

# Adaptive Cubatures on Triangle

## How to implement them

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ROGER 2007, Königswinter

# Outline

- 1 Introduction
- 2 A Meta Algorithm for Adaptive Integration
- 3 Our Approach
- 4 MATLAB Implementation
- 5 Examples and Tests

# Problem

- Our problem: calculate the definite integral

$$I_f := \int_B f(x) dx$$

$f : B \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}$ , given integrand,  $B$  given region.

# Problem

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$$I_f := \int_B f(x) dx$$

$f : B \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}$ , given integrand,  $B$  given region.

- The aim of constructing integration algorithm is to approximate  $I_f$  with a given error tolerance  $\varepsilon$  and as few function evaluations as possible.

# What is an adaptive integration algorithm

- **Adaptive algorithms** decide dynamically how many function evaluations are needed. The information for such decisions is derived from numerical experiments based on integrand. In general, no a priori information about the decision process is available. The efficiency and reliability of such algorithms depends upon the subdivision strategy.
  - The decision as to whether or not a subregion has to be further subdivided is based on either **local** and **global** knowledge. This leads to local and global subdivision strategy respectively.
  - Local knowledge is based only on the considered subregion.
  - Global knowledge is based on knowledge about all subregions of the integration region.
  - In any case, the depth of the subdivision process is determined dynamically.

# Notes

- For the 1D case the basic idea is as follows: Let  $[a, b]$  be a bounded interval. In order to compute

$$I = \int_a^b f(x) dx$$

we integrate  $f$  using two methods which provide us the approximations  $I_1$  and  $I_2$ . If the difference of this two approximations is less than a given tolerance, we accept the better of them, say  $I_2$ , as approximate value of integral. Otherwise, we divide  $[a, b]$  into two (or three) congruent parts; then proceed recursively on each part.

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- The idea is credited to Huygens, but in this form appear in [Davis, Rabinowitz 1984].

# Negative results

- [deBoor 1971] it is impossible to construct a correct program that integrates each given function.
- Moreover, for a given program, it is possible to find a function  $f$ , which is not correctly integrated ( [Kahan 1980]).
- Hence, the task of each implementer is to code programs which function correctly for a class of function as large as possible.



# The Rice's meta algorithm

- The Rice's meta algorithm 2 [Rice 1975] is an abstract description of the mechanisms involved in adaptive integration.
- It can be used as a starting point for the development of adaptive integration algorithms based on a given formula  $Q_N$  with an error estimator  $E$ .
- We reproduced it here in the form given in [Überhuber 1995]

# The Rice's meta algorithm

Meta algorithm for adaptive integration

**Input:**  $f, B, \varepsilon, Q_N, E$ .

**Output:** The approximate integral value  $q$  and the error estimation  $e$ .

$q := Q(f; B); e := E(f, B);$

insert  $(B, q, e)$  into the data structure;

**while**  $e > \varepsilon$  **do**

choose an element of the data structure (with index  $s$ );

Subdivide  $B_s$  into subregions  $B_\ell, \ell = 1, 2, \dots, L;$

Calculate approximations for integrals over  $B_1, \dots, B_L$

$q_\ell := Q_N(f; B_\ell), \quad \ell = 1, 2, \dots, L;$

Calculate corresponding error estimates;

$e_\ell := E(f; B_\ell), \quad \ell = 1, 2, \dots, L;$

remove old data  $(B_s, q_s, E_s)$  from the data structure;

Insert  $(B_1, q_1, e_1), \dots, (B_L, q_L, e_L)$  into the data structure;

$q := \sum_i q_i; \quad e := \sum_i e_i;$

**end while**

# The case of triangle

- As in the case of [Laurie 1982, Berntsen, Espelid 1992, Cools et al. 1997] our region  $B$  will be a collection of triangles.
- This allow:
  - A larger degree of generality
  - To restart the algorithm for refinement, performing the continuation of previous work.

