Global Optimization and Verified Numerical Techniques for the Solution of Mathematical Problems

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A Motivating Example: SIAM 100 $, 100 Digits Challenge 2002

The problem (#4) to be minimized:

$$\exp(\sin(50x)) + \sin(60e^y) + \sin(70\sin(x)) + \sin(\sin(80y)) -$$

$$- \sin(10(x+y)) + \frac{1}{4}(x^2+y^2).$$

The result obtained for the enclosure of the global minimum value for the search domain of $[-10.0, 10.0]$ was:

$$[\underline{-3.306868647475}316, \underline{-3.306868647475}196]$$

obtained a the cost of 0.26 CPU seconds, 75 memory units, 1975 function-, 1158 gradient-, and 92 Hessian inclusion function evaluations, and 238 iterations.

Motivating Example: Fractional Programming

Test problem (Benson, JOTA 112(2002), 1-19):

$$\max \frac{-x_1^2 - 3x_1 - x_2^2 + 3x_2 + 3.5}{x_1 + 1} + \frac{x_2}{x_1^2 - 2x_1 + x_2^2 - 8x_2 + 20}$$

subject to: $2x_1 + x_2 \leq 6$, $3x_1 + x_2 \leq 8$, $-x_1 + x_2 \geq -1$, and $x_1, x_2 \geq 1$.

Results:

Benson: $f(1.0200, 1.7100) = 4.0319$,

IHR: $f(1.0000, 1.7778) = 4.0603$ (at the cost of ≈ 1379 iterations),

Interval: $x^* \in ([1, 1]; [\underline{1.74382317}0661926, \underline{1.74382317}4387217])$, and $f(x^*) \in [\underline{4.06081916}4267911, \underline{4.06081916}0846712]$

at the cost of 0.02 seconds CPU time, 224 function-, and 114 gradient evaluations, and 76 iterations.

Interval inclusion function

- Instead of real numbers, we shall calculate with intervals.
- Definition of the interval arithmetic:

$$A \circ B = \{a \circ b \mid a \in A \text{ and } b \in B\}, A, B \in \mathbb{I}$$

$$(\mathbb{I} \text{ is set of } (i, j), \text{ where } i, j \in \mathbb{R}, \text{ and } i < j.)$$

$$\begin{gathered}
[a,b] + [c,d] = [a+c, b+d] \\
[a,b] - [c,d] = [a-d, b-c] \\
[a,b] * [c,d] = [\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)] \\
[a,b]/[c,d] = [a,b] * [1/d, 1/c] \ \text{ if } \ 0 \notin [c,d]
\end{gathered}$$

- Example: The range of the function $x - x^2$ on the interval $[0, 1]$ is $[0, 0.25]$, with interval arithmetic it is $[-1, 1]$.

Cases when the reliability of the optimum is not important

In practical applications, when the objective is to optimize cost or profit. In such cases approximate solutions are satisfactory.

The example of H.-P. Schwefel: the positions of heating elements were to be determined in nuclear power stations for Siemens such that the efficiency improves. The solution found by an evolutionary method was by more than 1% better than the earlier one. Although it remained unknown whether the found approximation was optimal, and also how far it was from the optimum, the client was satisfied ($> 10^8$ DEM).

Cases when reliability is a must

- Proving theoretical statements like
  - the Kepler-conjecture,
  - the Fekete-problems,
  - determination of the kissing numbers (how many congruent spheres can touch an n-dimensional one)
  - circle packing problems, or:
  - $\min\left(a^n + b^n - c^n\right)^2 + \sin^2 a\pi + \sin^2 b\pi + \sin^2 c\pi + \sin^2 n\pi$ where a, b, and c are nonnegative , and n is greater than two.
- certain practical problems, where the approximate solutions are of no value (e.g. whether there exists a cheaper way of production...)

Optimization with tolerances

The reformulated nonlinear optimization problem: find such an n-dimensional interval X^* for wich

$$\begin{aligned} f(x) &\leq f_\varepsilon \equiv f(x^*) + \varepsilon, & & (1) \\ g_j(x) &\leq 0 & j = 1, 2 \ldots, m. & & (2) \end{aligned}$$

holds for a given $\varepsilon > 0$ and *for all* $x \in X^*$.

We have introduced an interval arithmetic based algorithm for the solution of the above problem, that identifies a maximal interval X^* containing a user given seed point, which has sides parallel to the coordinate axes, and all points of which are feasible suboptimal points.

Applications of the optimization with tolerances

- The original problem was to design the composite material of the airplane wall for Boeing. We had to determine the angles with which the layers should be sticked together to obtain a cheap and light structure that still meets all the security constraints. We were able to solve 8 dimensional real life problems within minutes on a hardware from the year 1993.
- Recently we have applied our algorithm to civil engineering design problems, to determine the size of the foundation (footing) of buildings. The preliminary verified solutions of the highly nonlinear problems indicate the possibilities to substantially decrease the presently used safety constants applied by engineers.

An illustrating example for the building footing design problem

$$\min h\mu B^2$$

subject only to the soil breaking constraint:

$$\sigma_{Sd} \leq \sigma_{Eff},$$

$$1 \leq \mu \leq 5,$$

$$0.5\mu B \leq h \leq -a_s - 0.5,$$

$$B > 0,$$

$$-\frac{5}{6}B \leq a_x \leq \frac{5}{6}B,$$

$$-\frac{5}{6}\mu B \leq a_y \leq \frac{5}{6}\mu B.$$

where a_x, a_y, h, μ and B are the variables to be optimized, and:

$$R = P_z + \mu h B^2 \overline{\rho}_{rc},$$

$$\sigma_{Sd} = \frac{R}{\left(B - 2\left|\frac{P_z a_x + P_x h - M_y}{R}\right|\right)\left(\mu B - 2\left|\frac{P_z a_y + P_y h + M_x}{R}\right|\right)},$$

$$N_t = e^{\pi \tan\phi} \tan^2\left(45^o + \frac{\phi}{2}\right),$$

$$f = \frac{P_x}{P_z},$$

$$i_t = (1 - 0.7f)^3$$

$$\sigma_1 = \left(1 - \frac{1}{3\mu}\right)\gamma_1 B (N_t + 1)\tan\phi (1 - f)^3 j_B,$$

$$\sigma_2 = \left(1 + \frac{1}{2\mu}\right)\left(\gamma_2(|a_s| - 0.1)N_t i_t j_t + c(N_t - 1)\cot\phi\left(i_t - \frac{1 - i_t}{N_t - 1}\right) j_c\right),$$

$$\sigma_{Eff} = \alpha_1\alpha_2\alpha_3(\sigma_1 + \sigma_2).$$

The measured values, parameters of the example problem: $P_x = 13$ kN, $P_y = 103$ kN, $P_z = 1360$ kN, $M_x = 663$ kNm, $M_y = -23$ kNm. $\overline{\rho}_{rc} = 28.8\frac{kN}{m^3}$, $\phi = [26^o, 28^o]$, $\alpha_1 = 0.85$, $\alpha_2 = 0.85$, $\alpha_3 = 0.6$, $c = 0$,

$$\gamma_1 = \left[18\frac{kN}{m^3}, 20\frac{kN}{m^3}\right], \quad \gamma_2 = \left[16\frac{kN}{m^3}, 18\frac{kN}{m^3}\right],$$

$$a_s = -2.3m,\ j_B = 1,\ j_t = 1,\ j_c = 1.$$

The engineering calculation procedure resulted in the following values:

$$h = 1.70, \quad \mu = 1.41, \quad B = 2.40, \quad a_x = 0.00, \text{ and } a_y = 0.00.$$

The corresponding volume is 13.807 m^3.

