad \text{with } c_{n,\lambda,k} = \frac{(-1)^{n+\lambda+k} 2^{k}}{(k+1)(k-n)!} \frac{\prod_{l=1}^{\lambda} (k-2l+1)}{\prod_{l=1}^{\lambda} (k+2l+1)},\tag{40}$$

where by convention 1/n! has value 0 if n < 0. This series has an infinite radius of convergence and the coefficients verify the recurrence relation

$$4(k+1)c_{n,\lambda,k} = (k-n+1)(k-n+2)(k-2\lambda+1)(k+2\lambda+3)c_{n,\lambda,k+2}, \ k \ge 0.$$
(41)

Proof.- To do

The recurrence relation implies that

$$c_0 = c_2 = c_{2n_1} = 0, \ c_{2n_1+2} \neq 0, \tag{42}$$

where n_1 is defined by $n = 2n_1 + 2$ if n is even and $n = 2n_1 + 1$ if n is odd, and

$$c_1 = c_3 = c_{2m_1 - 1} = 0, \ c_{2m_1 + 1} \neq 0, \tag{43}$$

where m_1 is defined by $2m_1 = \max(n, 2\lambda)$ if n is even and $2m_1 + 1 = \max(n, 2\lambda + 1)$ if n is odd.

2 Numerical stability and exact values in arbitrary precision

2.1 Naive evaluation of $\bar{A}^n_{\lambda}(a, r)$

Functions $\bar{A}^n_{\lambda}(a, r)$ may be evaluated using recurrence relations (14) and (15). However there happens a loss of precision when n, λ, a or r increases and numbers are represented by floating point reals with fixed precision. A way to overcome this problem is to increase the precision of by floating point reals for intermediate computations. It is straightforward within a computer algebra system like Maple or others.

An heuristic (not rigorous) way to get exact numerical results for a given precision D is to successively compute the function for increasing precisions $D < D_1 < \ldots < D_n < D_{n+1}$ and to stop the computation when the rounding to D digits of the results for precisions D_n and D_{n+1} are equal. The precision D_n then gives a precise indication of the numerical instability of an algorithm and in particular a formula for \bar{A}^n_{λ} and given values of a and r.

The following functions in **calculAn.mpl** are used to implement this procedure.

```
exComp1 := proc(f,x)
  local oldprec,prec1,prec2,y1,y2;
  global INCPREC, CURPREC;
  oldprec:=Digits;
  y1 := f(x);
 Digits := Digits+INCPREC;
  CURPREC := Digits;
  y^2 := f(x);
  while not(evalf(y1,oldprec)=evalf(y2,oldprec)) do
   y1 := y2;
   Digits := Digits+INCPREC;
   CURPREC := Digits;
   y2 := f(x);
  od;
  Digits := oldprec;
  evalf(y1,oldprec);
end:
showPrec1 := proc(f,x)
   global CURPREC;
   CURPREC:=1;
   exComp1(f,x);
   CURPREC;
end:
exComp2 := proc(f,a,r)
  local oldprec,prec1,prec2,y1,y2;
  global INCPREC, CURPREC;
  oldprec:=Digits;
  y1 := f(a,r);
  Digits := Digits+INCPREC;
```

```
CURPREC := Digits;
  y2 := f(a,r);
  while not(evalf(y1,oldprec)=evalf(y2,oldprec)) do
   y1 := y2;
  Digits := Digits+INCPREC;
  CURPREC := Digits;
  y2 := f(a,r);
  od;
  Digits := oldprec;
  evalf(y1,oldprec);
end:
showPrec2 := proc(f,a,r)
   global CURPREC;
   CURPREC := 1:
   exComp2(f,a,r);
   CURPREC;
end:
```

Then come the definitions of $\bar{A}^n_{\lambda}(a,r)$ and $g^{(n)}_{\lambda}(a)$ using recurrence equations.

```
Anbar := proc(n,lambda,a,r)
  if r>a then RETURN(Anbar(n,lambda,r,a)); fi;
  if n=0 then
    RETURN(BesselK(lambda+1/2,a)*BesselI(lambda+1/2,r));
 fi;
  if n=1 then
    RETURN(a*r/(2*lambda+1)*(Anbar(0,lambda-1,a,r) - Anbar(0,lambda+1,a,r)));
 fi;
  (a<sup>2</sup>+r<sup>2</sup>)*Anbar(n-2,lambda,a,r) - 2*a*r/(2*lambda+1)*(
    lambda*Anbar(n-2,lambda-1,a,r) + (lambda+1)*Anbar(n-2,lambda+1,a,r));
end:
Gn := proc(n,lambda,a)
  if n=0 then
    RETURN(BesselK(lambda+1/2,a)*BesselI(lambda+1/2,a));
 fi;
  if n=1 then
    RETURN(a<sup>2</sup>/(2*lambda+1)*(Gn(0,lambda-1,a,tst) - Gn(0,lambda+1,a,tst)));
 fi;
  2*a^2*(Gn(n-2,lambda,a,tst) - 1/(2*lambda+1)*(
      lambda*Gn(n-2,lambda-1,a,tst) + (lambda+1)*Gn(n-2,lambda+1,a,tst)));
end:
```

This section to be completed.

2.2 Roots of $\bar{A}^n_{\lambda}(a,r)$

From equation (4) it follows that $A_{\lambda+1/2}^n(\zeta, a, r) > 0$ for $0 < r \le a$ if n = 0 or n = 1 or $\lambda = 0$. Let us denote by $Z_{\lambda}^{(n)}$ the subset of points (r, a) in r > 0, a > 0 such that $\bar{A}_{\lambda}^n(a, r) = 0$. For $\lambda = 1, n \ge 2$ and for $n = 2, 3, \lambda \ge 1, Z_{\lambda}^{(n)}$ is a single simple curve (as in figures 3 and 3). The set $Z_6^{(10)}$ is shown in figure 3. The points on the diagonal a = r are obtained for a = r =0.568310, 2.444904, 5.5934424, 11.269419, 28.131956 and the limit points (0, a) or (a, 0) are obtained

when a is a positive root of polynomial

$$a^{6} - 39a^{5} + 510a^{4} - 2640a^{3} + 4725a^{2} - 945a - 945$$
,

that is a = 0.732831, 3.008601, 6.388665, 11.132220, 18.070565.

It may be observed, but not yet proved, that $Z_{\lambda}^{(n)}$ is the union of $\min(\lambda, \lfloor \frac{n}{2} \rfloor)$ simple curves.

Although it may be deduced from the existence of non void sets $Z_{\lambda}^{(n)}$ that it is impossible to find a pure arithmetic algorithm to get functions $\bar{A}_{\lambda}^{n}(a,r)$ with a predefined relative precision using double floats, results of the previous subsection show that the loss of precision at the neighborhood of zeros is not the main obstacle.

3 Analytical study

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Figure 1: Number of false digits in the naive evaluation of $\bar{A}_4^2(a,r)$ by recurrence relation.



Figure 2: Number of false digits in the naive evaluation of $\bar{A}_4^2(a, r)$ by equation (30).



Figure 3: The function $g_6^{(10)}$.



Figure 4: The function $g_6^{(10)}$.



Figure 5: The function $g_6^{(10)}$.



Figure 6: The function $g_6^{(10)}$.



Figure 7: The function $g_6^{(10)}$.



Figure 8: Sets $Z_l^{(2)}$ for l = 1, ..., 6.



Figure 9: Sets $Z_1^{(n)}$ for n = 2, ..., 6.



Figure 10: The set $Z_6^{(10)}$.