Relato do Processo no USPTO da Patente: "Hyperbolic Smoothing Clustering and Minimum Distance Methods"

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Sequência da Apresentação

1 – Prolegômenos:

Penalização, Lagrangeano e Suavização Hiperbólica

2 – Suavização do Modelo Hidrológico SMAP

3 - Fundamental Smoothing Procedures

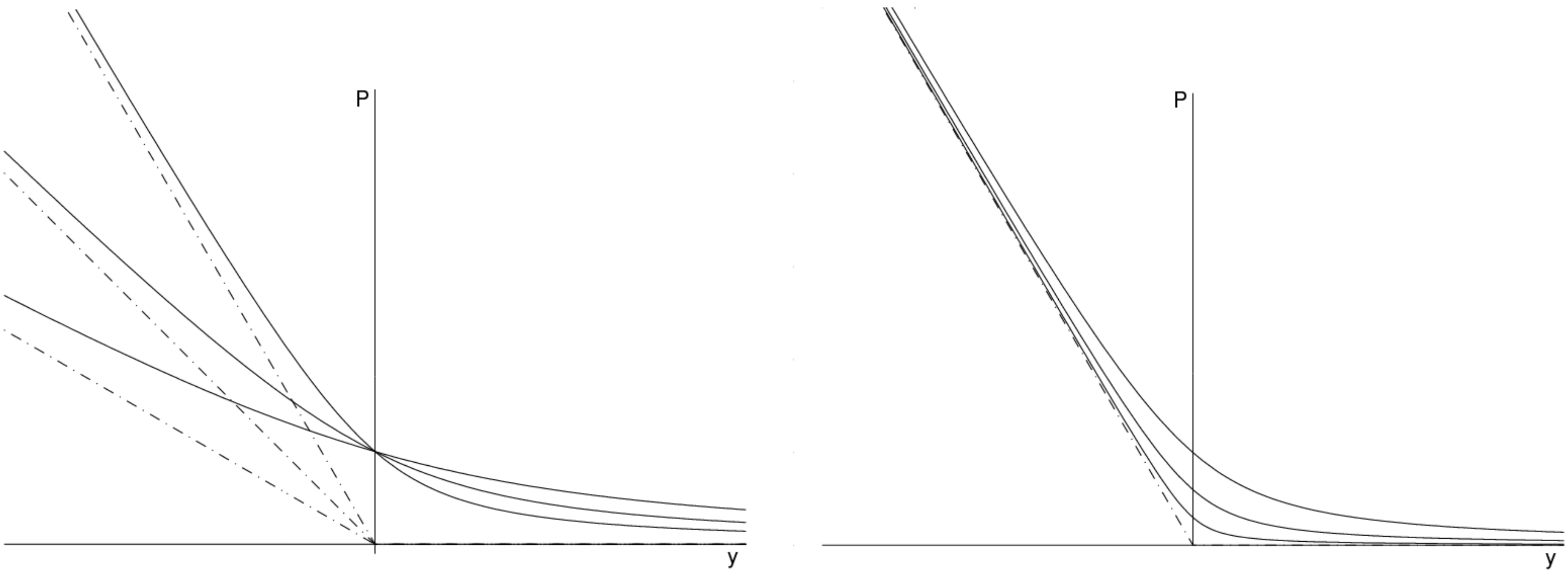
4 – Suavização de 3 Tradicionais Problemas Otimização

Covering, Clustering and Fermat-Weber Problems

5 – Tramitação da Patente no USPTO

6 – Acervo de Módulos Prontos

Origem: Penalização Hiperbólica Tese de Mestrado: 1979 a 1982



Penalização Hiperbólica

Hyperbolic Penalty

Methods of Penalty

$$
\begin{aligned}
&\text{minimize} \quad f(x) \\
&s.t. \quad h_i(x) = 0, \quad i \in I = \{1, \cdots, p\} \\
&\qquad\;\; g_j(x) \le 0, \quad j \in J = \{1, \cdots, p\} \\
&\qquad\;\; x \in \Re^n
\end{aligned}
$$

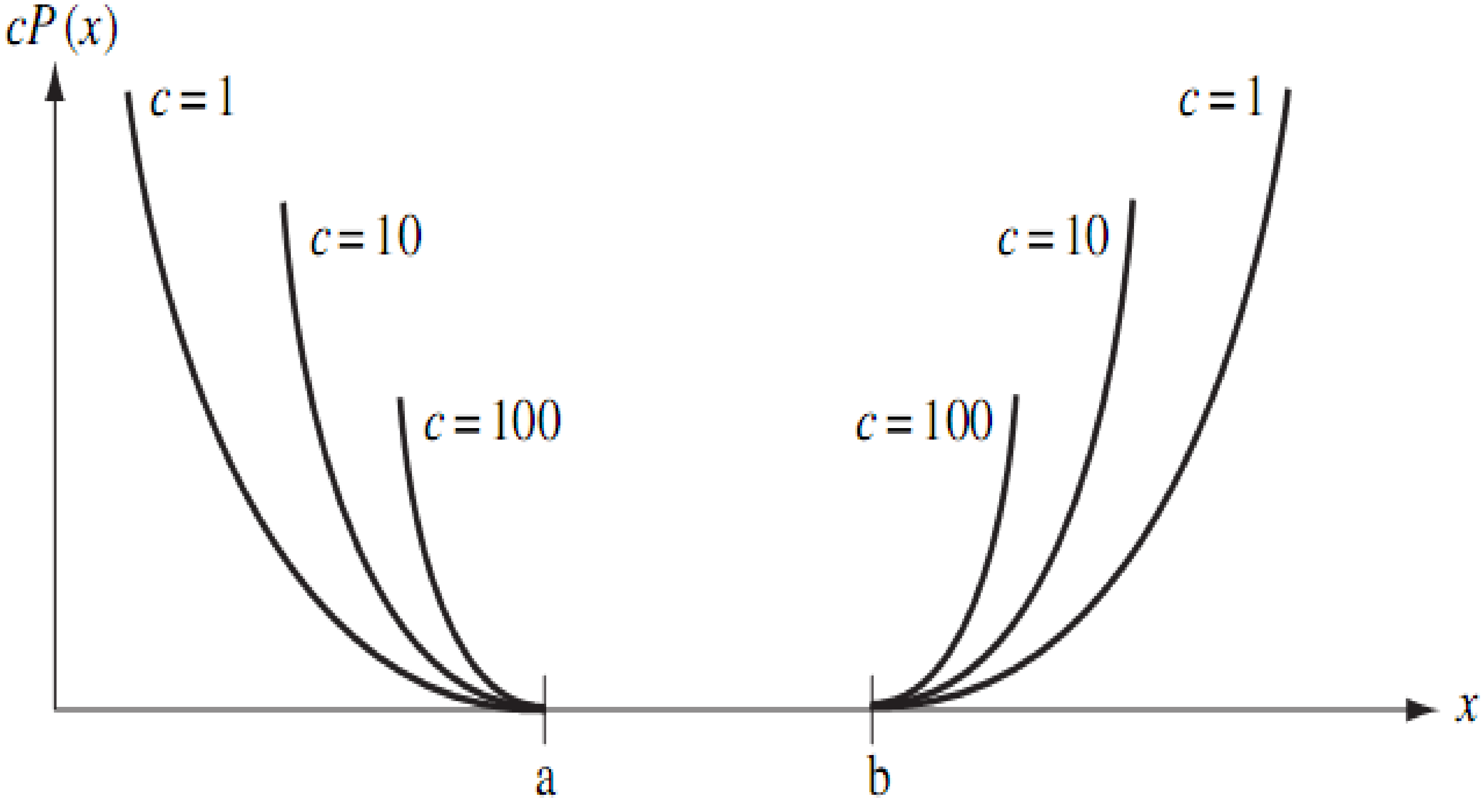
Penalty Methods

- Idea

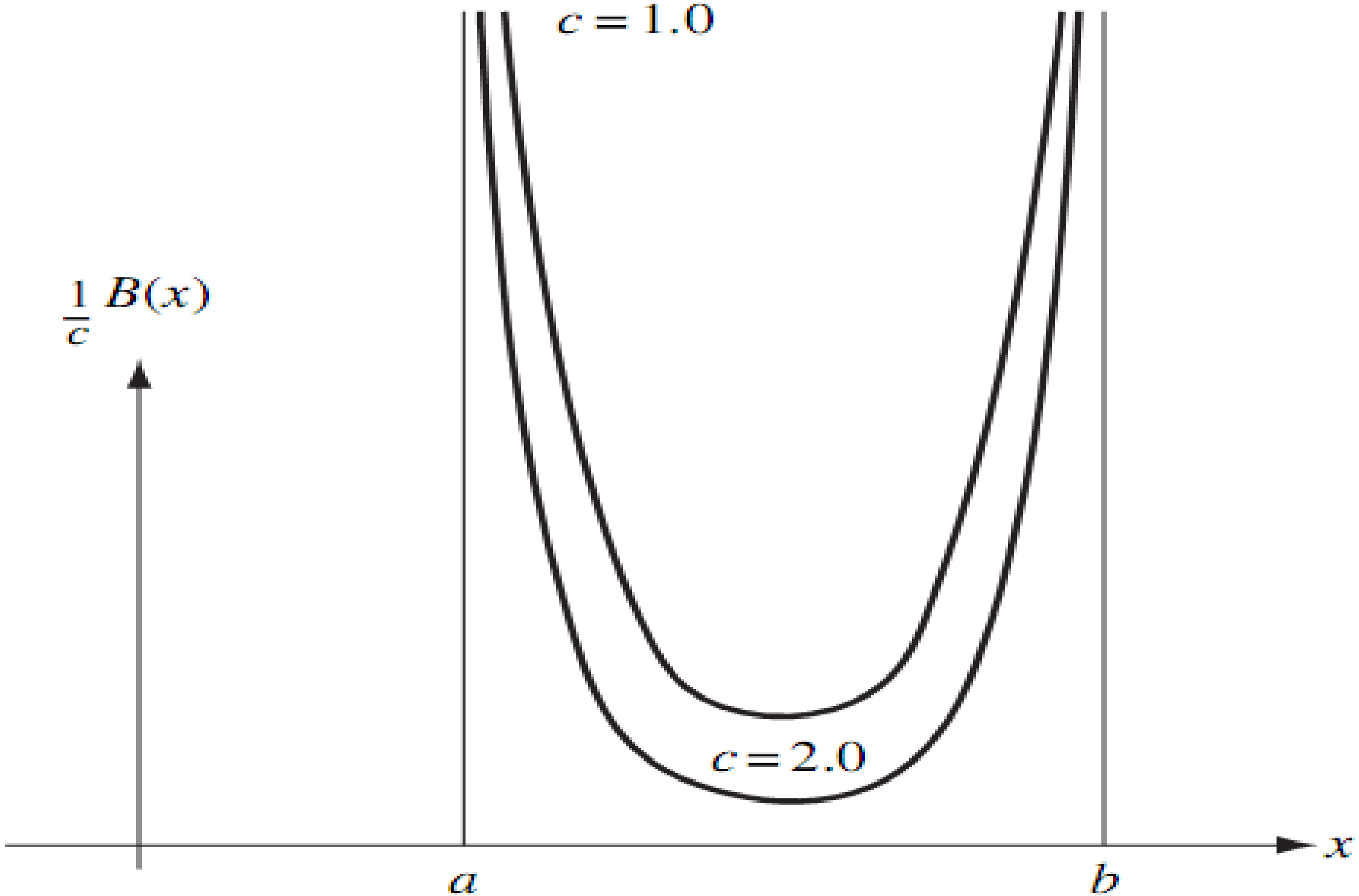
$$\underset{x \in \Re^n}{\text{minimize}} \quad F(x) = f(x) + P\left[g(x), h(x)\right]$$

- Methods penalty
  - outside penalty
  - inside penalty
- Non-parametric
- Exact
- Lagrangean

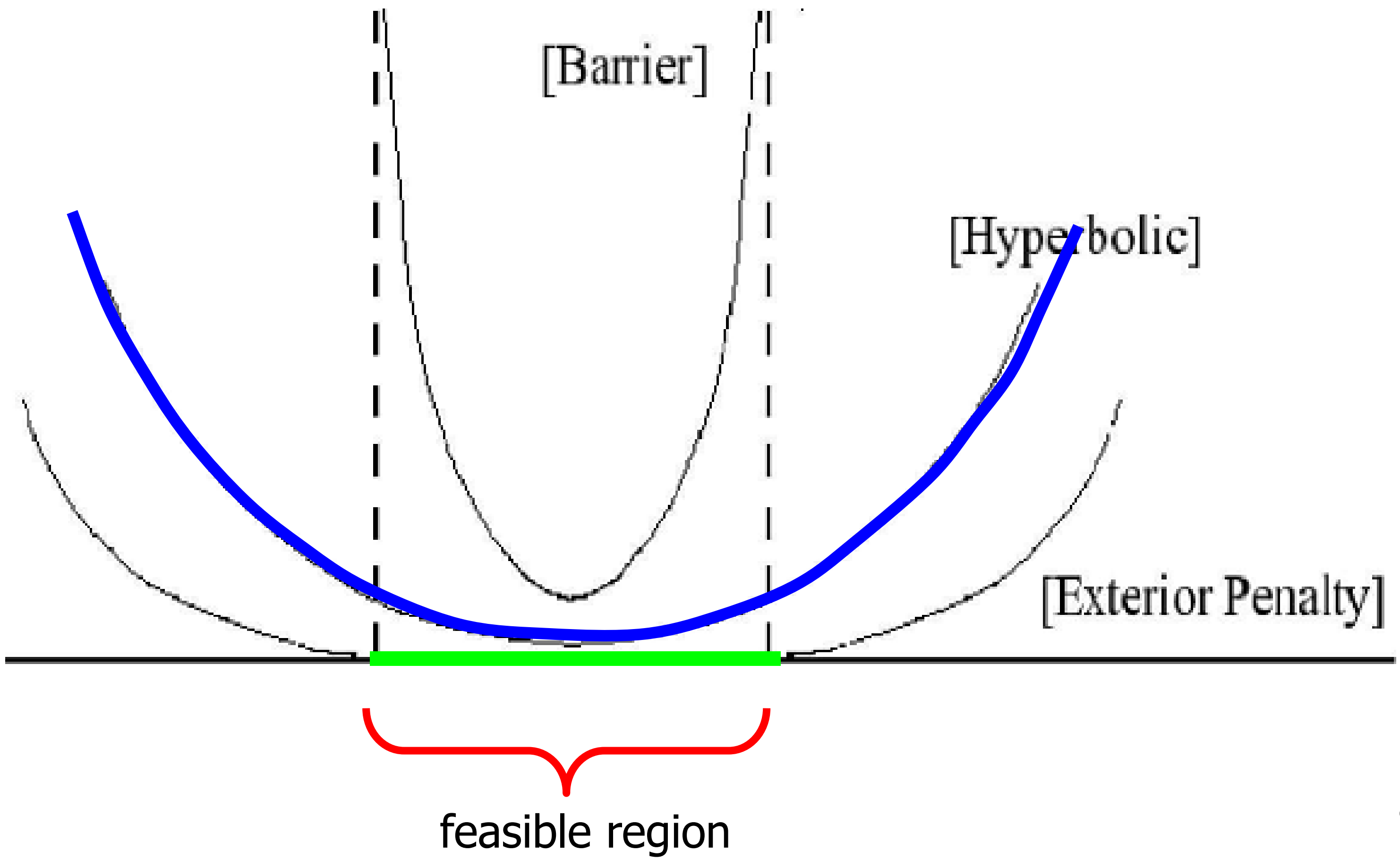
Exterior Penalty



Interior Penalty



First idea of Xavier Penalty (1977)