The obtained result tolerance box for the seed point which was the result of the engineering calculation, and for the suboptimality level of $f_\epsilon = 20.0$:

$$\begin{aligned}
&[\ \ 1.700000000000000, 1.730000000000000],\\
&[\ \ 1.390000000000000, 1.410000000000000],\\
&[\ \ 2.380000000000000, 2.411171875000000],\\
&[\ \ 0.000000000000000, 0.020000000000000],\\
&[-1.240000000000001, 0.015000000000000].
\end{aligned}$$

The total number of function evaluations was 52,313, and the computation time less than a second. The volume is between ca. 13.385 and 14.181. With other seed points much less feasible footings could be determined.

References on optimization with tolerances

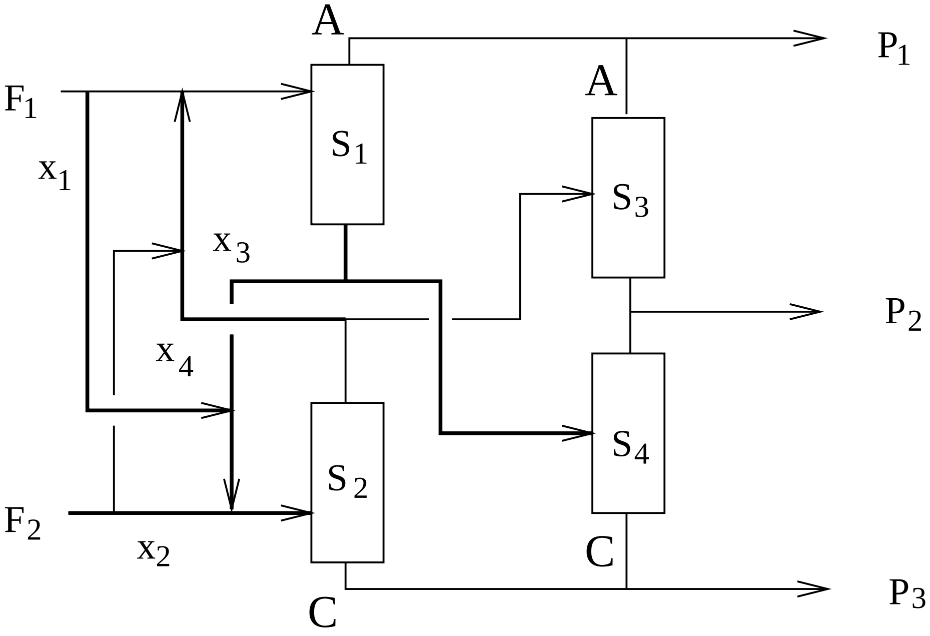
[1] Csallner, A.E., T. Csendes, and A.B. Kocsis: *Reliable numerical computation in civil engineering*. Numerical Algorithms 37(2004) 85-91.

[2] Csendes, T., Z.B. Zabinsky, and B.P. Kristinsdottir: *Constructing large feasible suboptimal intervals for constrained nonlinear optimization*. Annals of Operations Research, 58(1995) 279–293.

[3] Kristinsdottir, B.P., Z.B. Zabinsky, T. Csendes, and M.E. Tuttle: *Methodologies for tolerance intervals*. Interval Computations, 3(1993) 133–147.

[4] Kristinsdottir, B.P., Z.B. Zabinsky, M.E. Tuttle, and T. Csendes: *Incorporating manufacturing tolerances in optimal design of composite structures*, Engineering Optimization 26(1996) 1–23.

A separation network design problem



Find that separation network setting for the divisors $x_i \in [0.0, 1.0], (i = 1, 2, 3, 4)$ that allow a minimal cost functioning.

Results for the separator network design problem

The result obtained by a stochastic, clustering global optimization method based on real function evaluations

$f(x^*)$	x_1^*	x_2^*	x_3^*	x_4^*	NFE	CPU
62.550111	0.00296602	0.99875609	0.75149047	1.0000000	56 067	8.73
62.791640	0.01029729	0.99757082	0.84846761	1.0000000	27 232	4.45
62.851381	0.02461725	0.99482994	0.64821641	1.0000000	61 190	9.45
62.855458	0.00166749	0.99553307	0.86046189	1.0000000	51 263	8.13
62.836668	0.05248426	0.99983809	0.81663978	1.0000000	38 757	6.10
average					47 486.3	7.470

Results for the separator network design problem 2.

The interval arithmetic based B&B procedure have found the following result at the cost of 35,683 function evaluations, 3 minutes CPU time, and 10,000 memory units (containing one subinterval):

$$F(X^*) = [62.49, 62.69],$$

$$\begin{aligned} X^* \quad &= \quad [0.00000000000, 0.00097656250], [0.99804687500, 0.99902343750], \\ &\quad\; [0.71875000000, 0.72070312500], [0.99804687500, 1.00000000000] \end{aligned}$$