# Basic Elements

- A collection of triangles organized in a heap;  $M$  is the current number of triangles
- A quadrature rule  $Q$  to produce a local estimate to the integral over each triangle of the collection
- A procedure for error estimation  $E$
- A strategy for picking the next triangle to be processed — in our case the triangle on the top of the heap
- A subdivision strategy

# The algorithm

Initialize the triangle collection;  $M := m$ ;

Compute  $\hat{Q}_i$  and  $\hat{E}_i$ ,  $i = 1, 2, \dots, m$

$\hat{Q} = \sum_{i=1}^m \hat{Q}_i$ ;  $\hat{E} = \sum_{i=1}^m \hat{E}_i$ ;

**while**  $\hat{E} > \varepsilon$  **do**

{Control}

Pick the triangle  $T_k$  on top of heap;

{Subdivision}

Divide  $T_k$  in  $p$  parts;

{Process triangles}

Compute  $\hat{Q}_k^{(i)}$ ,  $\hat{E}_k^{(i)}$ ,  $i = 1, \dots, p$ ;

{Update}

$\hat{Q} := \hat{Q} + \sum_{i=1}^p \hat{Q}_k^{(i)} - \hat{Q}_k$ ;  $\hat{E} := \hat{E} + \sum_{i=1}^p \hat{E}_k^{(i)} - \hat{E}_k$ ;

Replace triangle  $T_k$  by  $p$  new triangles;

$M := M + p - 1$ ;

**end while**

# Data structures

- A collection of triangles  $\text{Tri}$ , organized as an array of triangles. Information for each triangle:
  - $V1, V2, V3$  - pointers to vertices (see Vertex below)
  - $VI$  - approximate of the integral
  - $EE$  - error estimation
- A collection of vertices,  $\text{Vertex}$ , organized as a matrix with two columns (coordinates)
- A heap of pointers to triangles,  $\text{Heap}$ . Ordered by  $EE$ . Triangle with maximum  $EE$  on top.

# Cubature rules

- The user may choose the cubature rule. A procedure that initializes the nodes and the coefficients is specified at invocation.
- The rule must be given in fully symmetric form, as in [Stroud 71] or in Ronald Cools' Encyclopedia of cubature formula [Encyclopedia].
- A procedure evaluates the cubature formula given in fully symmetric form.
- Supported: a 37 point PI rule of degree 13 [Berntsen, Espelid 1990] and a seven point PI rule of degree 5, due to Radon

# Error estimation

- Two methods:



# Error estimation

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# Error estimation

- Two methods:
- Embedded cubature formulas.
- Null rules.

# Embedded cubature formulas

- We shall use two cubature formulas

$$Q_j[f] = \sum_{i=1}^{N_j} f(x_{ij}, y_{ij}), \quad j \in \{1, 2\},$$

with degree of exactness  $d_j$ ,  $d_1 < d_2$ , where  $N_j$  is the number of nodes for  $Q_j$ .

- In order to reduce the number of function evaluation (and so the amount of work) one tries to choose  $Q_1$  and  $Q_2$  such that

$$\{(x_{i1}, y_{i1} : i = 1, \dots, N_1)\} \subset \{(x_{i2}, y_{i2} : i = 1, \dots, N_2)\}.$$

A pair  $(Q_1, Q_2)$  having this property is called an **embedded pair**.

- The difference  $|Q_1[f] - Q_2[f]|$  is used as an error estimation for  $Q_1$ .

# Null rules

## Definition

[Lyness 1965] A rule

$$N[f] = \sum_{i=0}^n u_i f(x_i) \quad (1)$$

is a **null rule** iff it has at least one nonzero weight, and in addition  $\sum_{i=0}^n u_i = 0$ . A null rule has the **degree**  $d$  if it integrates to zero all basic monomials of degree  $\leq d$  and fail to do so for a monomial of degree  $d + 1$ .

- A null rule of the form (1) has the degree at most  $n - 1$ .
- Null rules may be used as estimations of error.
- An estimation based on a single null rule is sometimes unreliable; in practice one uses combination of null rules of various degrees. [Berntsen, Espelid 1991]

## Error estimation using null rules

{Compute}

$$e_j := N_j[f], j = 1, \dots, 2k;$$

$$E_j := (e_{2j-1}^2 + e_{2j}^2)^{1/2}, j = 1, \dots, k;$$

$$r_j := E_j / E_{j+1}, j = 1, \dots, k - 1;$$

if  $r > 1$  then

$$\hat{E} = 10 \max_j E_j \text{ \{Nonasymptotic\}}$$

else if  $1/2 \leq r$  then

$$\hat{E} := 10r^1 E_1 \text{ \{Weakly-asymptotic\}}$$

else

$$E = 10 \cdot 4r^3 E_1 \text{ \{Strongly-asymptotic\}}$$

end if

- Since cubature rules and null rules are based on the same set of nodes, they are evaluated simultaneously.
- Embedded cubatures are considered combination of a cubature rule  $Q_1$  and a null rule  $Q_1 - Q_2$ .