Hyperbolic Penalty Method

The penalty method adopts the penalty function

$$P(y,\alpha,\tau) = -(1/2\tan\alpha)y + \sqrt{(1/2\tan\alpha)^2 y^2 + \tau^2}$$

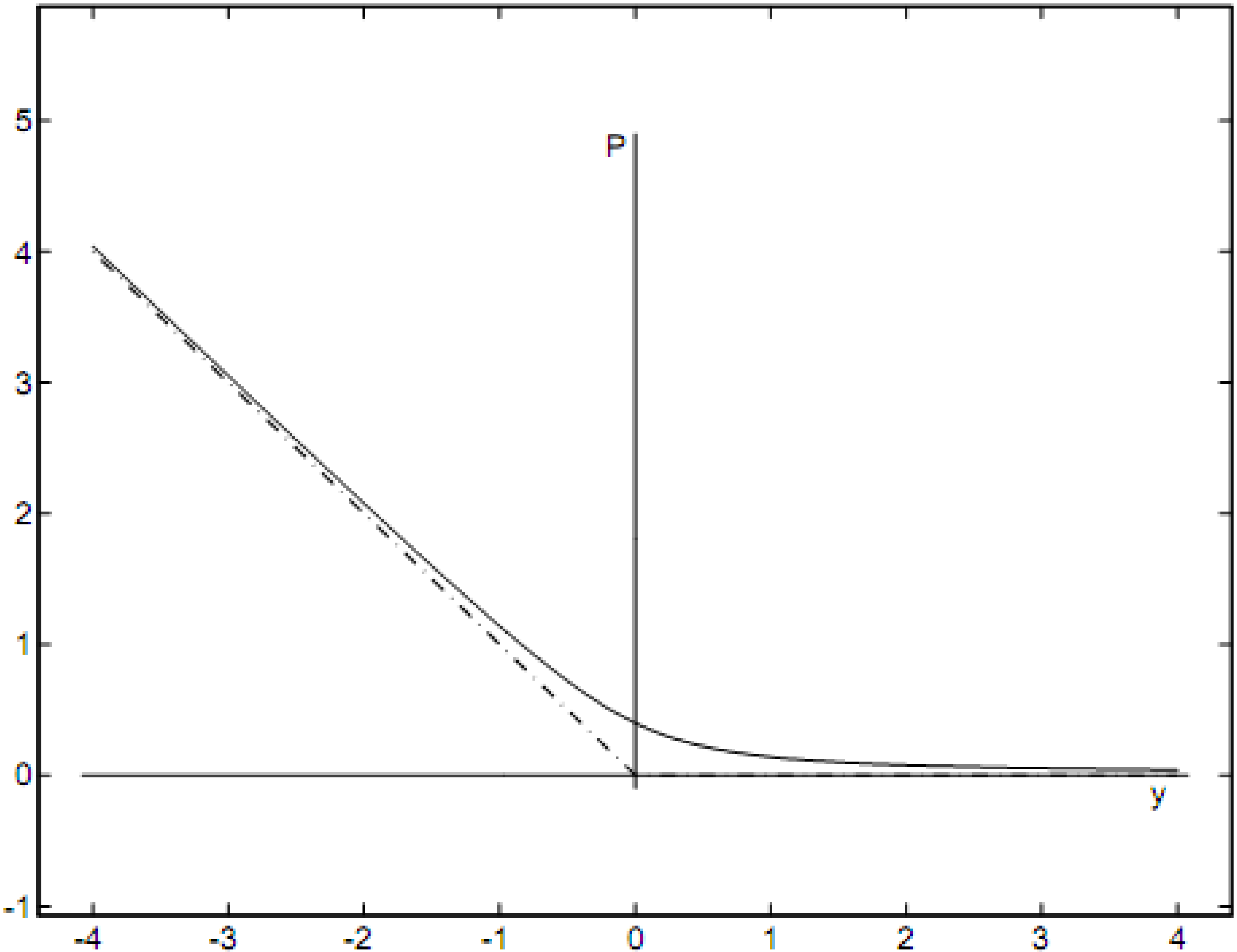
where $\alpha \in [0, \pi/2)$ and $\tau \geq 0$.

Alternatively the hyperbolic penalty function may be put in the more convenient form:

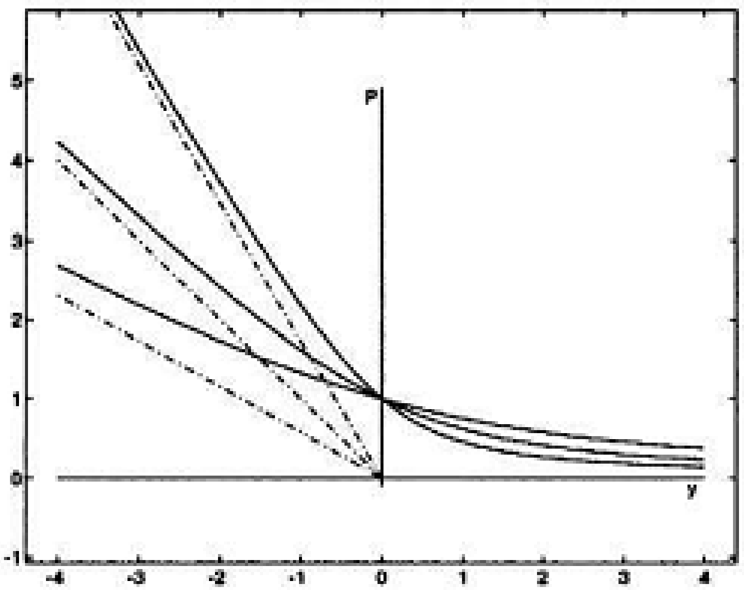
$$P(y,\lambda,\tau) = -\lambda y + \sqrt{\lambda^2 y^2 + \tau^2}$$

where $\lambda \geq 0$ and $\tau \geq 0$.