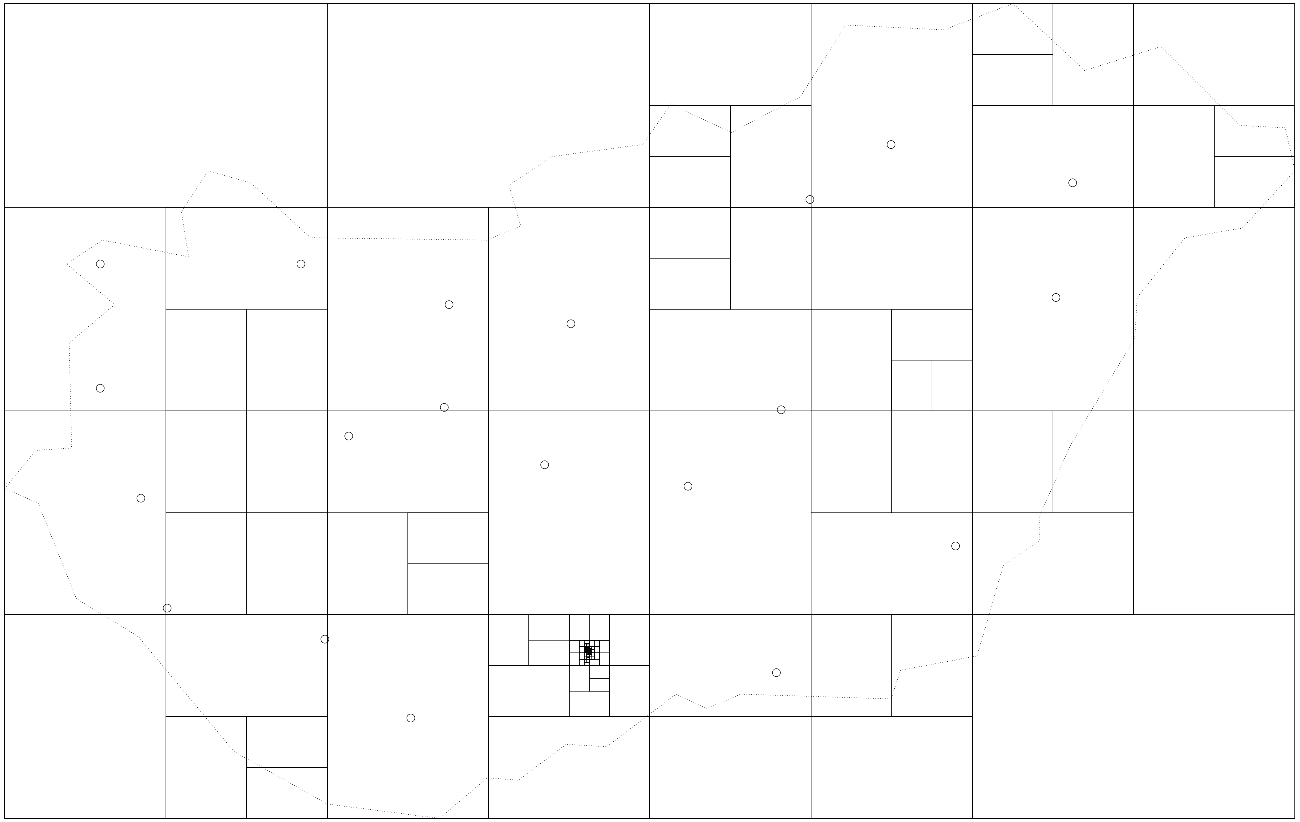
References on the process network synthesis problem

[1] Csallner A. E. (1993), *Global optimization in separation network synthesis*, Hung. J. Ind. Chem. **21**, 303–308.

[2] Csendes, T. (1998), *Optimization methods for process network synthesis — a case study*, In: Christer Carlsson and Inger Eriksson (eds.): Global & multiple criteria optimization and information systems quality. Abo Academy, Turku, pp. 113-132. `http://www.inf.u-szeged.hu/~csendes/publ.html`

[3] Floudas C. A. (1987), *Separation synthesis of multicomponent feed streams into multicomponent product stream*, AIChE J. **33**, 540–550.

A telling result of an obnoxious facility location problem[a]



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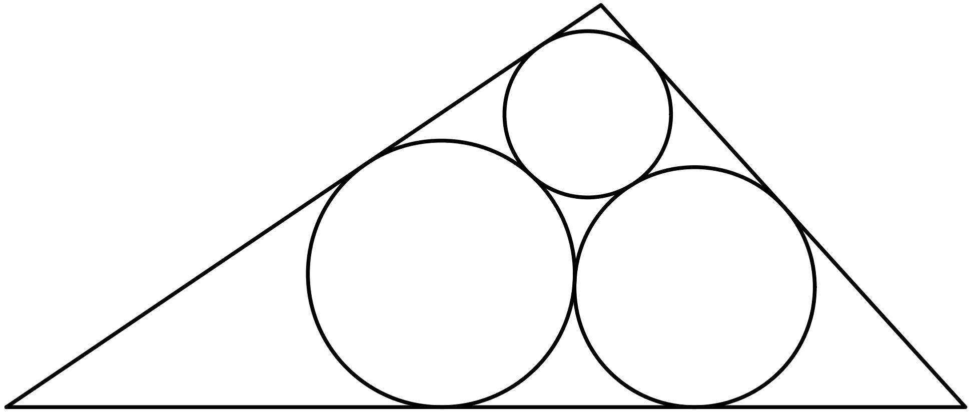
[a] Markót, M.C., J. Fernandez L.G. Casado, and T. Csendes: New interval methods for constrained global optimization. Mathematical Programming 106(2006) 287-318.

The Malfatti Problem

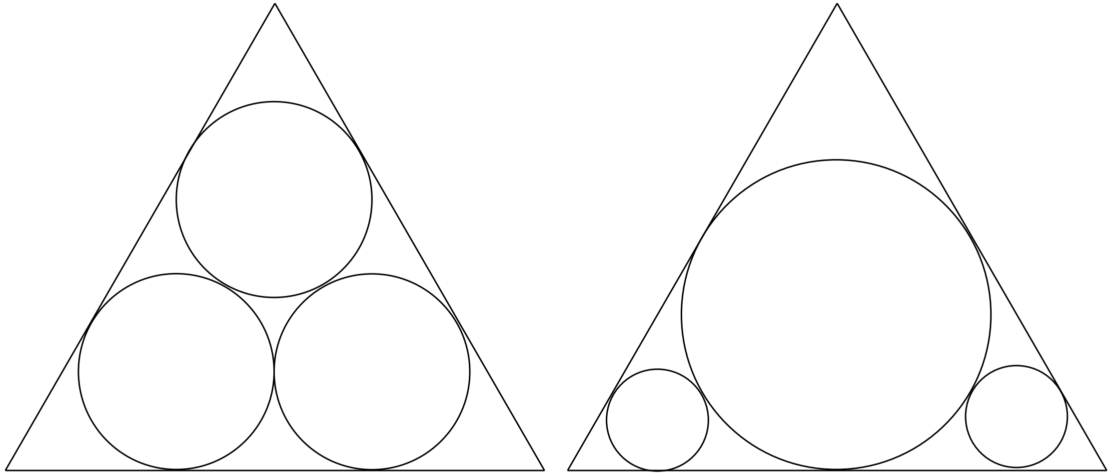
Gianfrancesco Malfatti (1731–1807) (Chokuen Ajima (1732–1798)): Consider a right prism with a right triangular base. How do we cut out three cylinders (perhaps of different sizes) from the prism, such that the total volume of the cylinders is maximal?



The Malfatti circles.

Denser Packings for the Malfatti Problem

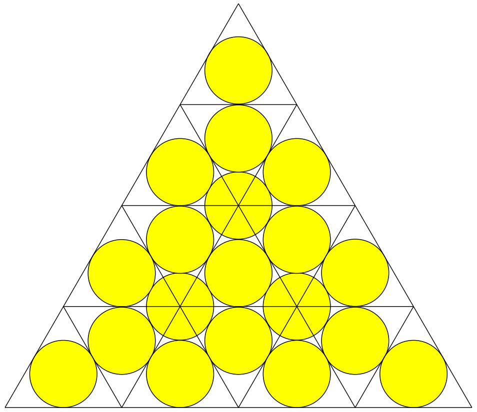
In 1930, H. Lob and H. W. Richmond showed that in an equilateral triangle a different packing can give a greater density than that of the Malfatti circles:



The Malfatti circles and a denser packing in an equilateral triangle.