# Subdivision

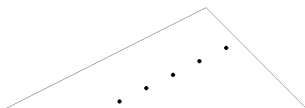
- The simplest subdivision is in four congruent triangles, determined by vertices and midpoints of edges
- A **more flexible method**
- Use subdivision directions parallel to the sides of the triangle
- 4th differences parallel to the sides are computed
- Let  $e$  be a unit vector along one side of triangle  $T_k$ ,  $h$  the length of the side,  $C$  the barycenter. Define the measure of variation of  $f$  in direction  $e$ :

$$D(e) = h^q \left| f \left( C - \frac{4}{15}he \right) - 4f \left( C - \frac{2}{15}he \right) + 6f(C) - 4f \left( C + \frac{2}{15}he \right) + f \left( C + \frac{4}{15}he \right) \right| \quad (2)$$

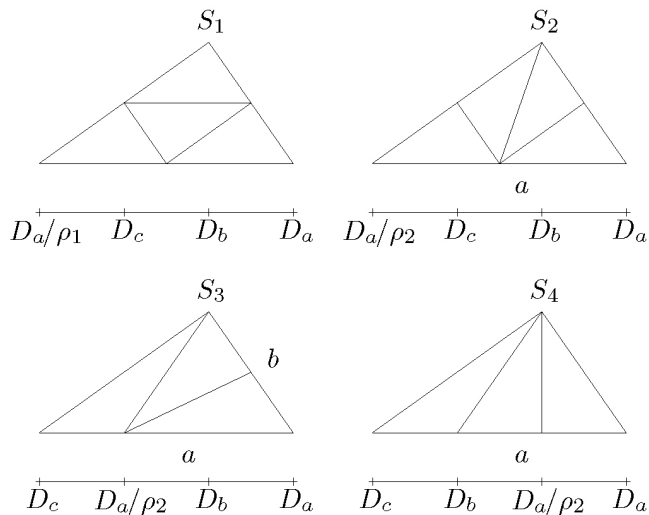
- Three heuristic constants  $q, \rho_1, \rho_2$  are involved

# Subdivision

- Define  $D_a = D(a / \|a\|)$ ,  
 $D_b = \dots$  using (2)
- The triangle is divided into four or three triangles according to magnitude of  $D_a, D_b, D_c$
- Requires 13 new function evaluations



# Subdivision types





## Algorithm — Choice of subdivision

- 1 Compute estimates  $D_a, D_b, D_c$  for sides  $a, b, c$
- 2 Relabel the sides so that  $D_a \geq D_b \geq D_c$
- 3 **If**  $D_c \geq D_a/\rho_1$  **then** choose  $S_1$ ;  
**else if**  $D_b \geq D_a/\rho_2$  and  $D_c \geq D_a/\rho_2$  **then** choose  $S_2$ ;  
**else if**  $D_b \geq D_a/\rho_2$  and  $D_c < D_a/\rho_2$  **then** choose  $S_3$ ;  
**else** choose  $S_4$   
**end if**

# MATLAB implementation - main function

- We code a flexible set of functions which allow to select the cubature formula and null rules. There exists also a restart facility that allows the refinement of previous result. The syntax of main function, `CubatureTriang` is

$$[\text{result}, \text{ee}, \text{stat}, \text{Tri}, \text{Vertex}, \text{VI}, \text{EE}] = \text{CubatureTriang}(\text{F}, \text{Tri}, \dots, \text{Vertex}, \text{VI}, \text{EE}, \text{opt}, \text{varargin})$$

- Parameters:

F - function to be integrated

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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`Tri` - collection of triangles