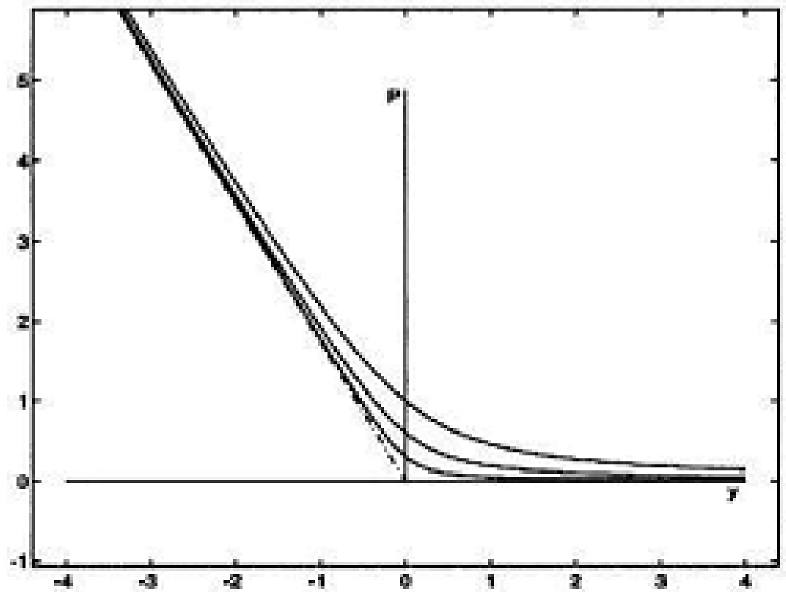
Hyperbolic Penalty Function



Hyperbolic Penalty Algorithm

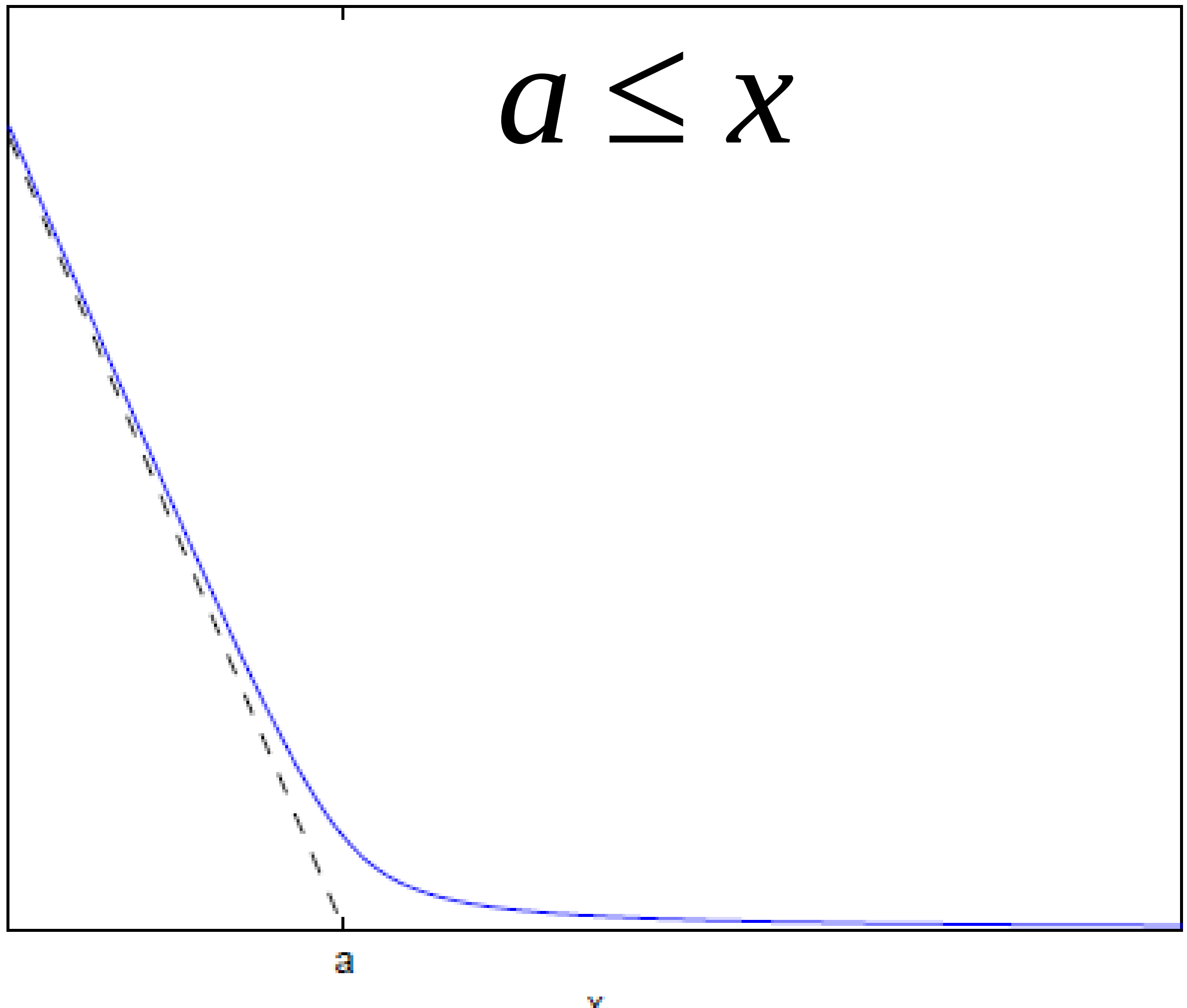


Phase 1

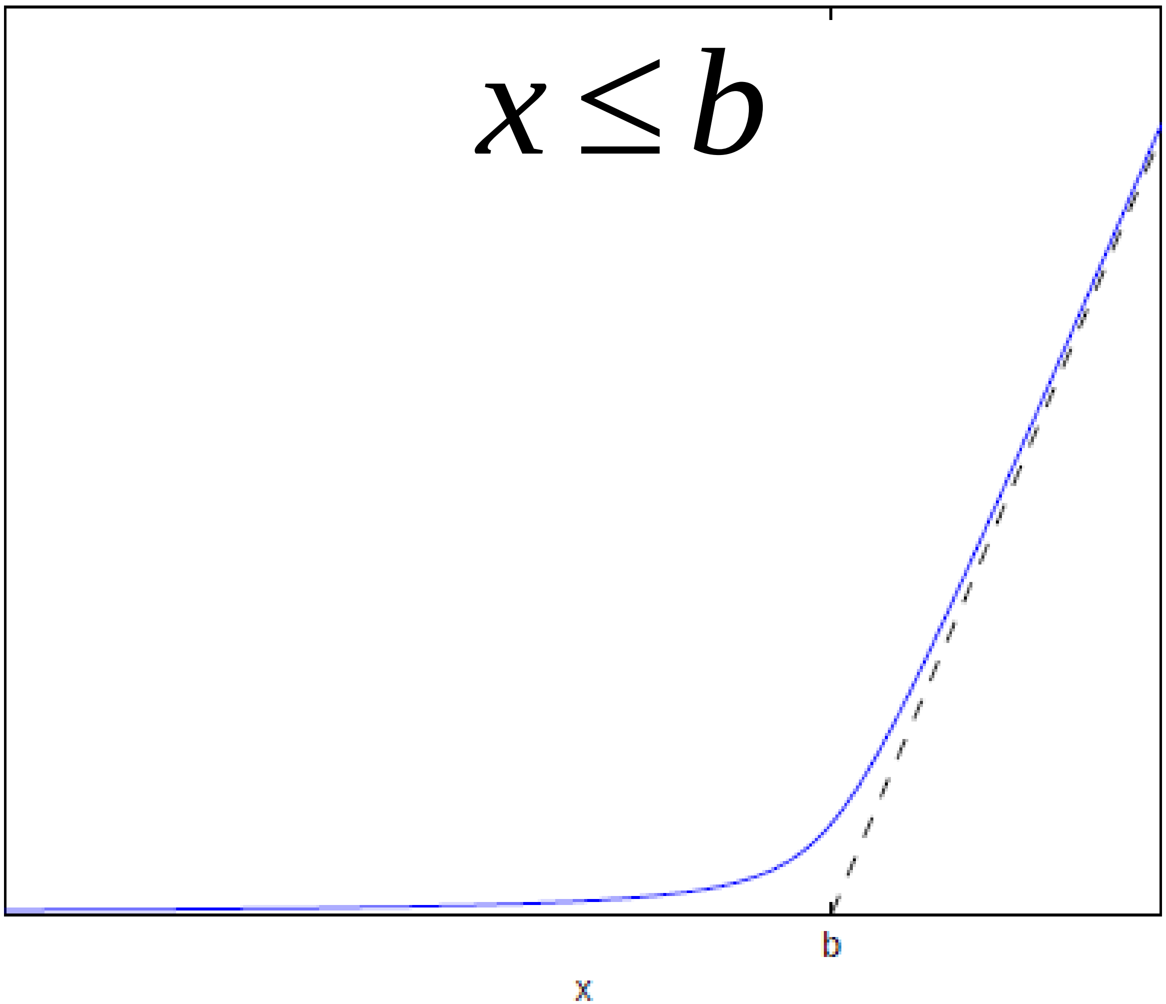


Phase 2

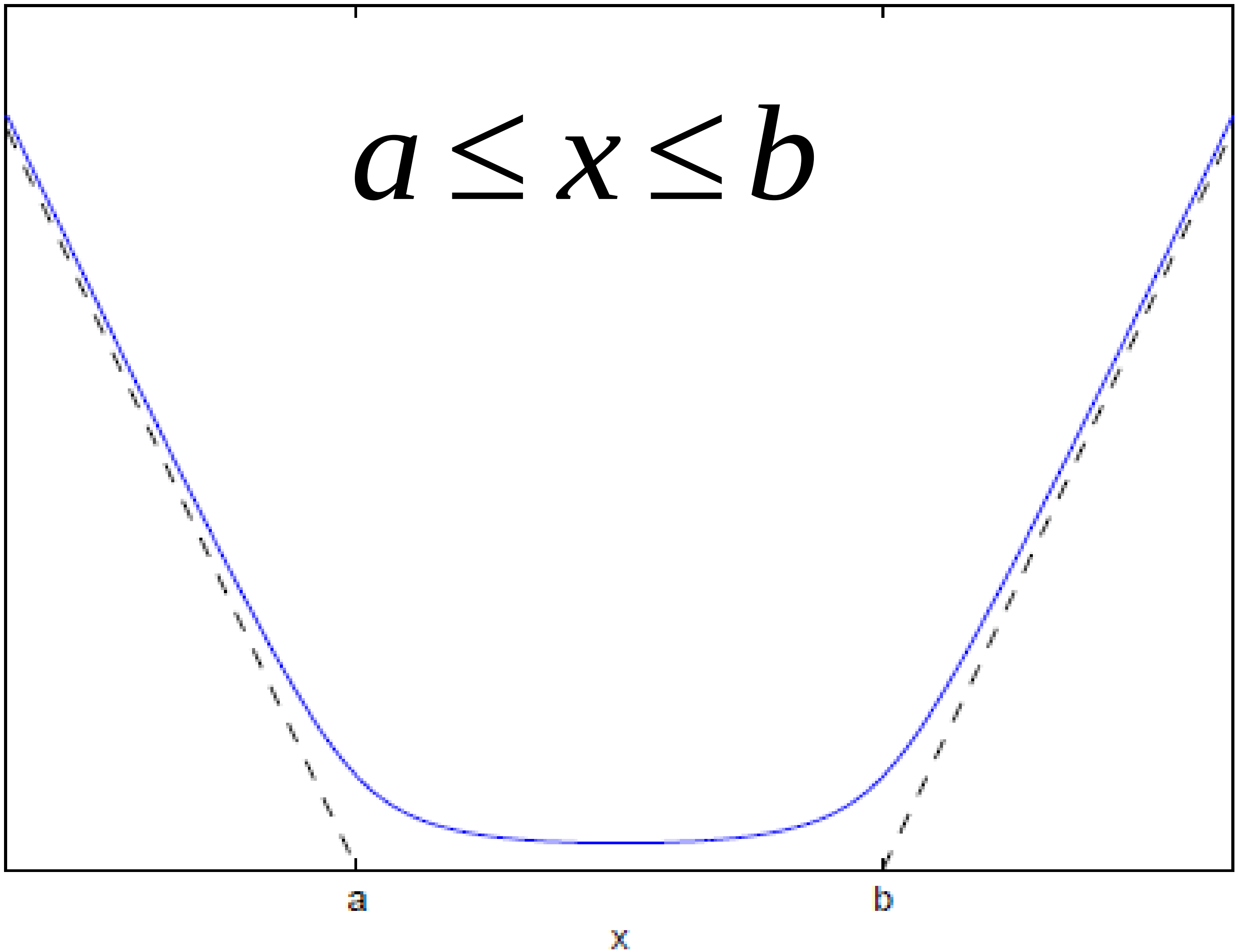
Hyperbolic penalty of the constraint $a \leq x$



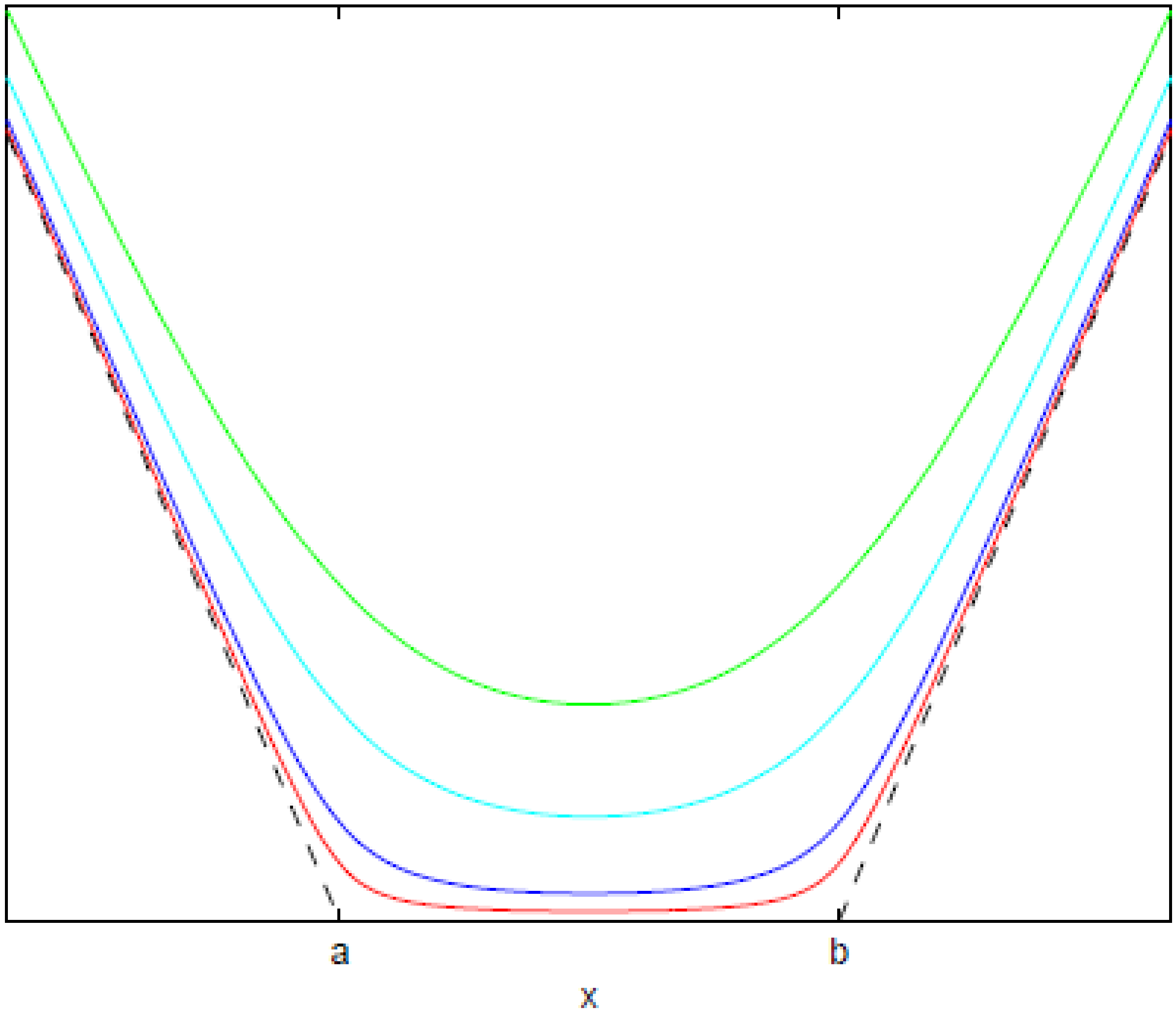
Hyperbolic penalty of the constraint $x \le b$



Pipeline effect



Sequence of pipelines



Hyperbolic Lagrangean

Dual Conections of the Hyperbolic Penalty

- Primal Problem

The general non-linear programming problem subject to inequality constraints is defined by:

$$\begin{array}{lll} \text{Minimize} & f(x) & \\ \text{such that:} & g_i(x) \geq 0, & i = 1, \ldots, m, \end{array}$$

where $f : \mathfrak{R}^n \longrightarrow \mathfrak{R}$ and $g_i : \mathfrak{R}^n \longrightarrow \mathfrak{R}$.

Dual Conections of the Hyperbolic Penalty

- KKT Necessary Conditions

x^*: a regular minimum point $\Rightarrow \exists\, \lambda^*$

$$\nabla f(x^*) - \sum_{i=1}^{m} \lambda_i^* \nabla g_i(x^*) = 0$$

$$\lambda_i^* \geq 0,\ \ i = 1, \cdots, m$$

$$\lambda_i^* g_i(x^*) = 0,\ \ i = 1, \cdots, m.$$

Dual Conections of the Hyperbolic Penalty

- Penalized Objective Function

$$\text{Minimize} \quad f(x) + \sum_{i=1}^{m} P(g_i(x), \lambda_i, \tau_i)$$

$$P(g_i(x), \lambda_i, \tau_i) = \quad \lambda_i g_i(x) + \sqrt{\lambda_i^2 g_i^2(x) + \tau_i^2}.$$

- $\bar{x}$: minimum point of the penalized objective function

$$\nabla f(\bar{x}) \quad \sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{x}) + \sum_{i=1}^{m} \frac{(\lambda_i^2 g_i(\bar{x}))}{(\lambda_i^2 g_i^2(\bar{x}) + \tau_i^2)^{1/2}} \nabla g_i(\bar{x}) = 0.$$

Dual Conections of the Hyperbolic Penalty

- Lagrange Multiples Estimates: $\widehat{\lambda}_i$, i=1,..., m

$$\nabla f(\bar{x}) \quad - \quad \sum_{i=1}^{m} \lambda_i \left[1 - \frac{\lambda_i g_i(\bar{x})}{\sqrt{\lambda_i^2 g_i^2(\bar{x}) + \tau_i^2}} \right] \nabla g_i(\bar{x}) \; = \; 0$$

$$\hat{\lambda}_i \quad = \quad \lambda_i \left[1 - \frac{\lambda_i g_i(\bar{x})}{\sqrt{\lambda_i^2 g_i^2(\bar{x}) + \tau_i^2}} \right].$$

- KKT Properties of $\widehat{\lambda}_i$

$$\nabla f(\bar{x}) - \sum_{i=1}^{m} \hat{\lambda}_i \nabla g_i(\bar{x}) = 0 \quad \text{OK!} \qquad\qquad \hat{\lambda}_i \geq 0 \quad \text{OK!}$$

But, the conditions: $\hat{\lambda}_i g_i(\bar{x}) = 0, i = 1, \cdots, m,$ are not satisfied!

Exact Penalty

- Simplified Hypothesis
  - The original problem is strictly convex;
  - x* is a regular minimum point

If $\lambda_i = \lambda_i^*$ then x^* is the minimum point of the penalized objctive function for ay values of parameters τ_i, i=1, ..., m.

$$\nabla f(\bar{x}) - \sum_{i=1}^{m} \lambda_i^* \left[1 - \frac{\lambda_i^* g_i(\bar{x})}{\sqrt{(\lambda_i^* g_i(\bar{x}))^2 + \tau_i^2}} \right] \nabla g_i(\bar{x}) = 0.$$

By taking $\bar{x} = x^*$, this equation is satisfied.

Hyperbolic Lagrangean

$$maximize_{\lambda \geq 0} \quad \phi(\lambda)$$

$$\phi(\lambda) = \quad minimum_x \quad \left[f(x) + \sum_{i=1}^{m} P(g_i(x), \lambda_i, \tau_i) \right]$$

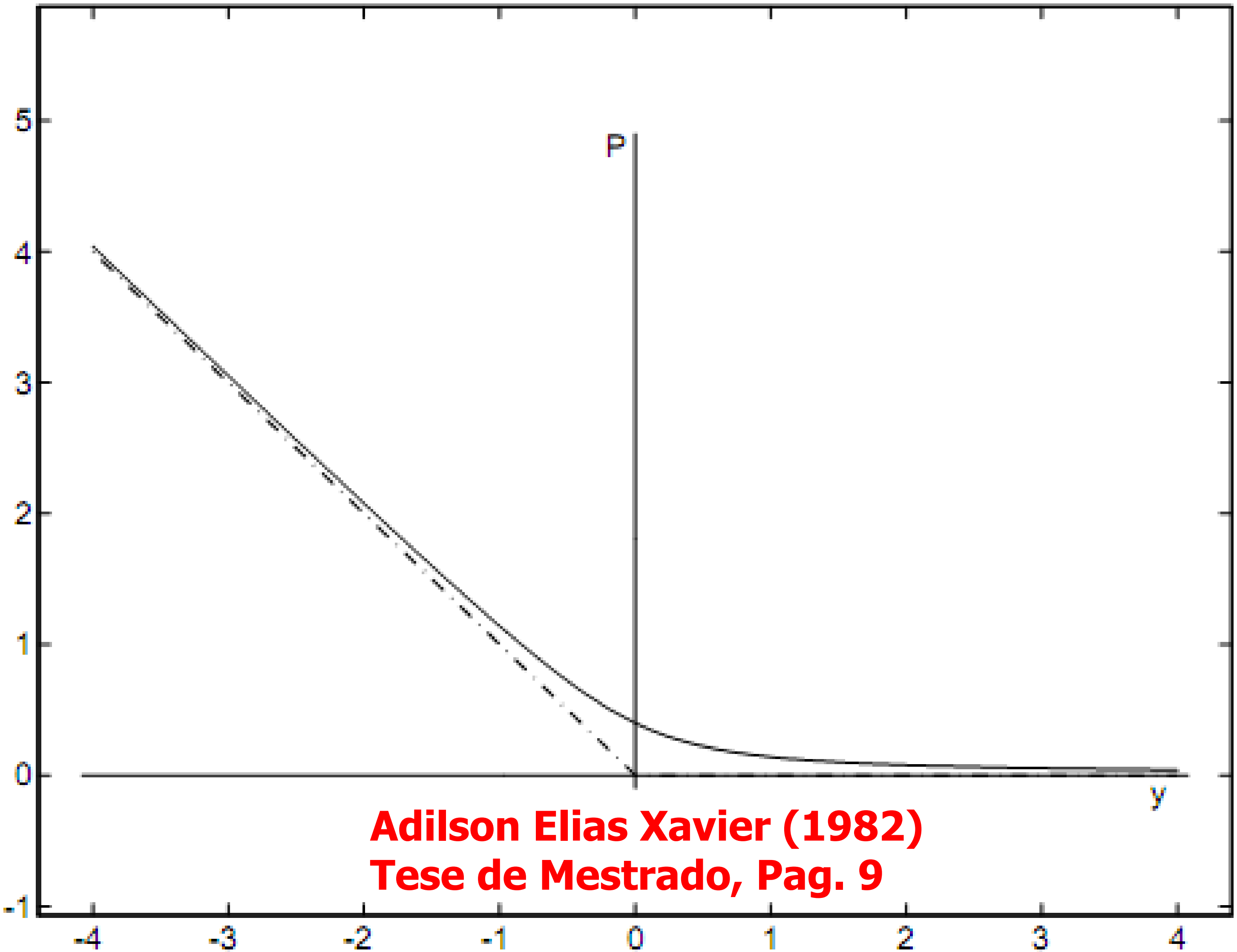
where

$$P(g_i(x), \lambda_i, \tau_i) = -\lambda_i g_i(x) + \sqrt{(\lambda_i g_i(x))^2 + \tau_i^2}.$$

Adequate hypothesis: REGULARITY and CONVEXITY!