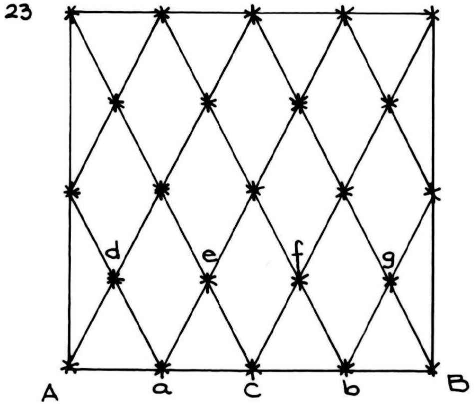
The Circle Packing Studies of Farkas Bolyai

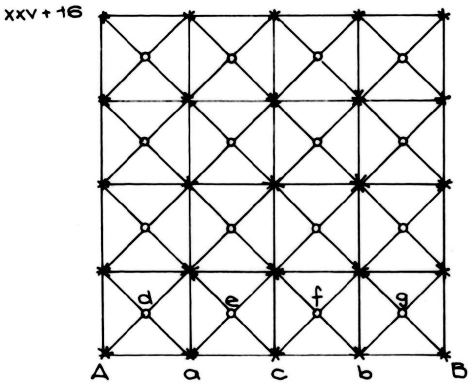
The Hungarian mathematician Farkas Bolyai (1775–1856) was the first who investigated the density of circle packing *sequences* in bounded regions. In his work, in the 'Tentamen' (1832–33) a dense packing of equal circles in an equilateral triangle was worked out:

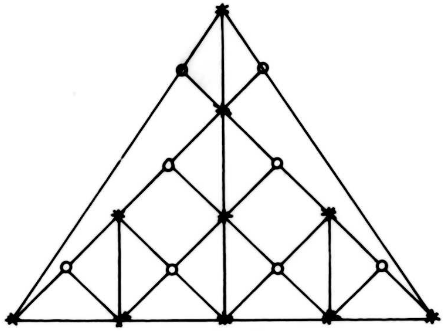


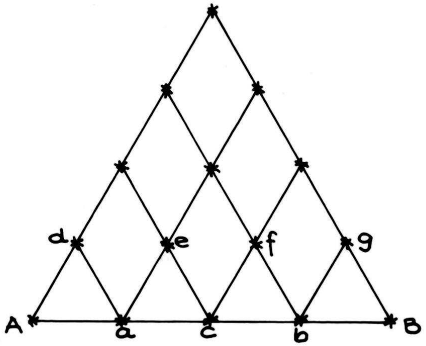
The example of Bolyai for packing 19 equal circles in an equilateral triangle.

Examples of Farkas Bolyai for Optimal Planting of Trees

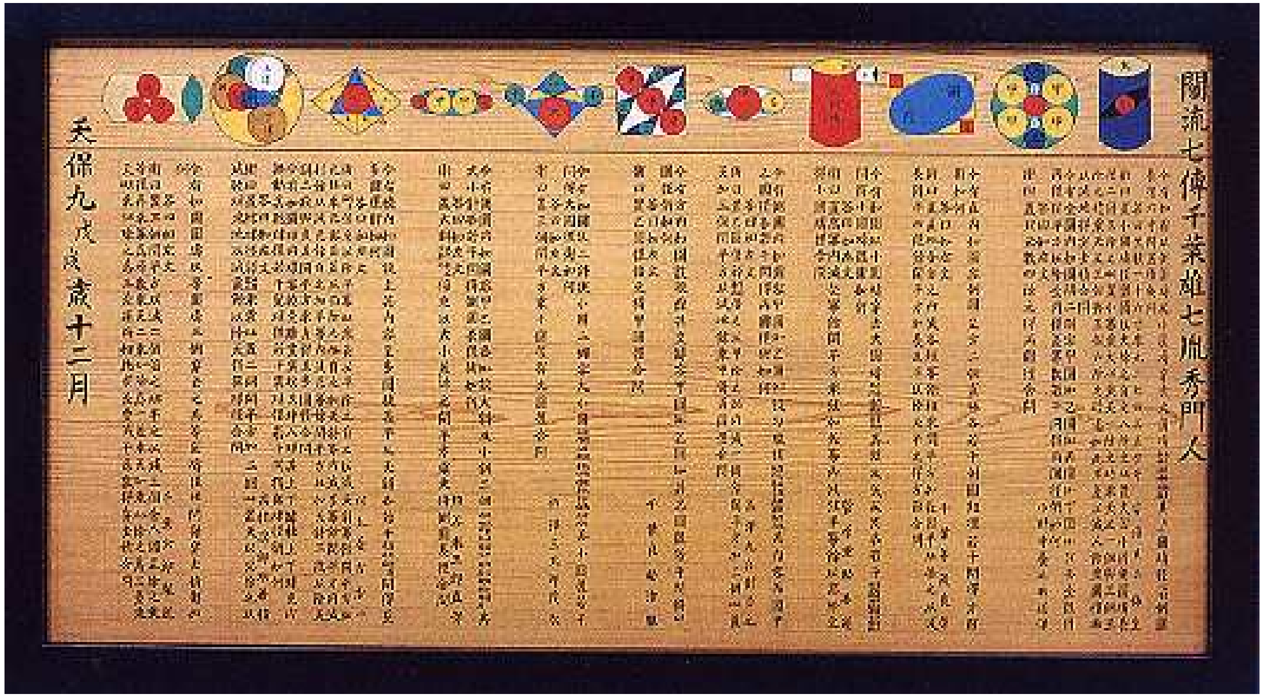








Packing Problems from the Ancient Japan



A Japanese Sangaku of the Edo period (1603–1867) deals with locating circles in various context. Sangakus were displayed in temples and Shinto shrines, probably for meditation purposes.

Circle Packing Problems

Locate a given number of n congruent circles without overlapping in the unit square with a maximal radius.

Locate a given number of n points in the unit square such that their minimal distance is maximal (point arrangement problem):

$$\max \quad \min_{1 \le i \ne j \le n} \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2},$$

$$\text{where } \; 0 \le x_i, y_i \le 1, \qquad i = 1, 2, \ldots, n.$$

These models are equivalent.

Optimization Models

The defined point arrangement problem is a bound constrained maximin optimization problem. The square root can obviously be omitted. The resulting model fits the interval inclusion function approach well.

Other equivalent problem formulations involve

- a linear optimization problem with nonlinear inequality constraints,
- a DC (difference of convex functions) programming problem, and
- an all quadratic (quadratically constrained quadratic) problem.

The Authors of Improved Approximate Packings between 1995 and 2006

Year	Authors	Results for n
1995	C. D. Maranas et al.	up to 30
1996	R. L. Graham and B. D. Lubachevsky	up to 61
1997	K. J. Nurmela and P. R. J. Östergård	up to 50
2000	D. W. Boll et al.	$32, 37, 48, 50$
2001	L. G. Casado et al.	up to 100
2002	M. Locatelli and U. Raber	up to 39
2005	B. Addis et al.	50 – 100
2006	P. G. Szabó and E. Specht	up to 200

Obstacles in the Optimization Problems

- they are of dimension $2n = 56, 58$, and 60, corrupted much by the dependency problem,
- to each global minimizer point there exist $n!$ equivalent ones due to the exchangeability of the circles,
- in addition to that, there are an enormous amount of symmetric equivalent solutions to be managed, and
- on the top of that – due to the existence of free circles (that can be moved slightly while keeping optimality) – a positive measure set of global minimizer points exists beyond the mentioned redundancies for $n = 28$ and 29.