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Vertex, VI, EE, opt, varargin)
```

- Parameters:

`Vertex` - collection of vertices

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- Parameters:

VI - value of integral for a triangle

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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

EE - error estimation for a triangle

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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`opt` - options: `errabs`, `errel`, `restart`, `initf`, `trace`, `nfev` -

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```
[result, ee, stat, Tri, Vertex, VI, EE]= CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`initf` - initialization function; return cubature parameters:

`weights`, `nodes`, null rules type;

call: `[W,G,m,p]=initf`



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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`result` - approximate of integral

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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`ee` - error estimation

# MATLAB implementation - main function

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```
[result, ee, stat, Tri, Vertex, VI, EE] = CubatureTriang(F, Tri, ...  
Vertex, VI, EE, opt, varargin)
```

- Parameters:

`stat` - statistics: number of function evaluations, number of triangles, success/failure.

# MATLAB implementation - cubature and null rules

- Cubature rule and null rules are given in fully symmetric form.
- The function `fselcub` approximate the integral and the error on the current triangle.
- The selection of cubature and null rules is performed via the `initf` parameter of `CubatTri`. Implemented:
  - Berntsen & Espelid 13 degree formula with eight null rules, function `BerntsenEspelid`
  - embedded 5-7 degree cubature formula, function `ecf57` [Cools, Haegemans 1988].
  - embedded 5-7 degree cubature formula, function `ecf58` [Laurie 1982].
- The user can code his own function if he/she obeys the call syntax.

# MATLAB implementation - Data structures management

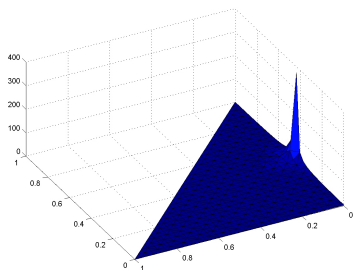
- Function `NewVertex` inserts a new vertex into the `Vertex` matrix
- Function `NewTriangle` inserts a triple of pointers (indices) to the vertices of triangle into the array `Tri`
- Function `InsertIntoHeap` takes a pointer to the current triangle and its error estimation and insert the pointer into heap at an appropriate place, updating the heap
- Function `ExtractMaxFromHeap` extract the top triangle from heap and update the data structures.

# Examples and tests - Test families

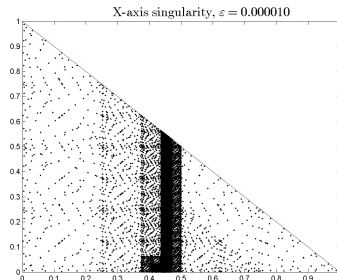
	Test family	Attributes
1	$f_1(x, y) = ( x - \beta_1  + y)^{d_1}$	X-axis singularity
2	$f_2(x, y) = \begin{cases} 1 & \sqrt{(x - \beta_1)^2 + (y - \beta_2)^2} < d_2 \\ 0 & \text{otherwise} \end{cases}$	Discontinuous
3	$f_3(x, y) = \exp(-\alpha_1 x - \beta_1  - \alpha_2 y - \beta_2 )$	$C_0$ function
4	$f_4(x, y) = \exp(-\alpha_1^2(x - \beta_1)^2 - \alpha_2^2(y - \beta_2)^2)$	Gaussian
5	$f_5(x, y) = (\alpha_1^{-2} + (x - \beta_1)^2)^{-1}(\alpha_2^{-2} + y^2)^{-1}$	X-axis peak
6	$f_6(x, y) = (\alpha_1^{-2} + (x - \beta_1)^2)^{-1}(\alpha_2^{-2} + (y - \beta_2)^2)^{-1}$	Internal peak
7	$f_7(x, y) = \cos(2\pi\beta_1 + \alpha_1x + \alpha_2y)$	Oscillatory

- $d_j$  - difficulty parameters,  $j = 1, \dots, 7$
- $\alpha_1, \alpha_2, \beta_1, \beta_2$  - random parameters uniformly distributed on  $[0, 1]$ .
- $\alpha_1, \alpha_2$  scaled such that  $\alpha_1 + \alpha_2 = d_j$