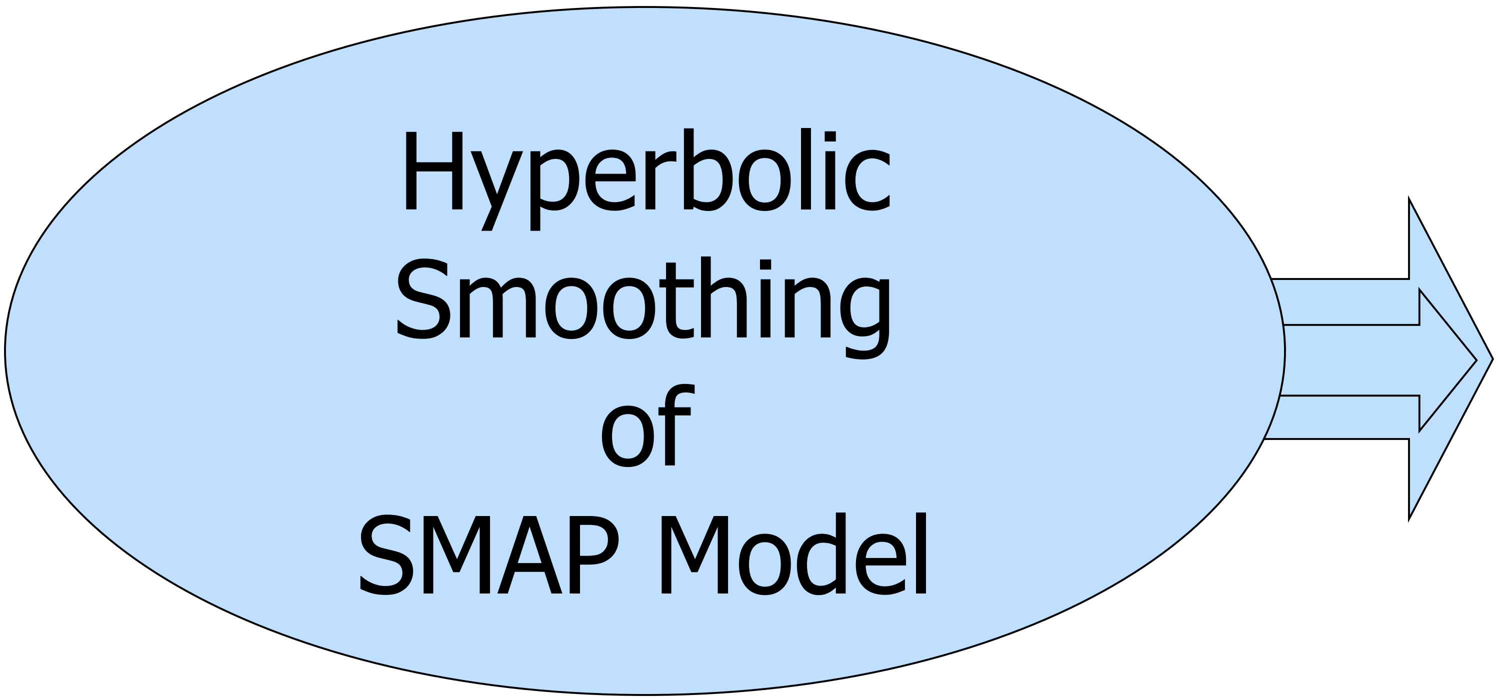
Hyperbolic Smoothing

Hyperbolic Penalty Function = Hyperbolic Smoothing of Zangwill Penalty

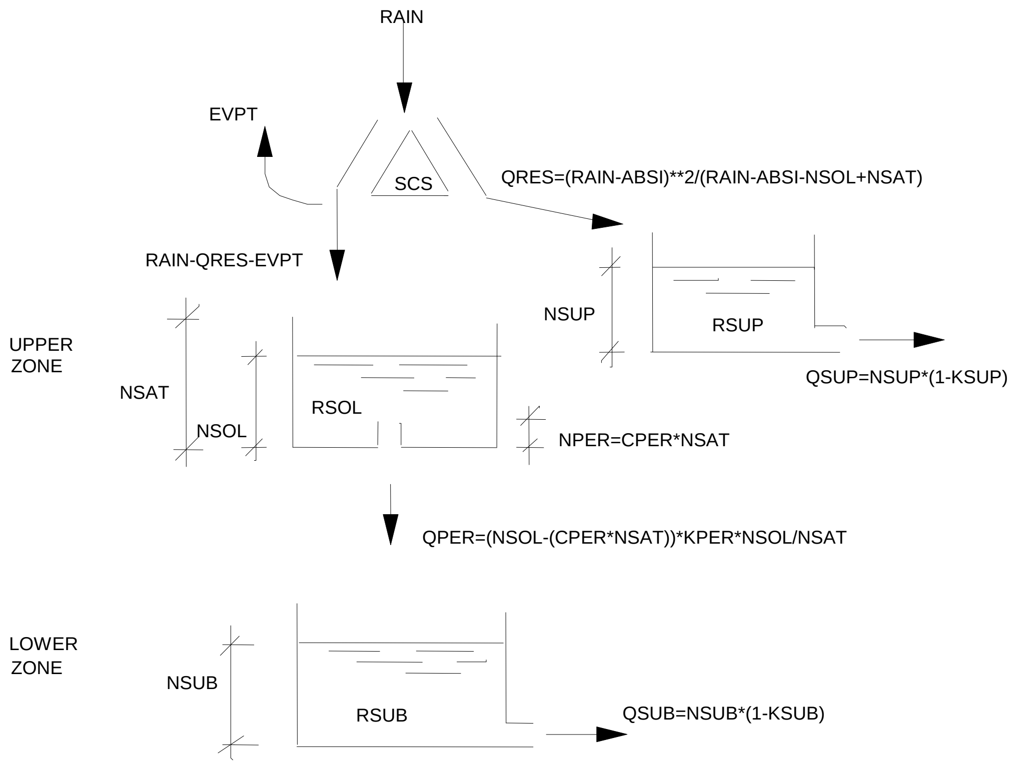


Adilson Elias Xavier (1982)
Tese de Mestrado, Pag. 9

SMAP:
hydrological run-on run-off model

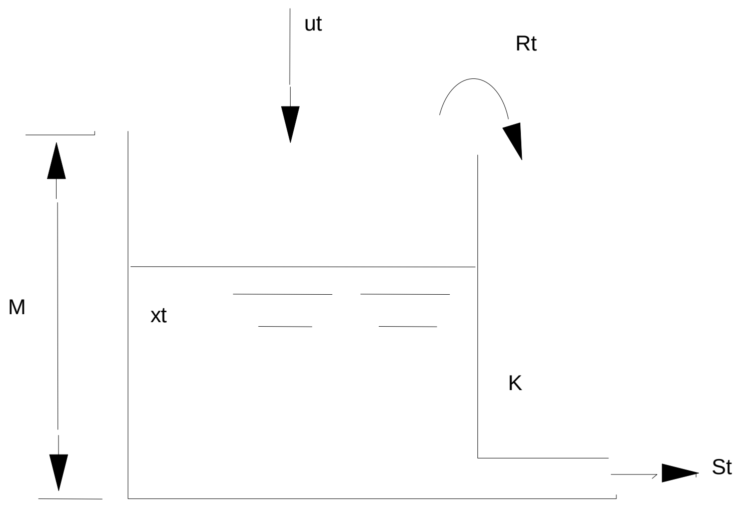


Scheme of the SMAP model



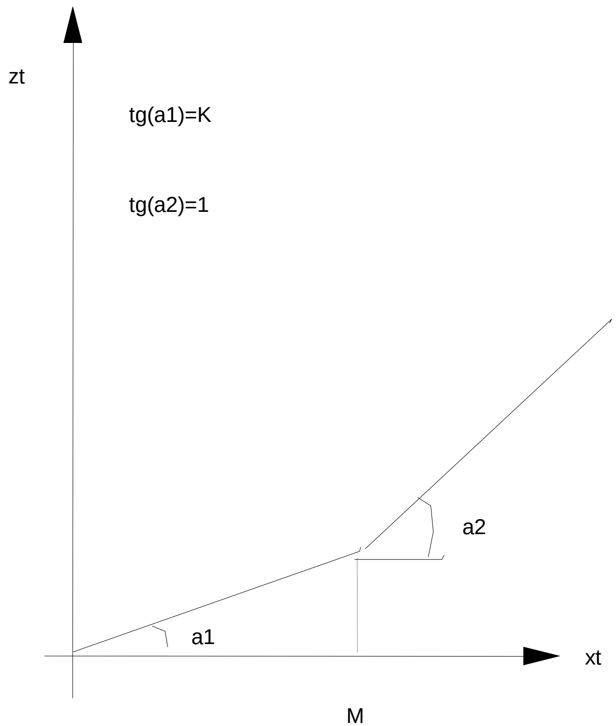
Scheme of the SMAP model

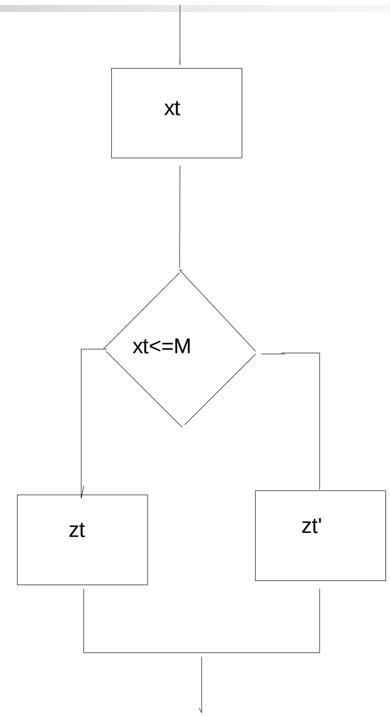
Superior Reservoir of SMAP Model



$$x_t = x_{t-1} + u_t$$
$$R_t = 0, \qquad if\ x_t \le M$$
$$R_t = x_t - M, \qquad if\ x_t > M$$
$$S_t = K(x_t - R_t)$$
$$z_t = S_t + R_t$$
$$z'_t = S_t, \qquad when \qquad R_t = 0$$