Main Components of the Reliable Solution Algorithm

- Enumeration of subproblems that may only contain a single solution: tiling,
- forcing a preset order of the circles (first one is the upper left,...),
- identifying free circles and their representation by a single center point each,
- the active area approach modified for interval representation to make use of the geometrical properties as an accelerating device, and
- a balanced branch-and-bound framework algorithm with an efficient mix of algorithm parameters.

The Tiling Technique

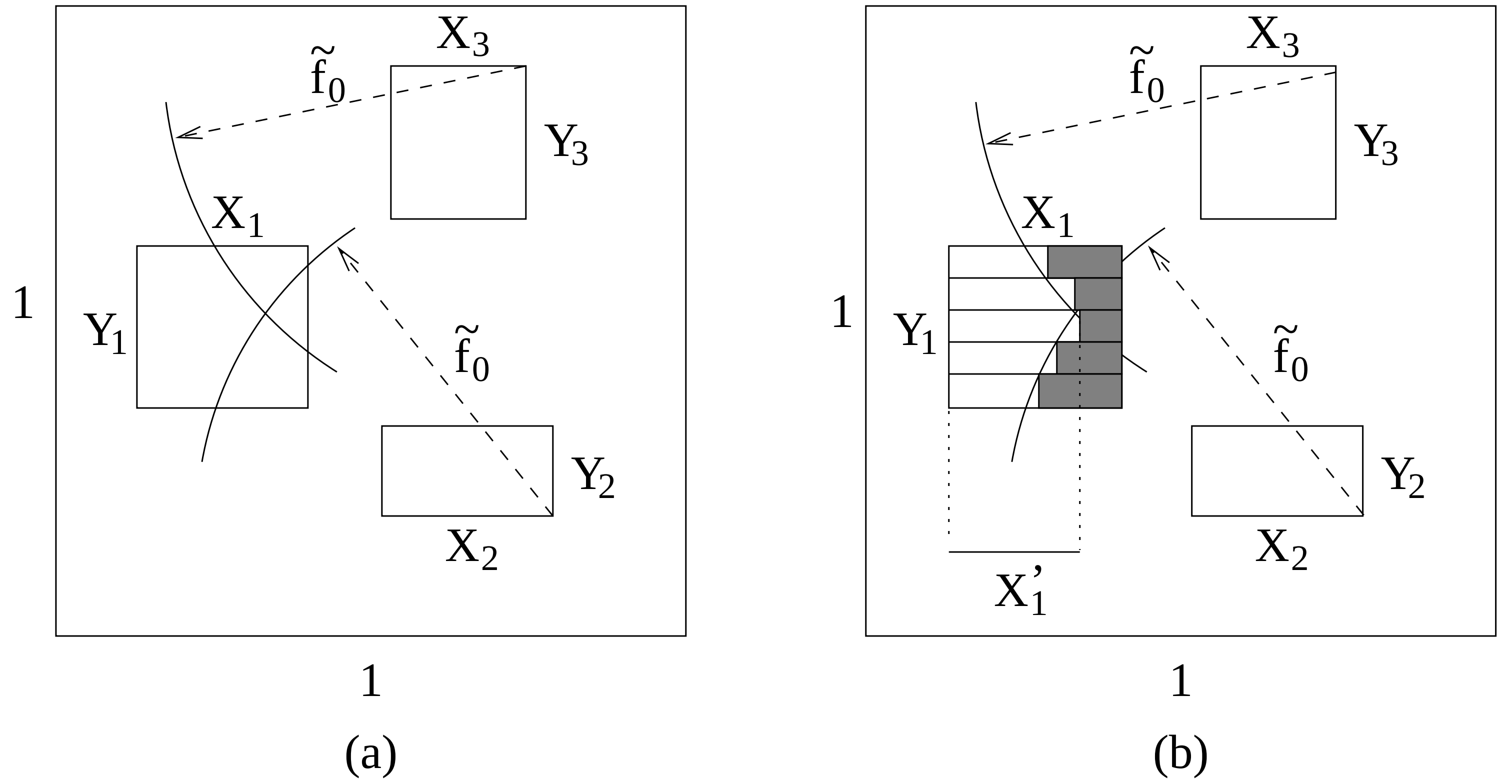
First assume that an $\tilde{f}_0$ lower bound for the optimum of the point arrangement problem is known.

Then divide the unit square into a number of s closed, non-overlapping regions (usually into rectangles), having a maximal diameter less than $\tilde{f}_0$.

Now for a solution having a function value greater than or equal to $\tilde{f}_0$, any such region (called ‘tile’) can contain at most one point of the solution.

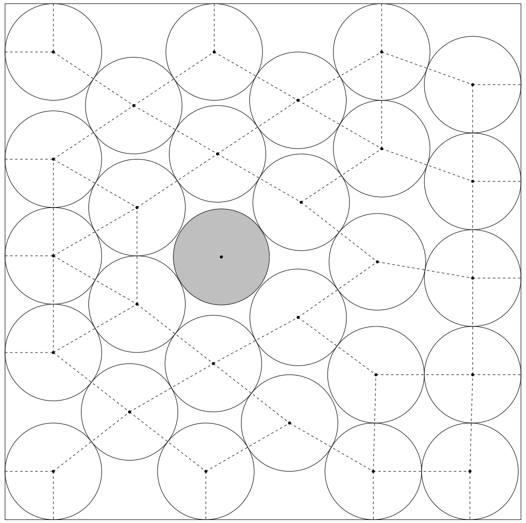
This fact enables us to choose n tiles from the total number of s tiles in all possible ways, and run the optimization method for every such tile combination.

The Active Area Method

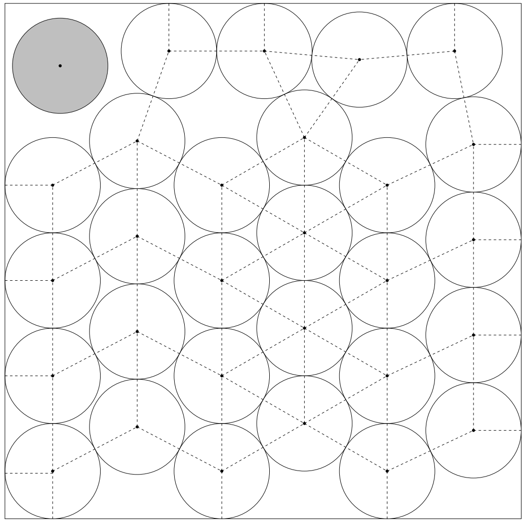


An illustration of the method of active areas with temporary one-directional splittings. The shaded rectangles could be deleted based on the known upper bound on the optimal radius length $\tilde{f}_0$.