# Test - family 1



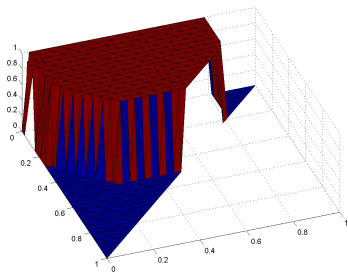
(a) Graph of  $f_1$



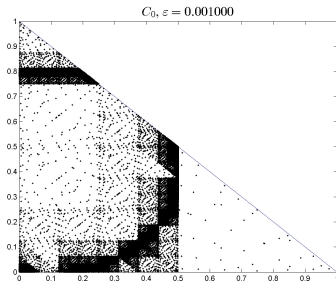
(b) Evaluation points

Figure: Test for family 1

# Test - family 2



(a) Graph of  $f_2$

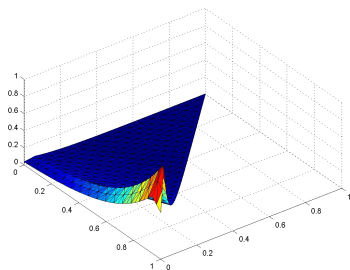


(b) Evaluation points

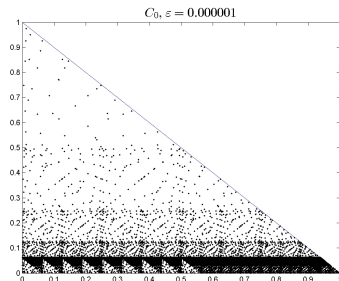
Figure: Test for family 2



# Test - family 3



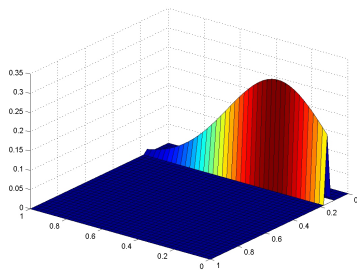
(a) Graph of  $f_3$



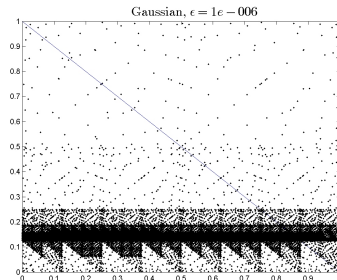
(b) Evaluation points

Figure: Test for family 3

# Test - family 4



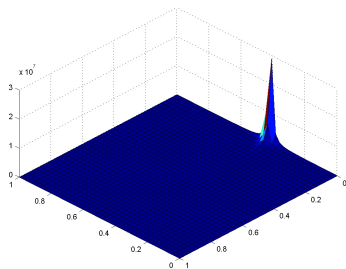
(a) Graph of  $f_4$



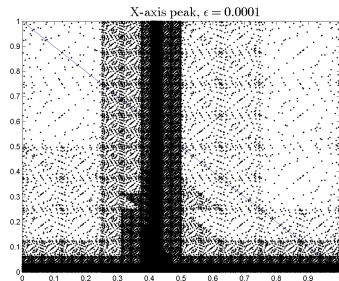
(b) Evaluation points

Figure: Test for family 4

# Test - family 5



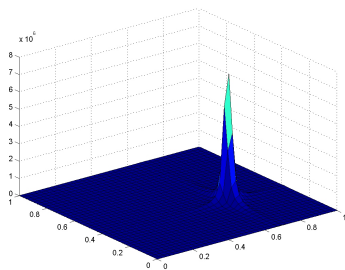
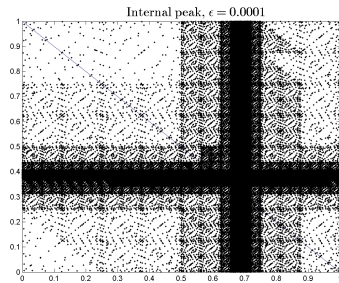
(a) Graph of  $f_5$