Original Flowchart of calculations: Superior Reservoir





SMOOTHING TECHNIQUE USED

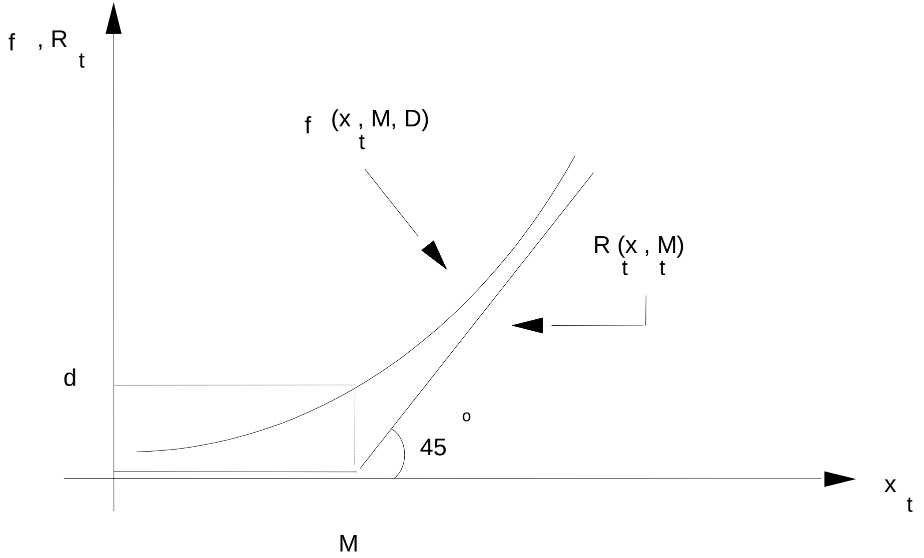


Figure 4. Functions ϕ and R in terms of x_t

Flowchart of smoothed calculations: Superior Reservoir

$$x_t = x_{t-1} + u_t$$

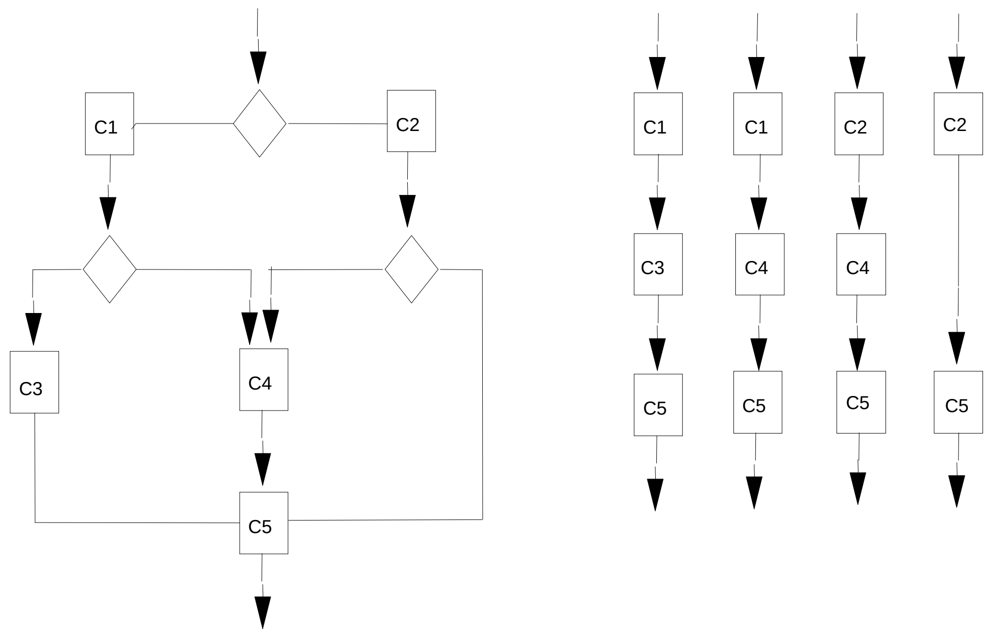
$$R_t = \phi(x_t, M, d)$$

$$S_t = K(x_t - R_t)$$

$$z_t = R_t + S_t$$

Representation of the flowchart of the smoothed model

Paths of Original SMAP MODEL



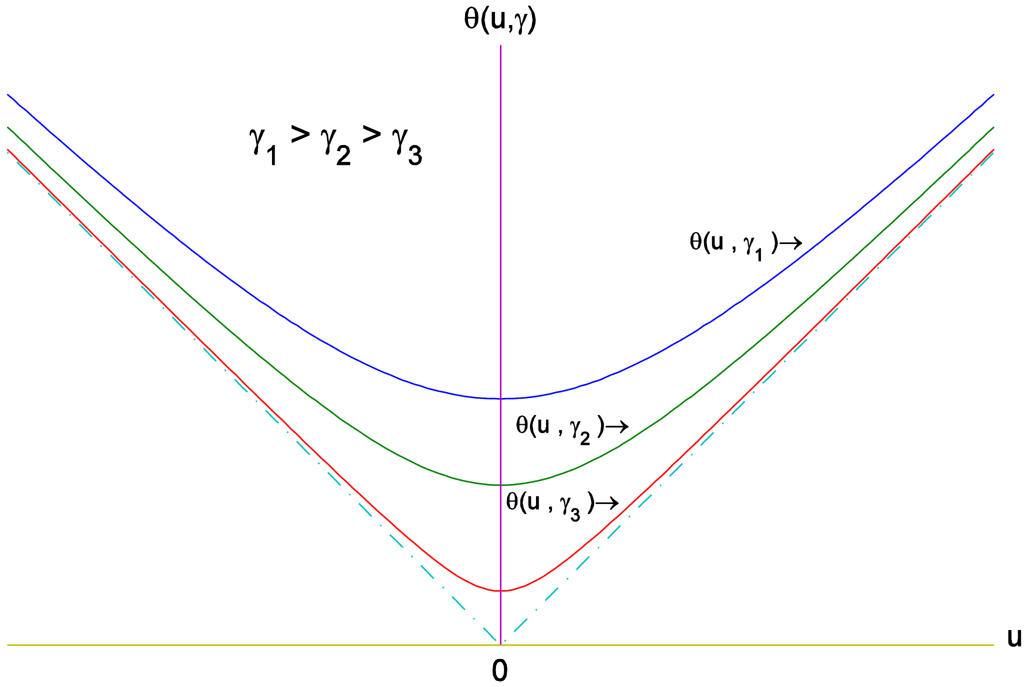
Flowchart of 3 "IFs" and **the 4 operational paths**

After Hyperbolic Smoothing: Only One Path

Fundamental Smoothing Procedures

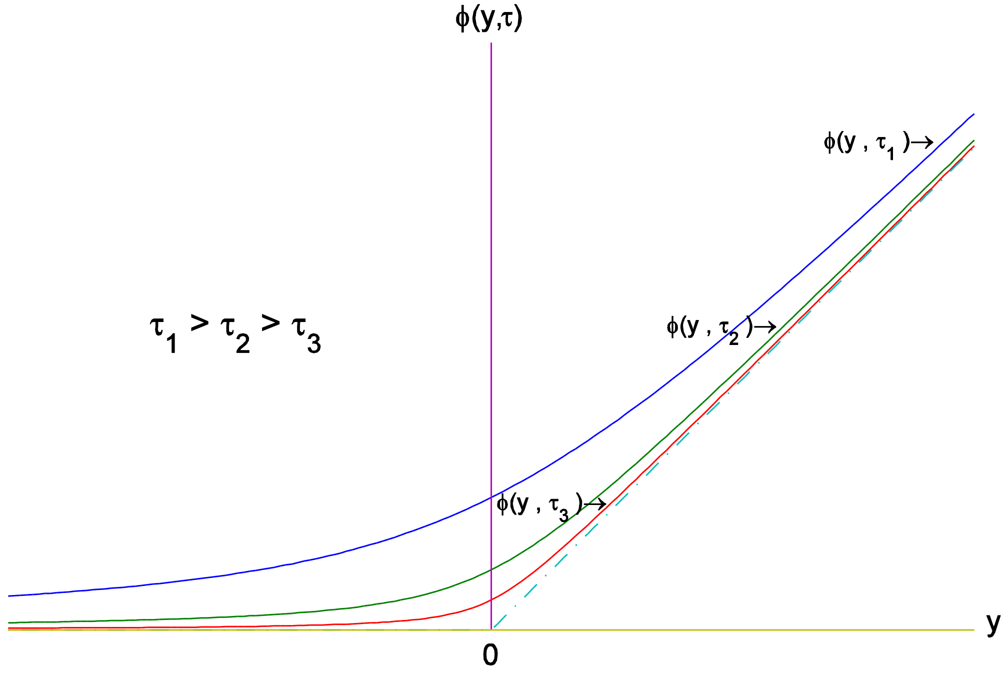
Fundamental Smoothing Procedures

Smoothing of the absolute value function

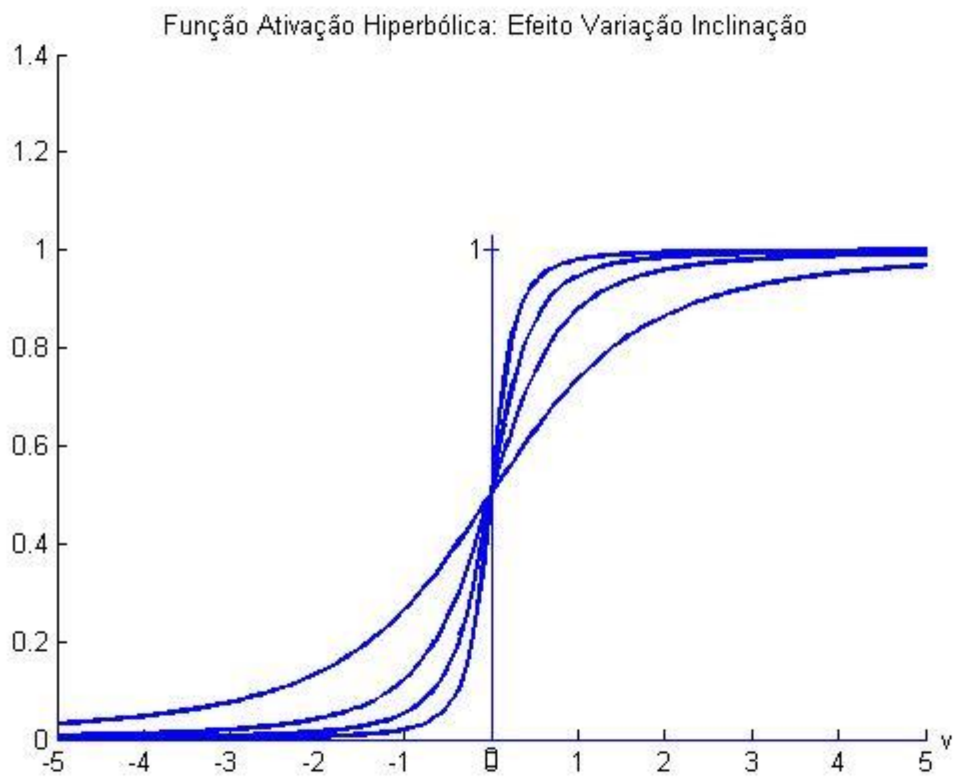


Fundamental Smoothing Procedures

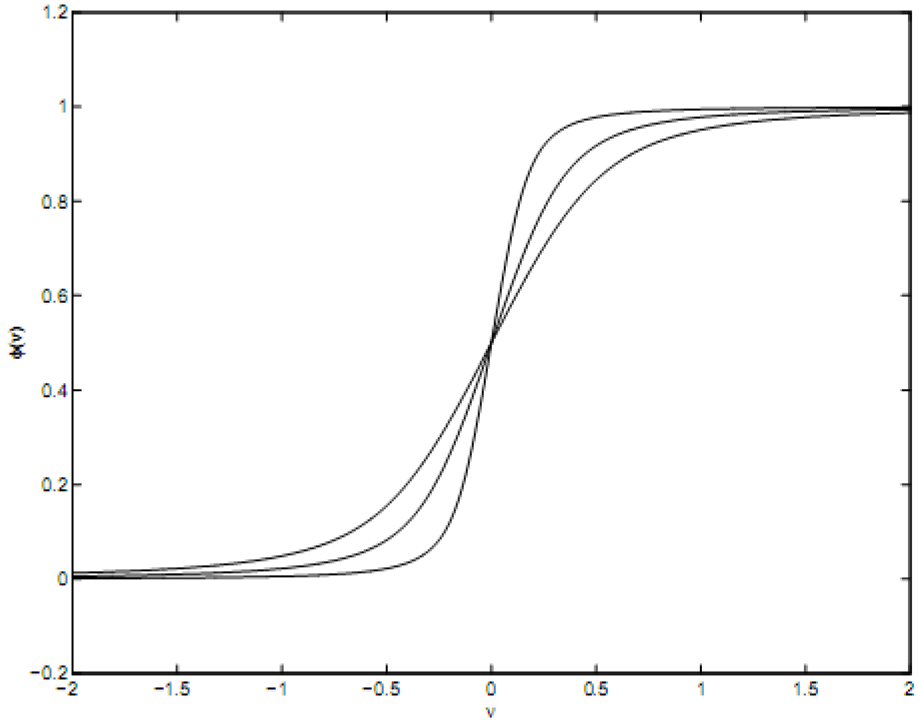
Smoothing of the function ψ



Additional Smoothing Procedures: 1 - Hyperbolic Neural Activation Function

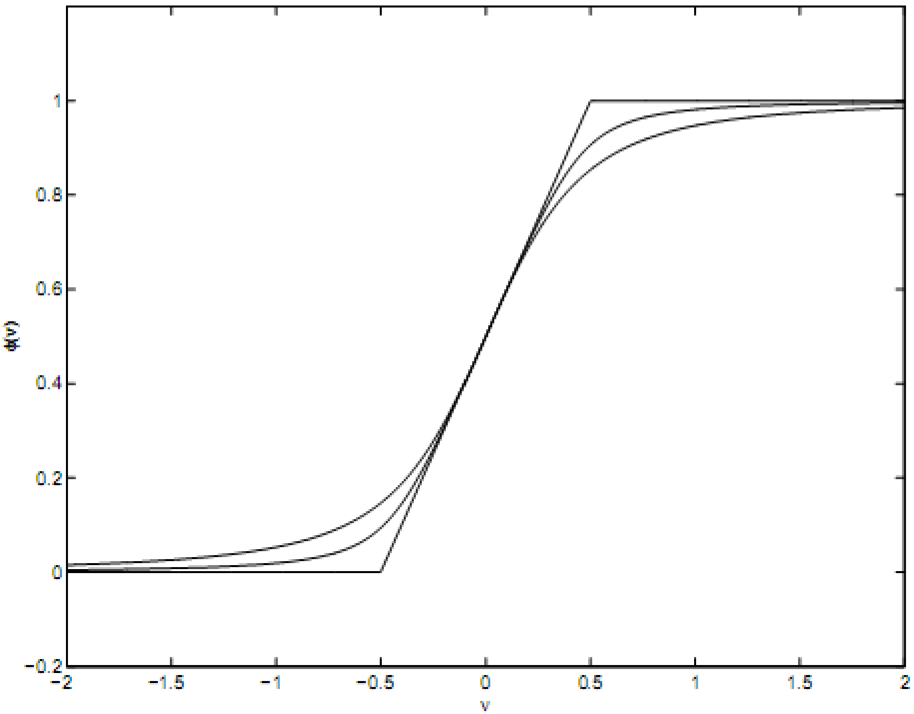


2 - Bi-hyperbolic Neural Activation Function



Função ϕ_X – Efeito da Variação do Parâmetro λ

2 - Bi-hyperbolic Neural Activation Function



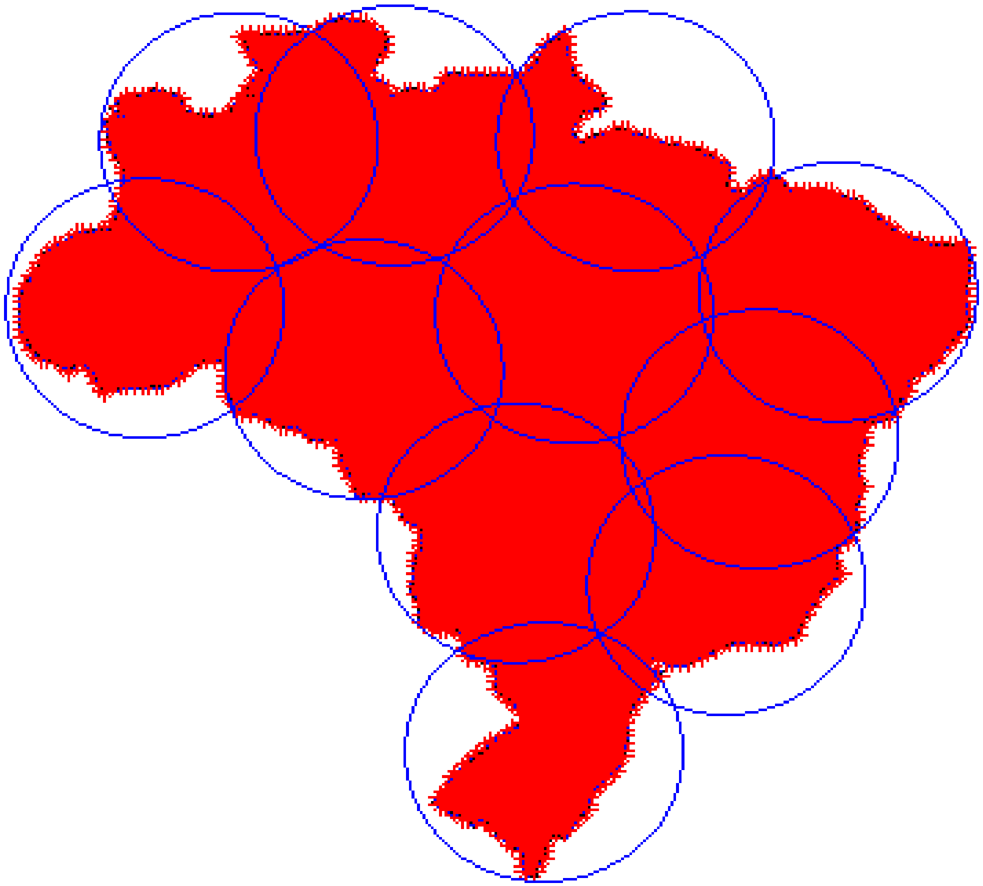
Função ϕ_X – Efeito da Variação do Parâmetro τ