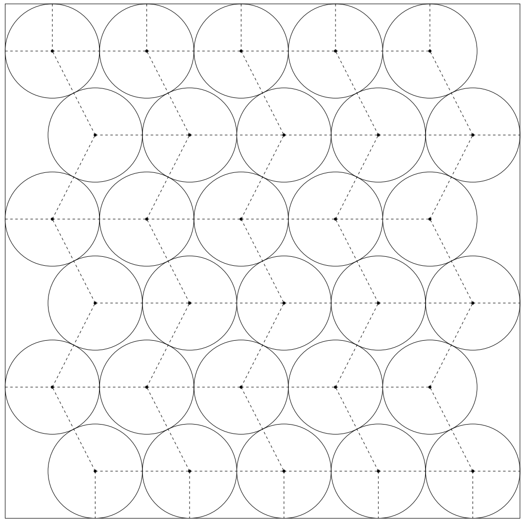
The Solutions of Circle Packing Problems for 28-30 Circles



n = 28



n = 29



n = 30

The shaded circles can be moved a bit keeping the optimality (i.e. the set of global minimizer points is of positive measure). The contact of two neighboring circles is indicated by connecting lines.

Details of the Solutions of the Circle Packing Problems

Hardware: PC, Pentium IV 1800 MHz processor, 1 GB RAM.

Software: Linux, GNU C/C++, C–XSC Toolbox, PROFIL/BIAS.

Obtained bounds on the radius values:

$F^*_{28} = [\underline{0.23053549364266}73, \underline{0.23053549364267}43], w \approx 7 \cdot 10^{-15}$,

$F^*_{29} = [\underline{0.2268829007442}089, \underline{0.2268829007442}240], w \approx 2 \cdot 10^{-14}$,

$F^*_{30} = [\underline{0.22450296453108}81, \underline{0.22450296453109}03], w \approx 2 \cdot 10^{-15}$.

Total running times: $\approx$ 53, 50, and 21 hours, respectively.

Ca. one million subintervals were necessary to store for the solutions.

The verified optimization technique could decrease the uncertainty in the place of the optimizer points by more than 711, 764, and 872 orders of magnitude, respectively.

The Authors of the Known Optimal Packings

Year	Authors	Results for n
1965	J. Schaer and A. Meir	$8, 9$
1970	B. L. Schwartz	6
1983	G. Wengerodt	16
1987	G. Wengerodt	14
1992	R. Peikert et al.	$10 - 20$
1999	K. J. Nurmela and P. R. J. Östergård	$7, 21 - 27$
2004	M. Cs. Markót	28
2005	M. Cs. Markót and T. Csendes	$29 - 30$

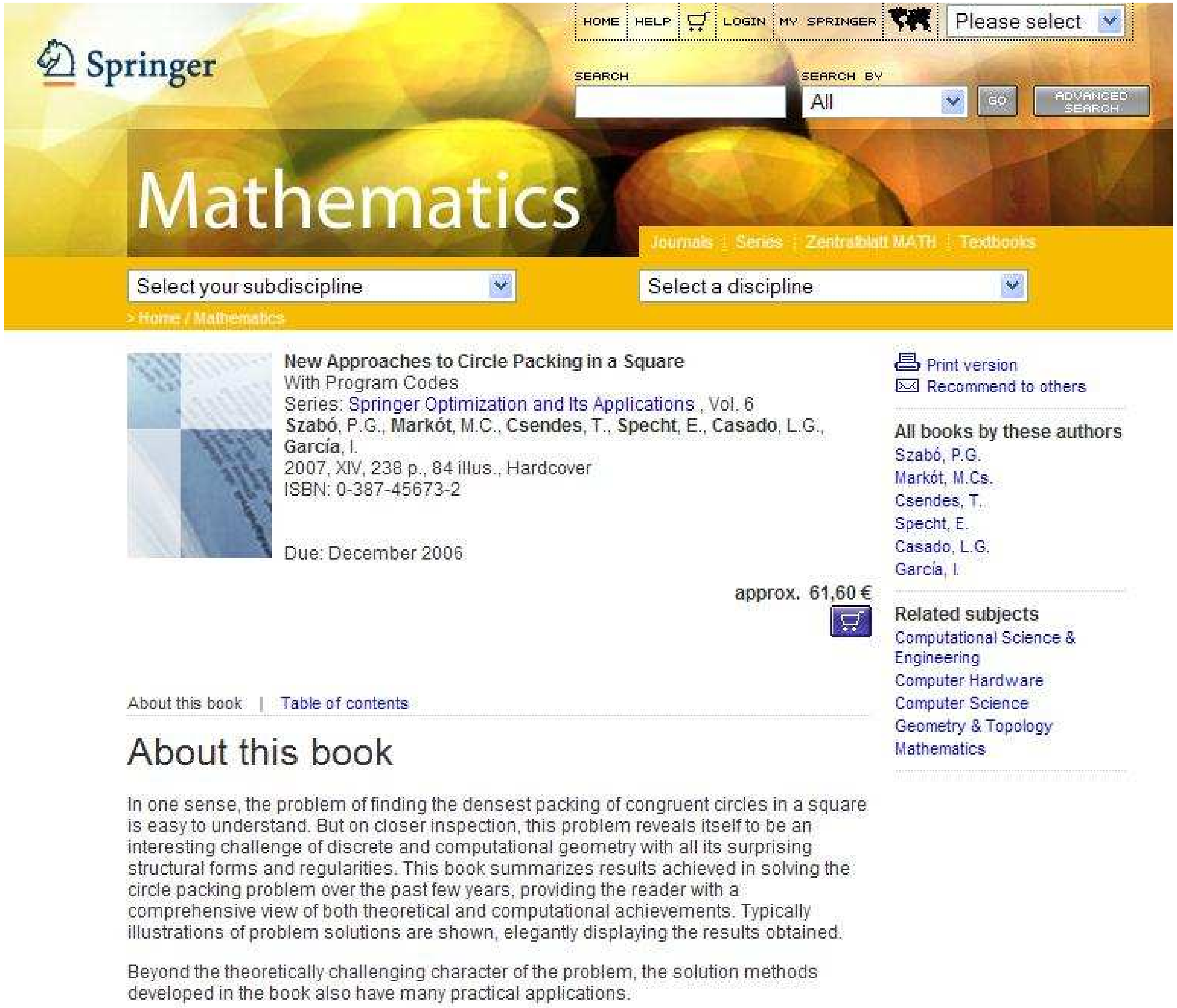
Publications on Circle Packing

Markót, M.Cs.: Optimal Packing of 28 Equal Circles in a Unit Square–the First Reliable Solution. Numerical Algorithms 37(2004) 253-261.

Markót, M.C. and T. Csendes: A new verified optimization technique for the ”packing circles in a unit square” problems. SIAM J. on Optimization 16(2005) 193-219.

Markót, M.Cs. and T. Csendes: A reliable area reduction technique for solving circle packing problems. Computing, 77(2006) 147-162.

Szabó, P.G., M.Cs. Markót, T. Csendes, E. Specht, L.G. Casado, and I. García: New Approaches to Circle Packing in a Square (With Program Codes), Springer, 2006, 250 pages + CD, in print.