(b) Evaluation points

Figure: Test for family 5

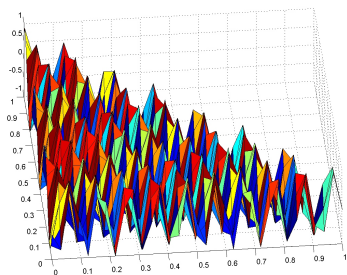
## Test - family 6

(a) Graph of  $f_6$ 

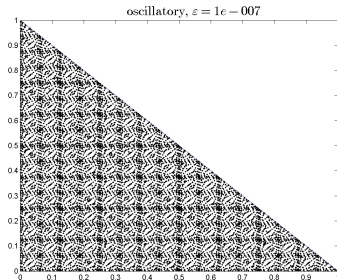
(b) Evaluation points

Figure: Test for family 6

# Test - family 7



(a) Graph of  $f_7$

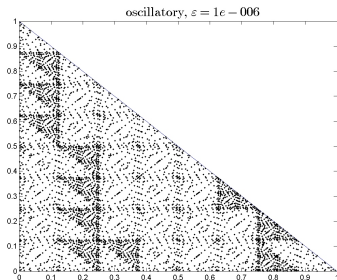


(b) Evaluation points

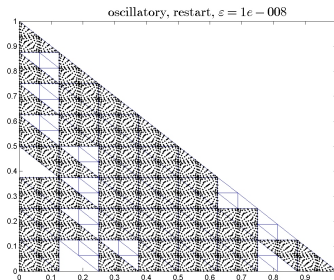
Figure: Test for family 7

# Test with restart

Family 7, first call for  $\text{errabs}=1e-6$ , then restart with  $\text{errabs}=1e-8$ .



(a) First step

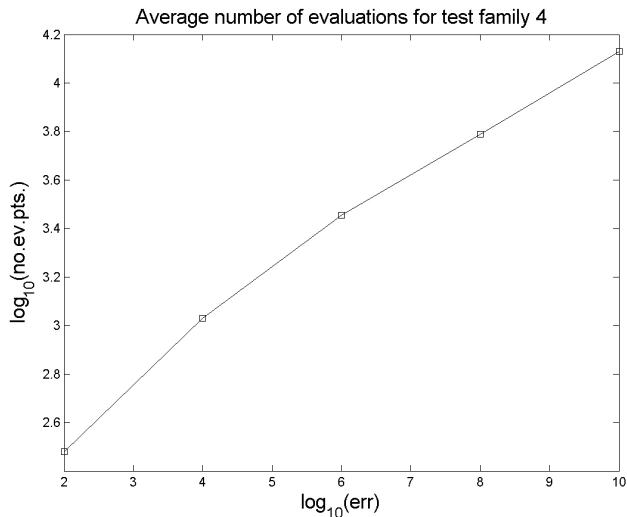


(b) Second step, restart

Figure: Test for family 7 with restart

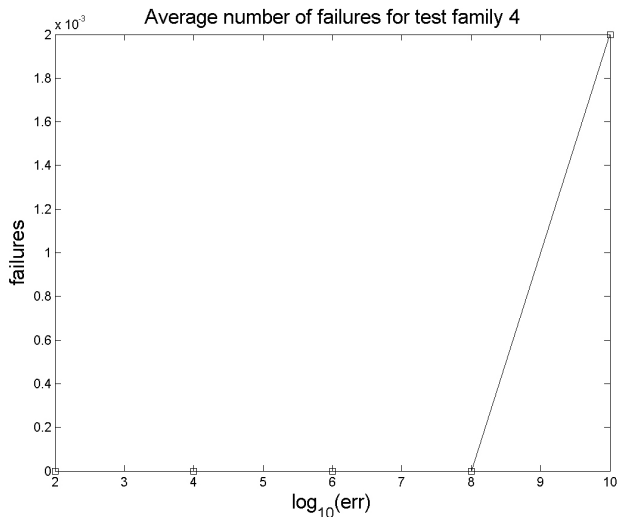
# Number of function evaluation - family 4