Covering Problems

Publications

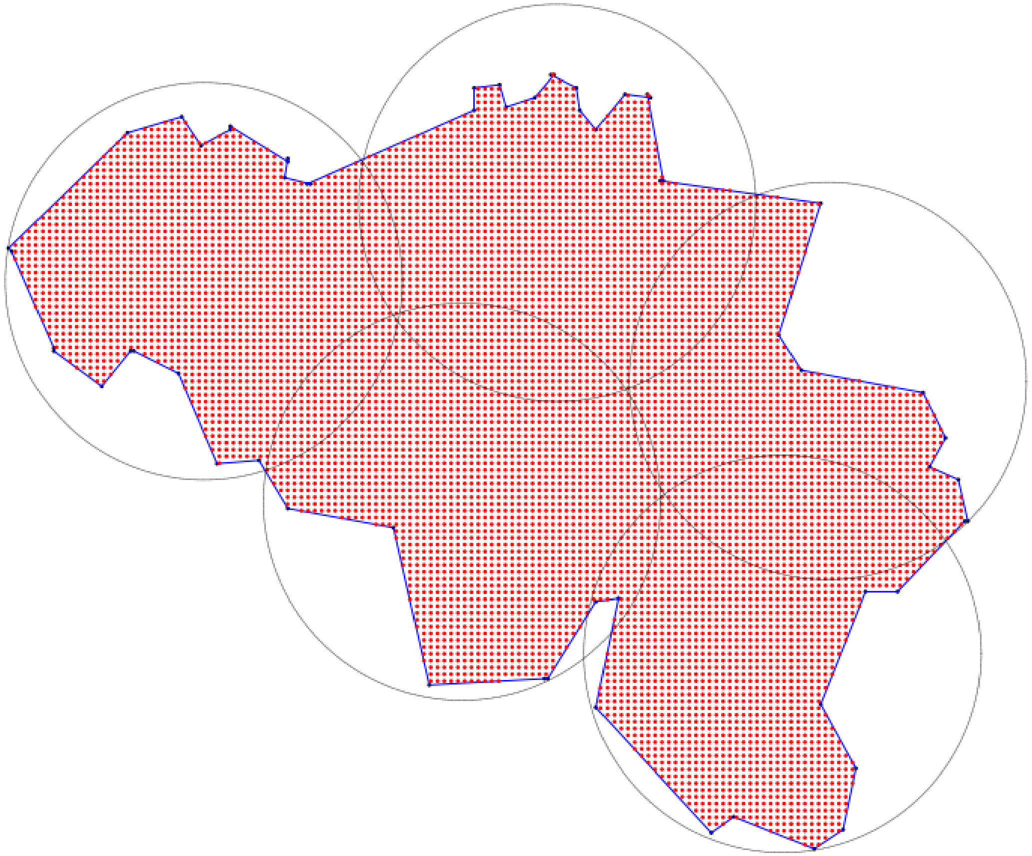
A. E. Xavier e A. A. F. Oliveira (2005), “Optimum Covering of Plane Domains by Circles Via Hyperbolic Smoothing Method”, **Journal of Global Optimization, Volume 31 Number 3, March 2005, Pages 493-504 , Springer**, http://dx.doi.org/10.1007/s10898-004-0737-8

Covering of a planar region by 11 Circles - 8986 pixels



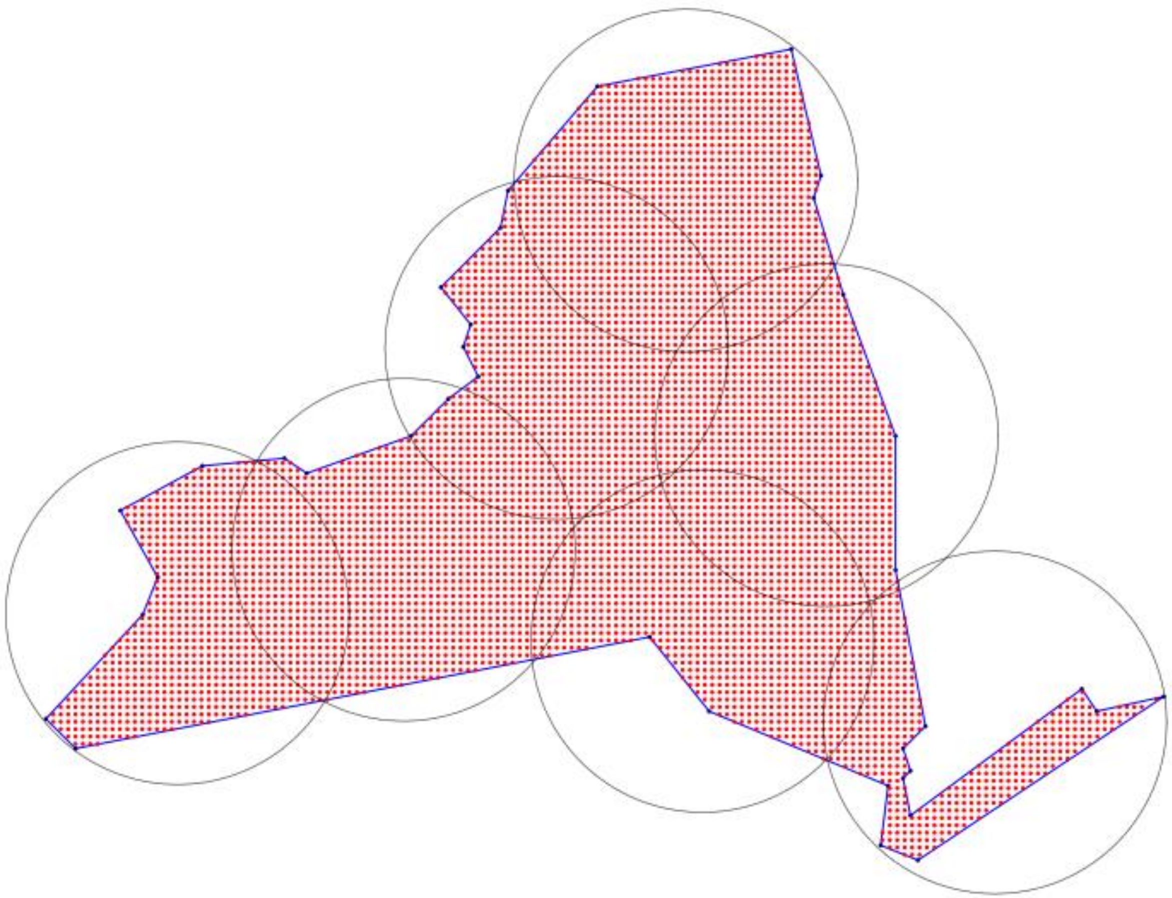
Covering Problems

Coverages of Netherlands



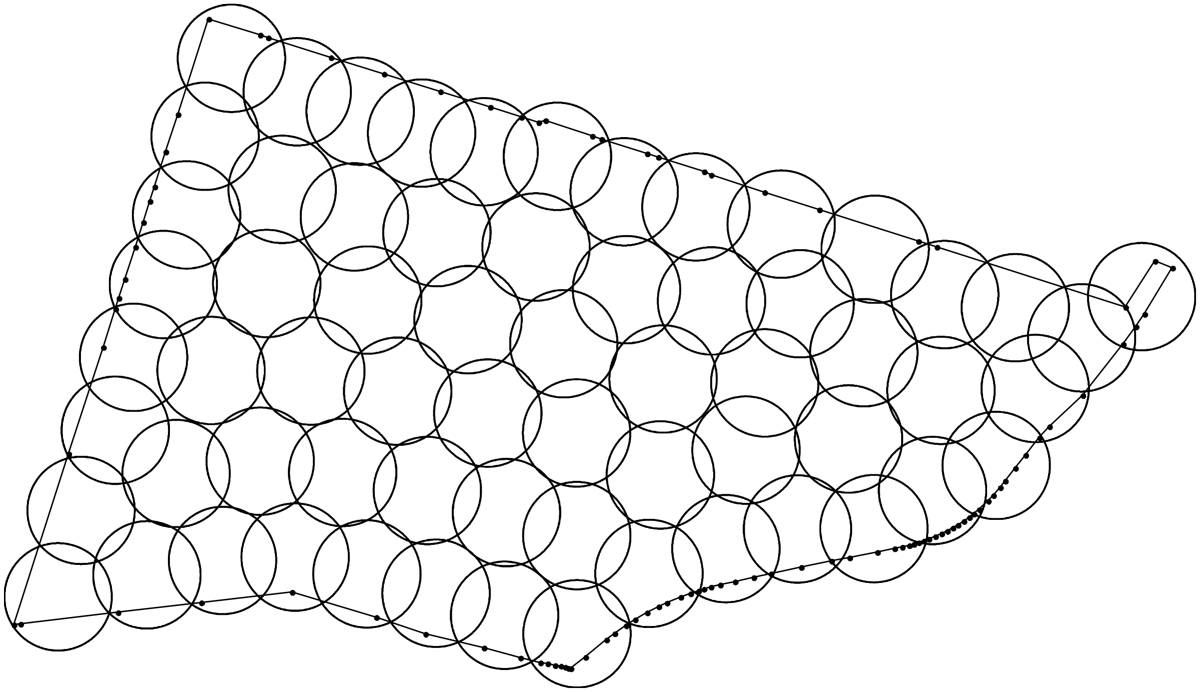
Covering Problems

Coverages of the state of New York



Covering Problems

Coverages of Dionisio Torres District – Fortaleza - Brazil



64 circles

Covering Problems

We consider the special case of covering a finite plane domain S optimally by a given number q of circles. We first discretize the domain S into a finite set of m points $s_j, j = 1, \cdots, m$. Let $x_i, i = 1, \cdots, q$ be the centres of the circles that must cover this set of points

$$X^* = \arg\min_{X \in \Re^{2q}} \max_{j=1,\cdots,m} \min_{i=1,\cdots,q} \left\| s_j - x_i \right\|_2$$

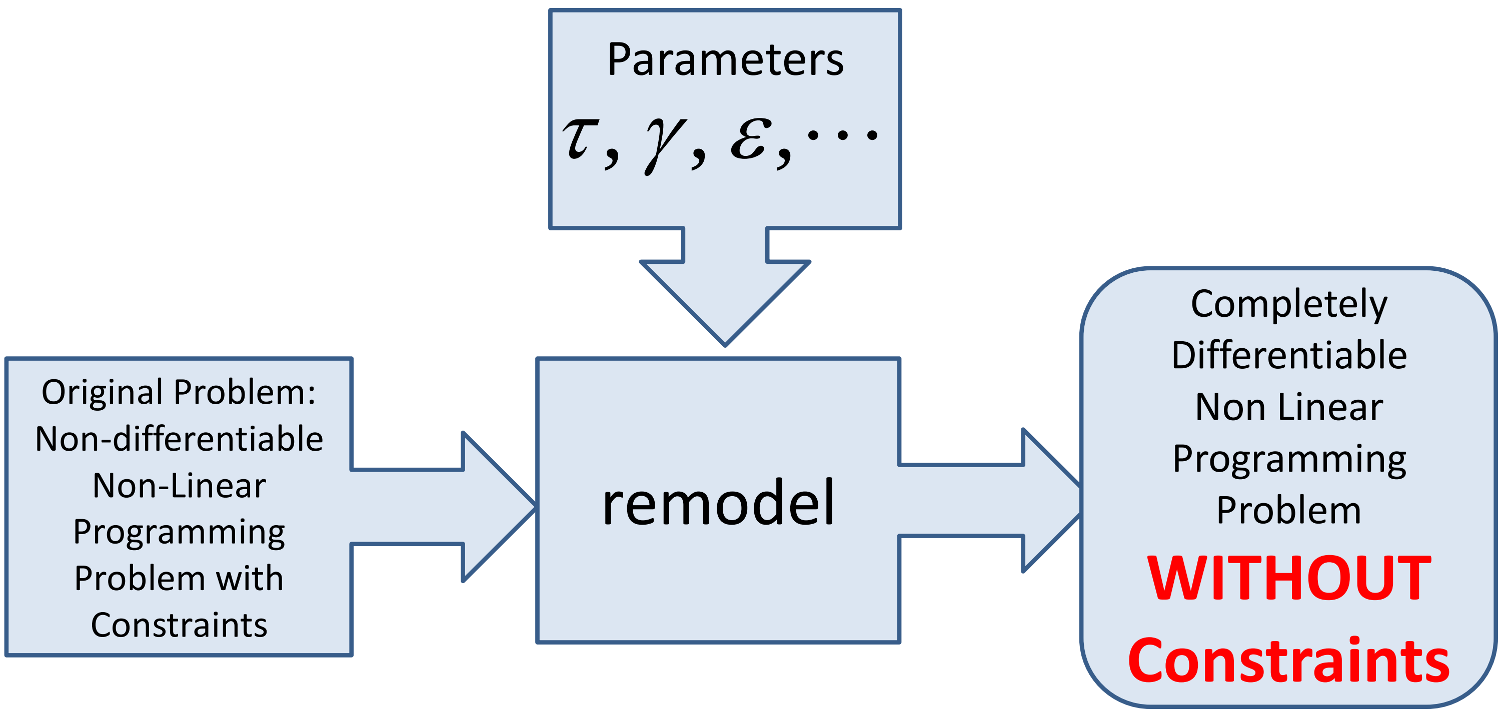
Covering Problems

By performing an ε perturbation and by using the FE approach, the three-level strongly nondifferentiable $\min - \max - \min$ problem can be transformed in a one-level completely smooth one:

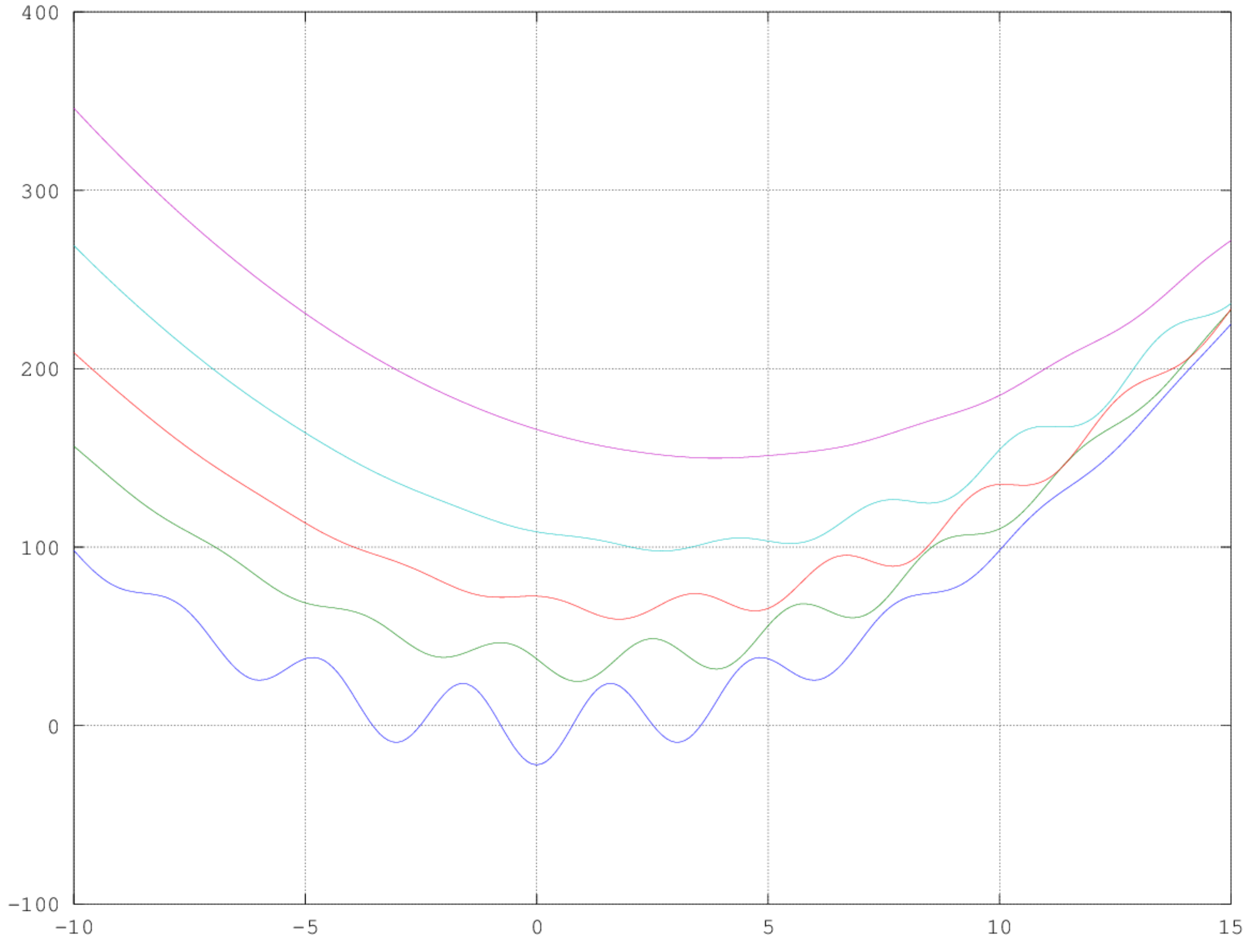
$$\text{minimize} \quad z$$

$$\text{subject to:} \quad \sum_{i=1}^{q} \phi\left(z - \left\| s_j - x_i \right\|_2, \tau\right) \geq \varepsilon, \quad j = 1, \cdots, m$$

Hyperbolic Smoothing Transformations



Additional Effect Produced by the Smoothing Procedures: Elimination of Local Minimum Points



Clustering

Problems

Publications – Part 1

Adilson Elias Xavier, “The Hyperbolic Smoothing Clustering Method”, **Pattern Recognition, Vol. 43, pp. 731-737, 2010**
doi:10.1016/j.patcog.2009.06.018

Adilson Elias Xavier and Vinicius Layter Xavier, "Solving the Minimun Sum-of-Squares Clustering Problem by Hyperbolic Smoothing and Partition into Boundary and Gravitational Region ", **Pattern Recognition, Vol. 44, pp. 70-77, 2011.**
doi:10.1016/j.patcog.2010.07.004

Publications – Part 2

Adilson Elias Xavier and Vinicius Layter Xavie& Sergio Barbosa Villas-Boas "*Solving the Minimum of L1 Distances Clustering Problem by the Hyperbolic Smoothing Approach and Partition into Boundary and Gravitational Regions*", **Studies in Classification, Data Analysis and Knowledge Organization,** Editors-in-chief: Bock, H.-H., Gaul, W.A., Vichi, M., Weihs, C. Springer-Verlag GmbH, Heidelberg, 2013, http://www.springer.com/series/1564.

A.M. Bagirov, B. Ordin, G. Ozturk and A.E. Xavier, *"An incremental clustering algorithm based on hyperbolic smoothing"*, **Computational Optimization and Applications.**
Vol. 61 Issue 1, pp. 219-241, 2015.
DOI 10.1007/s10589-014-9711-7

Clustering Problems

S denote a set of m patterns or observations

q a given number of clusters.

$x_i, i = 1, \cdots, q$ set of centroids of the clusters $x_i \in \Re^n$

Given a point s_j, we initially calculate the Euclidean distance to the nearest center.

$$z_j = \min_{i=1,\cdots,q} \left\| \mathrm{s}_{\mathrm{j}} - \mathrm{x}_{\mathrm{i}} \right\|_2$$

Clustering Problems

The minimum sum of the squares (MSSC) of these distances:

$$\text{minimize} \quad \sum_{j=1}^{m} z_j^2$$

$$\text{subject to:} \quad \mathrm{z_j} = \min_{\mathrm{i}=1,\cdots,\mathrm{q}} \left\| \mathrm{s_j} - \mathrm{x_i} \right\|_2, \quad j = 1, \cdots, m$$

Clustering Problems

By using HS approach, it is possible to use the Implicit Function Theorem to calculate each component $z_j, j = 1, \cdots, m$ as a function of the centroid variables $x_i, i = 1, \cdots, q$ and to obtain the unconstrained problem

$$\text{minimize} \qquad f(x) = \sum_{j=1}^{m} z_j(x)^2$$

where each $z_j(x)$ is obtained by the calculation of a zero of

$$h(x, z_j) = \sum_{i=1}^{q} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \quad j = 1, \ldots, m.$$

Computational Results HSCM

- Sobral city, 13280 patterns

Results for Sobral City Instance

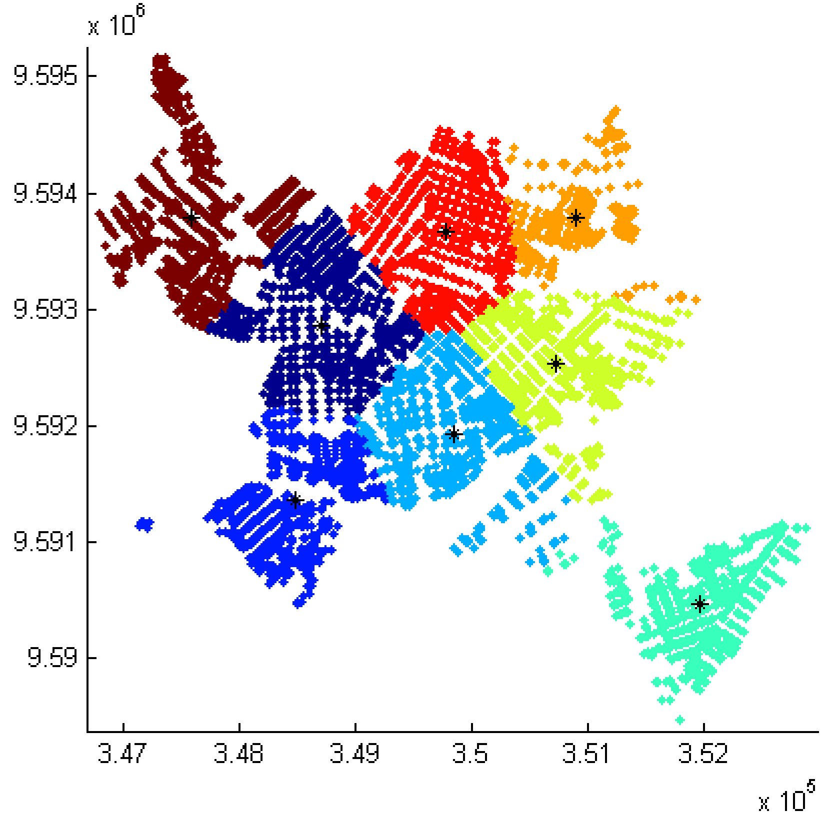
q	f_{HSC}	$Time_{HSC}$ (s)	$f_{j-means}$	$Time_{j\text{-}means}$ (s)	E	$Ratio$
8	0.40663×10^{10}	95.55	0.40674×10^{10}	2220.61	0.03	23.24
9	0.35783×10^{10}	78.11	0.38988×10^{10}	18.08	8.96	0.23
10	0.31477×10^{10}	127.89	0.56343×10^{10}	2259.02	78.99	17.66
11	0.27637×10^{10}	107.08	0.27637×10^{10}	26142.94	0.00	244.14

$$E = \frac{100(f_{j-means} - f_{HSC})}{f_{HSC}}$$

$$Ratio = \frac{Time_{j-means}}{Time_{HSC}}$$

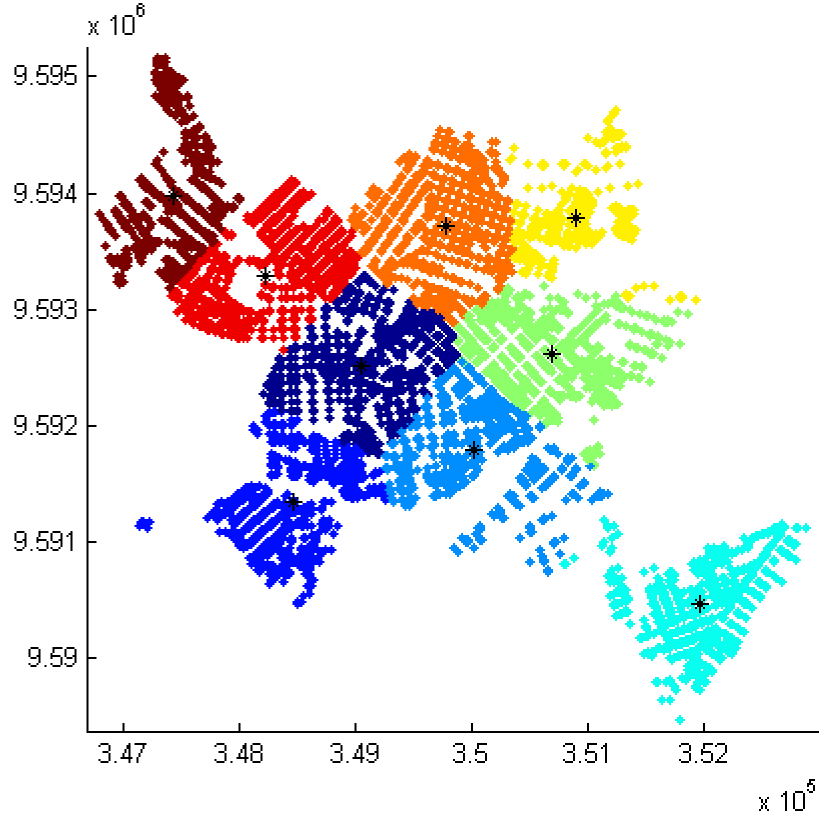
Computational Results HSCM

- Sobral city (q = 8)



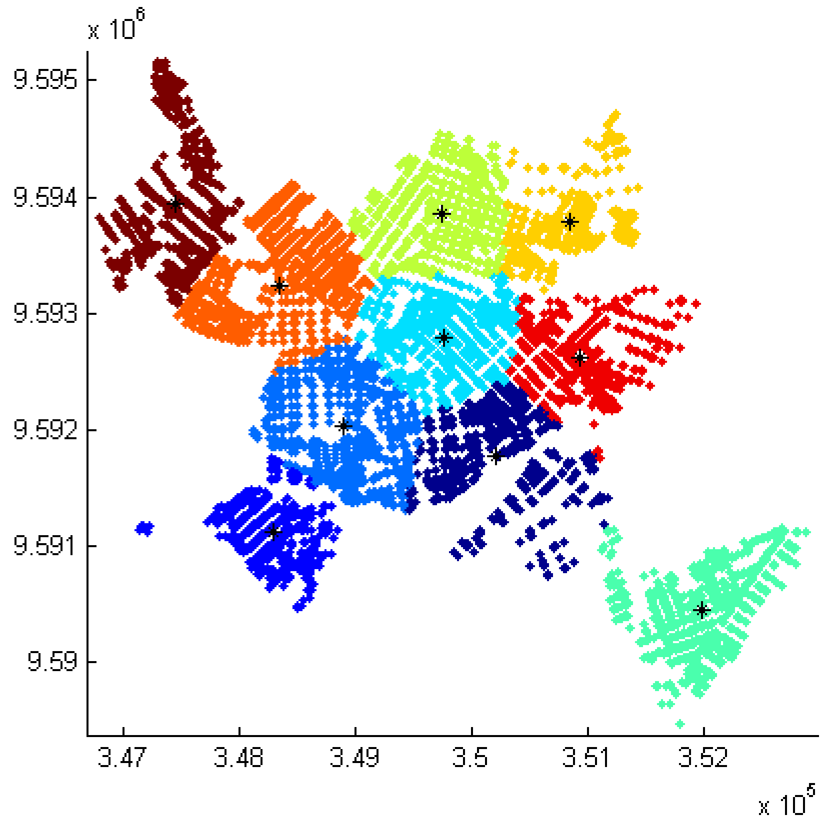
Computational Results HSCM

- Sobral city (q = 9)



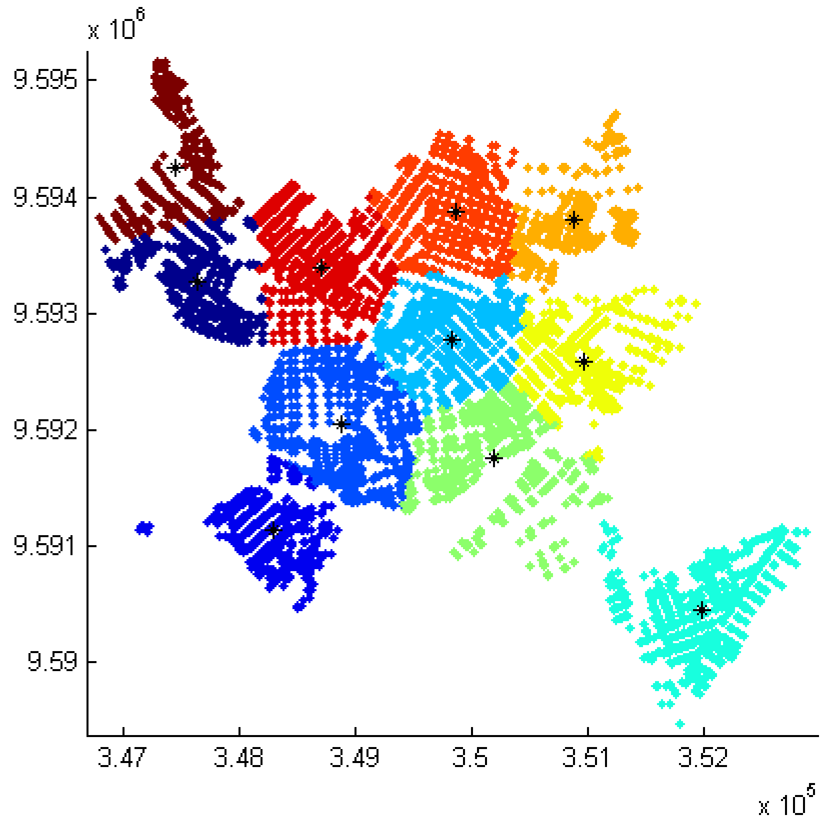
Computational Results HSCM

- Sobral city (q = 10)