New Approaches to Circle Packing in a Square
With Program Codes
Series: Springer Optimization and Its Applications , Vol. 6
Szabó, P.G., **Markót**, M.C., **Csendes**, T., **Specht**, E., **Casado**, L.G., **García**, I.
2007, XIV, 238 p., 84 illus., Hardcover
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approx. 61,60 €

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About this book

In one sense, the problem of finding the densest packing of congruent circles in a square is easy to understand. But on closer inspection, this problem reveals itself to be an interesting challenge of discrete and computational geometry with all its surprising structural forms and regularities. This book summarizes results achieved in solving the circle packing problem over the past few years, providing the reader with a comprehensive view of both theoretical and computational achievements. Typically illustrations of problem solutions are shown, elegantly displaying the results obtained.

Beyond the theoretically challenging character of the problem, the solution methods developed in the book also have many practical applications.

Chaos Verification for Hénon Mapping Iterations

Consider the Hénon transformation $\mathcal{H}(x, y) = (1 + y - px^2, qx)$ with the parameter values of $p = 1.4$ and $q = 0.3$. The task is to verify the following relations for all points of the region $Q_0 \cup Q_1$:

$$\mathcal{H}^7(Q_0 \cup Q_1) \subset \mathbb{R}^2 \setminus E,$$

$$\mathcal{H}^7(a \cup d) \subset O_2,$$

$$\mathcal{H}^7(b \cup c) \subset O_1,$$

where E, O_1, and O_2 are given sets, and a, b, c, d are the sides of the parallelograms Q_0 and Q_1.

The Hénon Mapping with the Related Sets

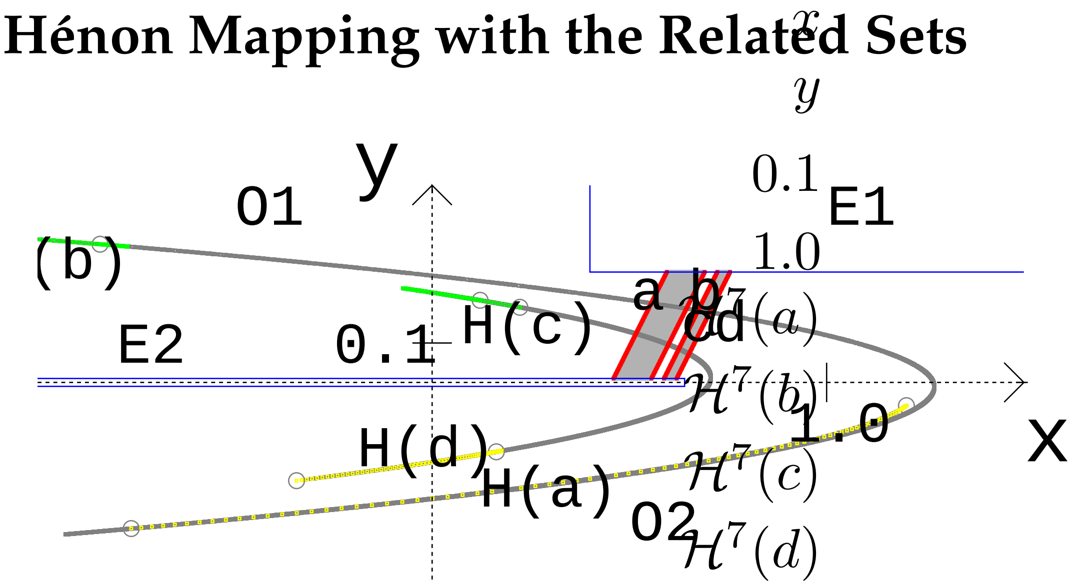


Illustration of the H^7 transformation for the classic Hénon parameters $A = 1.4$ and $B = 0.3$ together with the chaotic region of two parallelograms.

The Applied Checking Algorithm

The applied algorithm first encloses the sets Q_0 and Q_1 in a 2-dimensional interval, in the starting interval.

Then an adaptive subdivision technique generates such a tiling of the starting interval that either:

- For all subintervals all the required relations hold (in case they contain points of the respective sets Q_0 or Q_1), or
- it is shown that a small subinterval (of a user set size) exists that contradicts at least one of the relations.

Theoretical Results

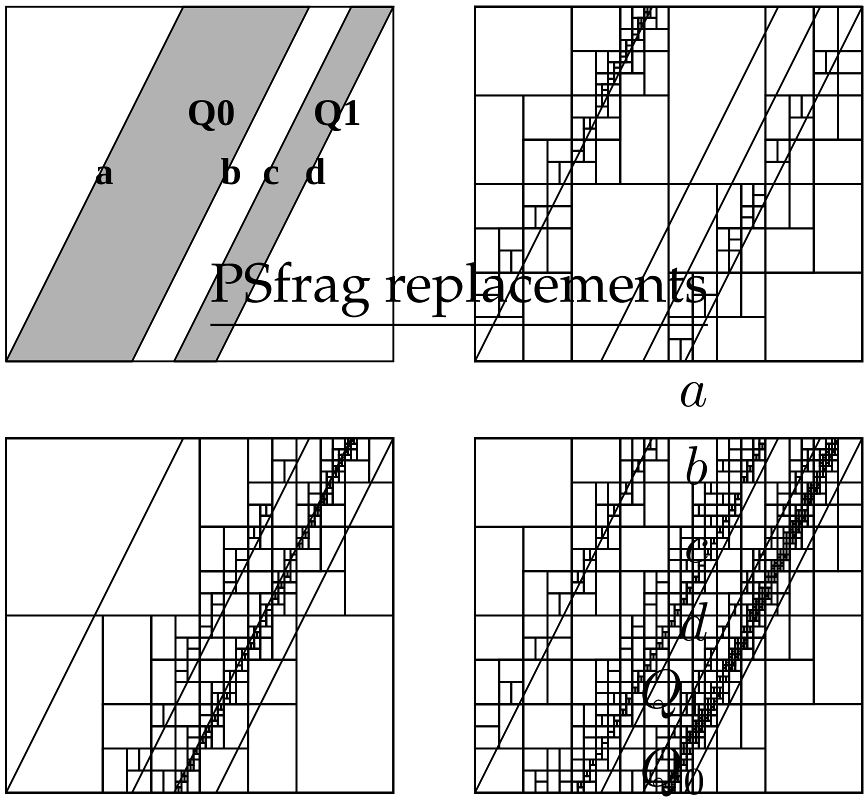
Theorem 1 *Assume that the underlying mapping* $\mathcal{T}$ *is given by an inclusion function* T *that has the zero convergence property,* $\varepsilon = 0$*, and* $\mathcal{T}(Q) \subset \mathcal{O}$ *holds. Then the checking algorithm concludes after a finite number of iteration steps that the condition of chaotic behaviour is fulfilled.*

Theorem 2 *Assume that the underlying mapping* $\mathcal{T}$ *is given by an inclusion function* T*,* $\varepsilon = 0$*, and there exist a point* $x \in Q$ *such that* $\mathcal{T}(x) \notin \mathcal{O}$*. Then the checking algorithm cannot conclude after a finite number of iteration steps whether the condition of chaotic behaviour is fulfilled.*

Numerical Results

```
 Starting interval:

[ 0.46000000000000001998, 0.75500000000000000445] [ 0.01000000000000000020,
0.28000000000000002665]

1. condition: successful proof! Number of function evaluations: 273 Largest
depth of the stack: 11

2. condition: successful proof! Number of function evaluations: 523 Largest
depth of the stack: 13

3. condition: successful proof! Number of function evaluations: 1613 Largest
depth of the stack: 14
```

Result Subintervals for the Chaos Verification



The parallelograms and the starting interval covered by the verified subintervals for which the given condition holds.