$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error



## Number of failures - family 4

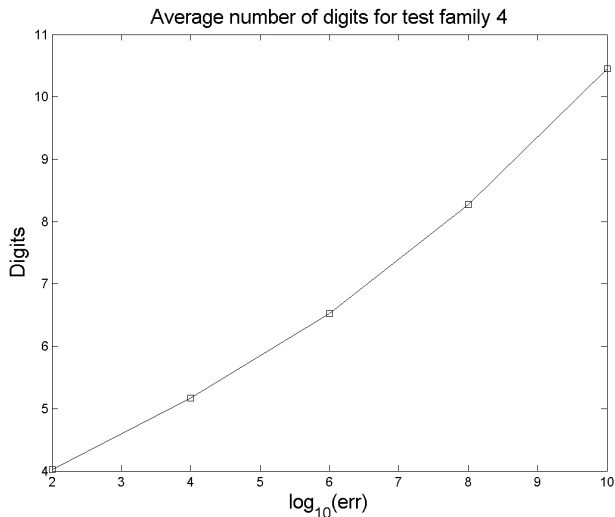
$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error





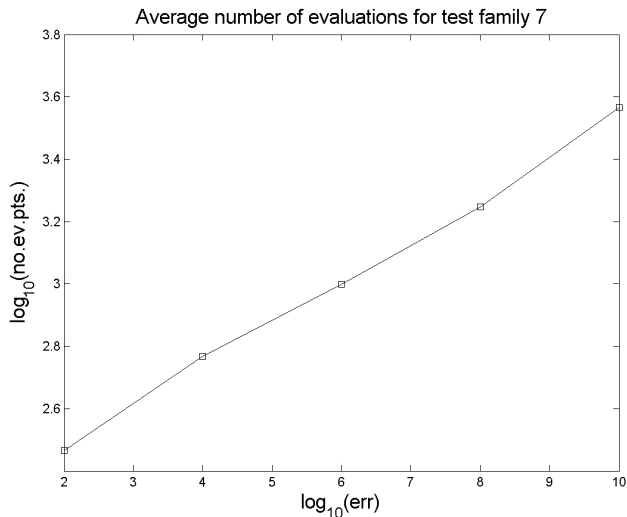
# Number of correct digits - family 4

$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error



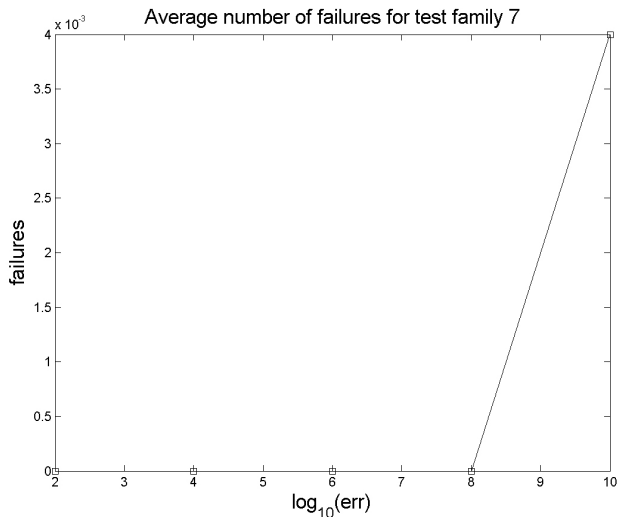
# Number of function evaluation - family 7

$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error



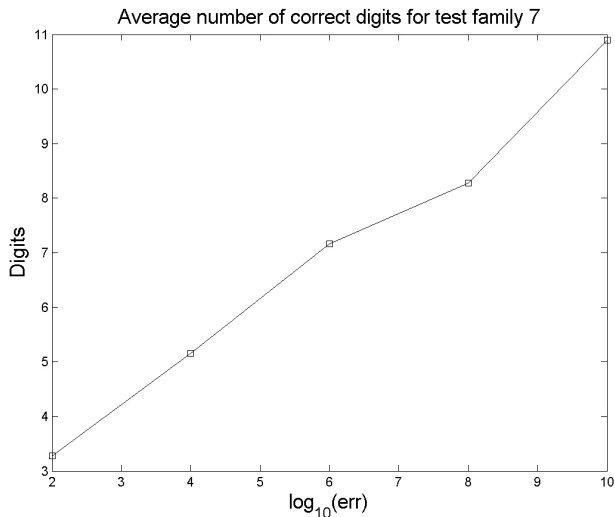
## Number of failures - family 7

$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error






# Number of correct digits - family 7

$\varepsilon = 10^{-2}, 10^{-4}, \dots, 10^{-10}$ , 500 samples for each error



# References I

-  J. Berntsen, T. O. Espelid:  
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