A Global Optimization Model to Locate Chaotic Places

Summing it up, we have considered the following bound constrained problem for the T inclusion function of the mapping $\mathcal{T}$:

$$\min_{x \in X} g(x), \tag{3}$$

where

$$g(x) = f(x) + p\left(\sum_{i=1}^{m} \max_{z \in T(I)} \inf_{y \in S_i} d(z, y)\right),$$

X is the n-dimensional interval of admissible values for the parameters x to be optimized, $f(x)$ is the original, nonnegative objective function, and $p(y) = y + C$ if y is positive, and $p(y) = 0$ otherwise. C is a positive constant, larger than $f(x)$ for all the feasible x points, m is the number of conditions to be fulfilled, and S_i is the aimed set for the i-th condition.

On the Defined Global Optimization Problem

Theorem 3 *For the defined bound constrained global optimization problem the following properties hold:*

1. In case a global optimization algorithm finds a point for which the objective function g *has a value below* C*, i.e. when each penalty term* $\max_{z\in T(I)} \inf_{y\in S_i} d(z, y)$ *is zero, then all the conditions of chaos are fulfilled by the found region represented by the corresponding optimal parameters* x *found. At the same time, the checking routine provides a guaranteed reliability computational proof of the respective subset relations.*

2. In case the given problem does not have a parameter set within the bounds of the parameters to be optimized such that the corresponding region would fulfill the criteria of chaos, then the optimization of $g(x)$ *cannot result in an approximate optimizer point with an objective function value below* C*.*

Some Results Achieved with the Introduced Global Optimization Model

- New chaotic places were located for other iterates of the Hénon mapping (e.g. for the more difficult case of the 5th iterate).
- It was proven that the region found for the 7th iterate does not ensure chaos for the 5th one.
- We have identified those A and B values that ensure the existence of a chaotic region in the classic two parallelograms.
- Chaotic behaviour was proved for exotic parameter Hénon mappings (e.g. for a negative mapping parameter q).

References on the Hénon-Chaos Problem

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An Improved Estimation for the Entropy of the Hénon Mapping

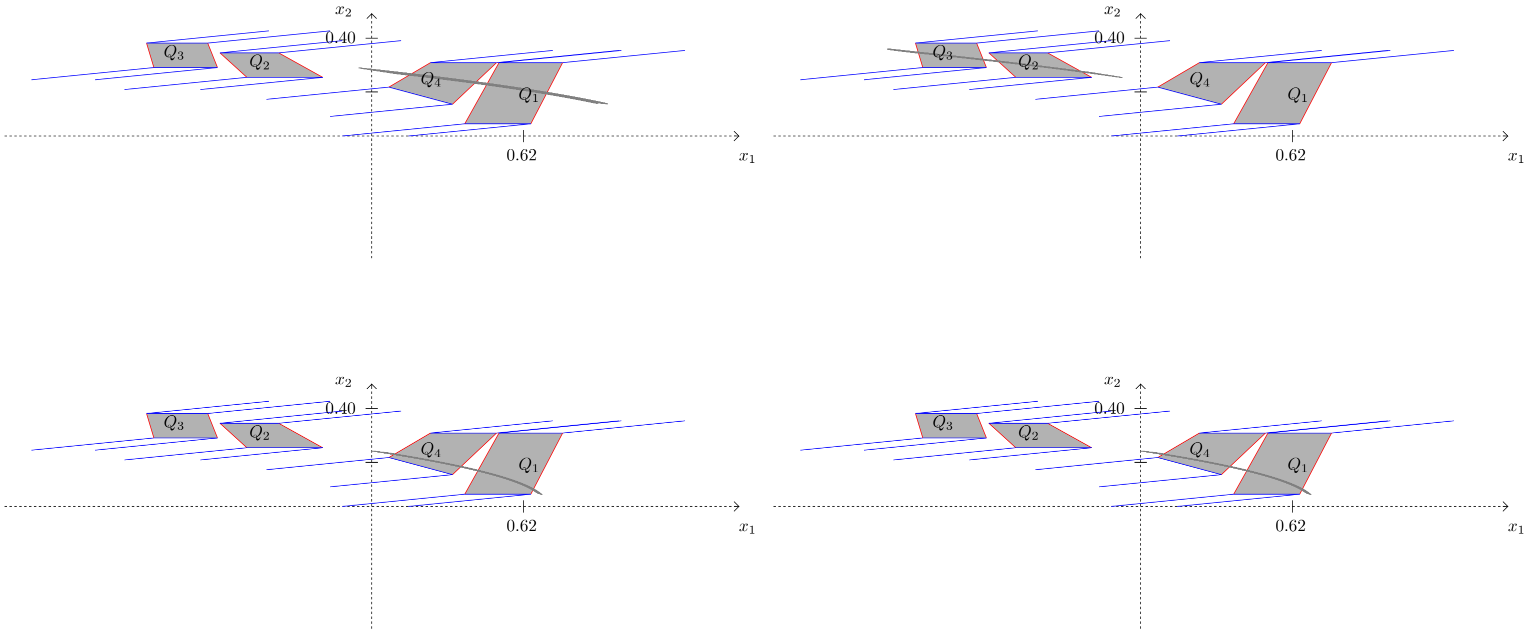
The entropy of a nonlinear mapping is defined as the maximal logarithm of the largest eigenvalue of possible covering matrices.

We tried the following covering matrix:

	Q_1	Q_2	Q_3	Q_4
Q_1	1			2
Q_2		2	2	
Q_3	2			2
Q_4		2	2	

The logarithm of the largest eigenvalue (1.479) of the corresponding matrix is 0.382. The predecessor of this covering has the entropy value of 0.338, the best known value is 0.430, while the conjectured maximal one is 0.465.

The Obtained Coverings for $\mathcal{H}^2(Q_1)$, $\mathcal{H}^2(Q_2)$, $\mathcal{H}^2(Q_3)$, and $\mathcal{H}^2(Q_4)$, Respectively



Ongoing Investigations

- Providing a computer aided proof for Wright's conjecture on a delayed differential equation
- Proving that the forced damped pendulum is chaotic
- Construction of a control force function that makes the upper fixpoint of a pendulum stable
- Validation and improvement of the best known entropy value for the Hénon mapping
- Providing a complete characterization of the Hénon mapping iterations regarding chaotic behaviour

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