Computational Results HSCM

- Sobral city (q = 11)



Fermat-Weber Problem

Publications

Xavier, V.L.: Resolução do Problema de Agrupamento segundo o Critério de Minimização da Soma de Distâncias**, M.Sc. thesis - COPPE - UFRJ, Rio de Janeiro, 2012**

Xavier, V.L., França, F.M.G., Xavier, A.E. and Lima, P.M.V., *"A Hyperbolic Smoothing Approach to the Multisource Weber Problem"*, **accepted for publication on the Special Issue of Journal of Global Optimization dedicated to EURO XXV 2012, Vilnius, Lithuania.**

Fermat-Weber Problem

The Fermat-Weber problem considers the placing of q facilities in order to minimize the total transportation cost:

$$\text{minimize} \quad \sum_{j=1}^{m} w_j z_j$$

$$\text{subject to:} \quad \mathrm{z_j} = \min_{\mathrm{i}=1,\cdots,\mathrm{q}} \left\| \mathrm{s_j} - \mathrm{x_i} \right\|_2, \quad j = 1,\cdots,m$$

Fermat-Weber Problem

By using HS approach, it is possible to use the Implicit Function Theorem to calculate each component $z_j, j=1,\cdots,m$ as a function of the centroid variables $x_i, i=1,\cdots,q$. In this way, the unconstrained problem is obtained

$$\text{minimize} \quad f(x) = \sum_{j=1}^{m} w_j z_j(x)$$

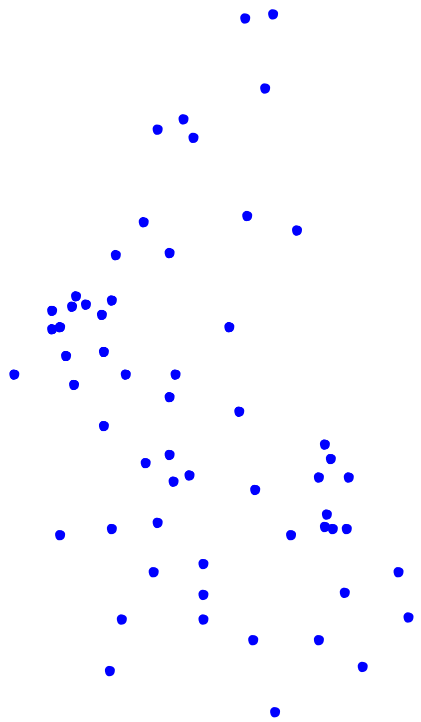
Fermat-Weber Problem

Where each $z_j(x)$ results from the calculation of the single zero of each equation below, since each term ϕ above strictly increases together with variable z_j :

$$h_j(z_j, x) = \sum_{j=1}^{m} \phi(z_j - \theta(s_j, x_i, \gamma), \tau) - \varepsilon = 0, \qquad j = 1, \cdots, m$$

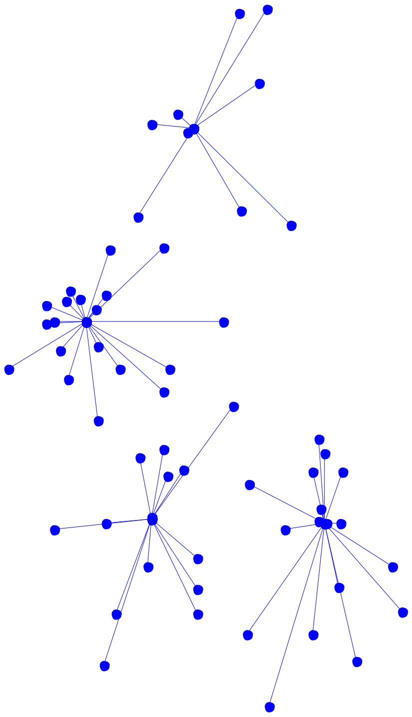
Fermat-Weber Problem

German Towns: coordinates of 59 towns (Späth, 1980)



Fermat-Weber Problem

4 facilities



Patente

Eventos Precedentes 1

1. COPPETEC – Exigência Aprovação Comitê Professores meados de 2004
2. Relatorio Tecnico PESC ES-675-5 Abril 2005 versão original do Hyperbolic Smoothing Clustering Method
3. Submissão Pattern Recognition da versão original do Hyperbolic Smoothing Clustering Method 20 maio 2008
4. EURO Continous Optimization 2008 – Neringa, Lituânia primeira divulgação internacional 20 a 23 maio 2008
5. Envio código fonte versão original do Hyperbolic Smoothing Clustering Method para Bagirov julho 2018

Eventos Precedentes 2

1. Parecer de referee da Pattern Recognition pedindo resultados computacionais com instâncias maiores (única exigência)
2. Realização de novos experimentos com instâncias maiores => TSPLIB Pla85900
3. Descoberta da dinâmica do processo de convergência que é precoce para a imensa maioria das observações
4. Idéia do esquema "*Partition into Boundary Band Zone and Gravitational Regions*"

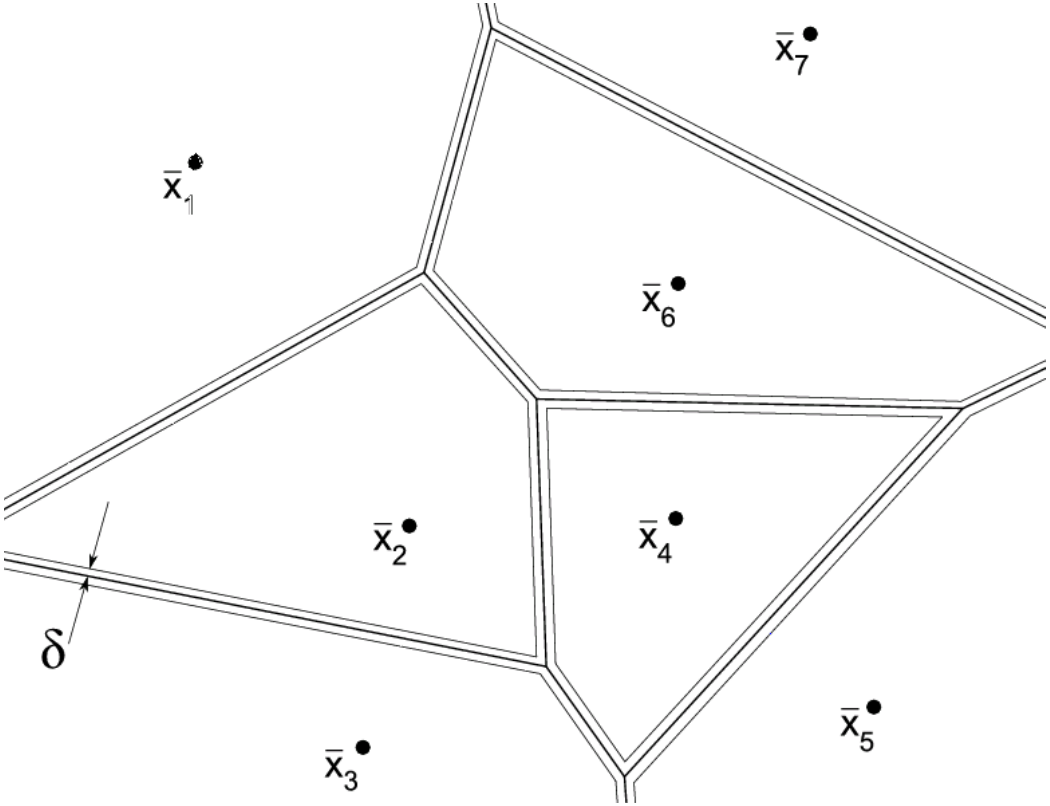
The Partition into Boundary Band Zone and Gravitational Regions

The basic idea of the approach is the partition of the set of observations in two non overlapping parts:

- the first set corresponds to the observation points that are relatively close to two or more centroids;

- the second set corresponds to the observation points that are significantly close to a unique centroid in comparasion with the other ones.

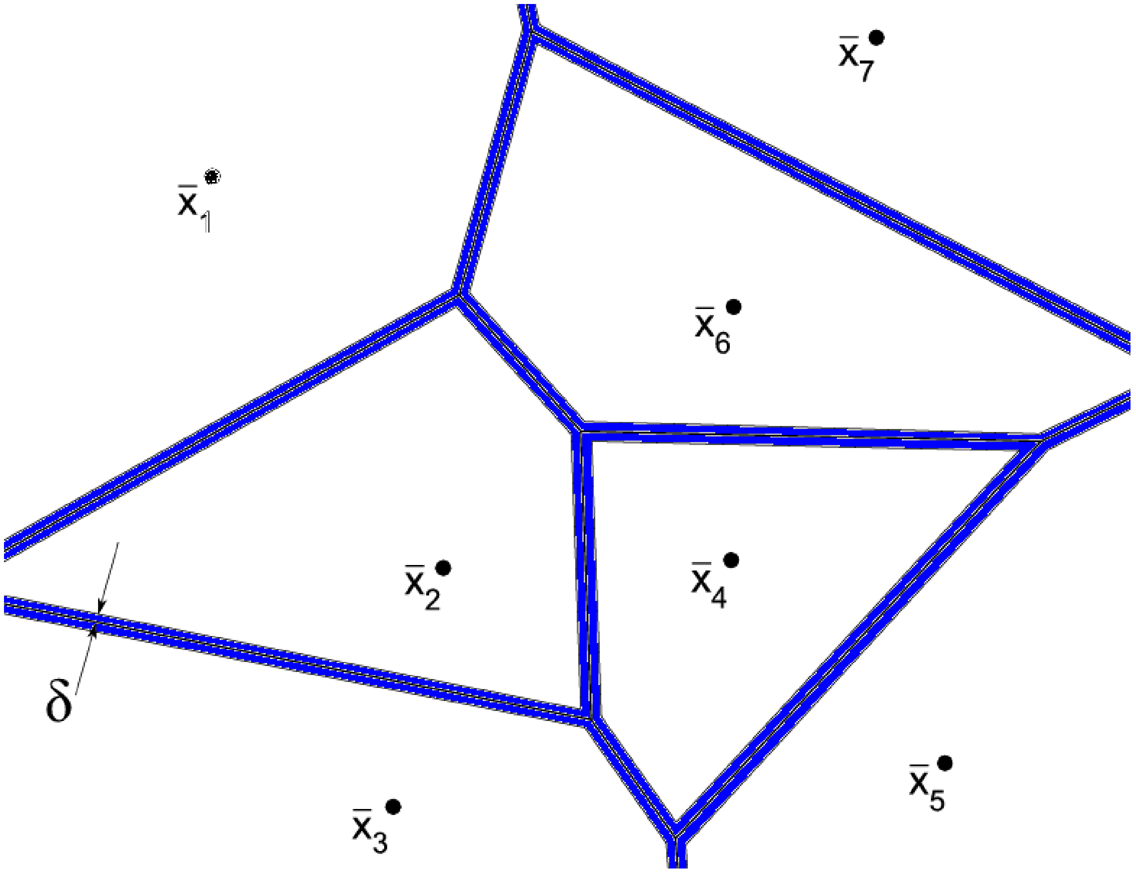
Partition of the Set of Observations



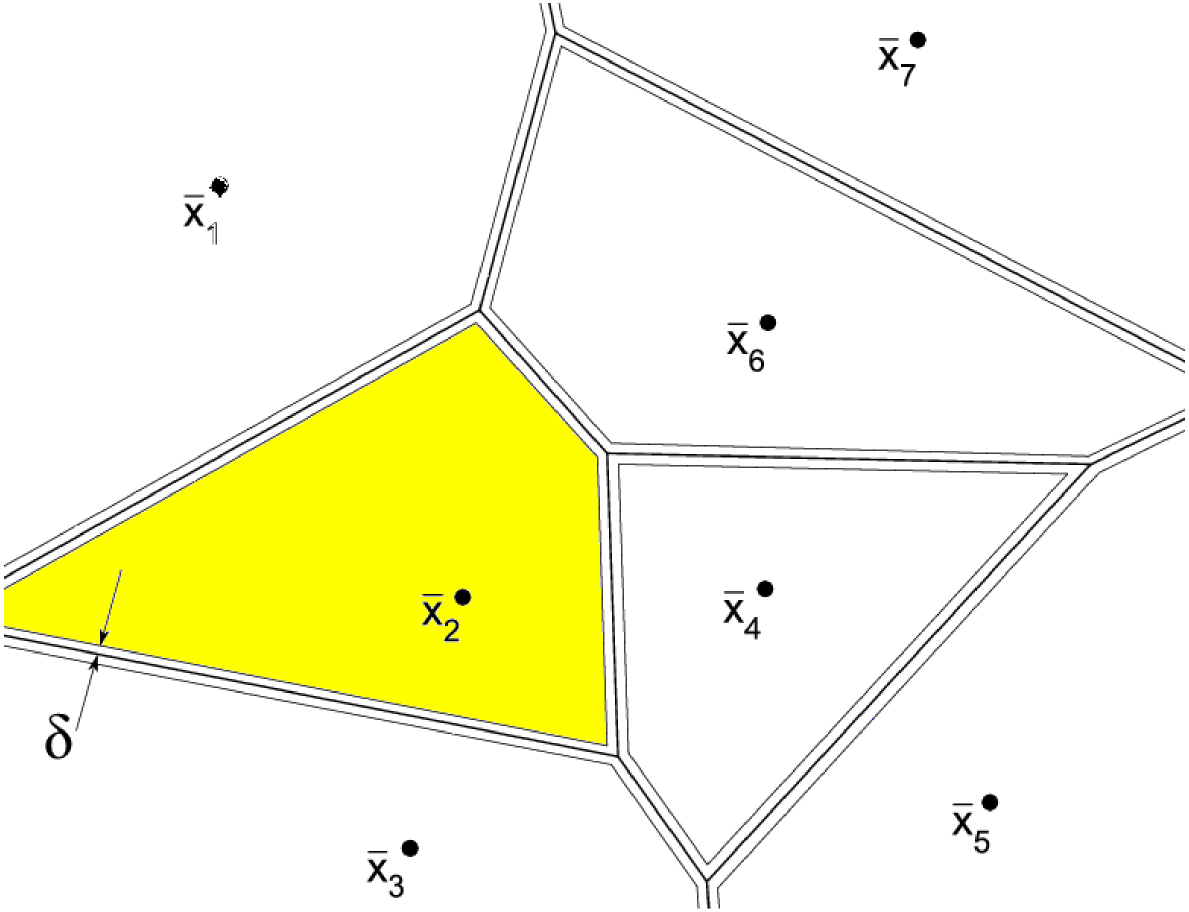
$\bar{x}$: the referencial point

δ: the band zone width

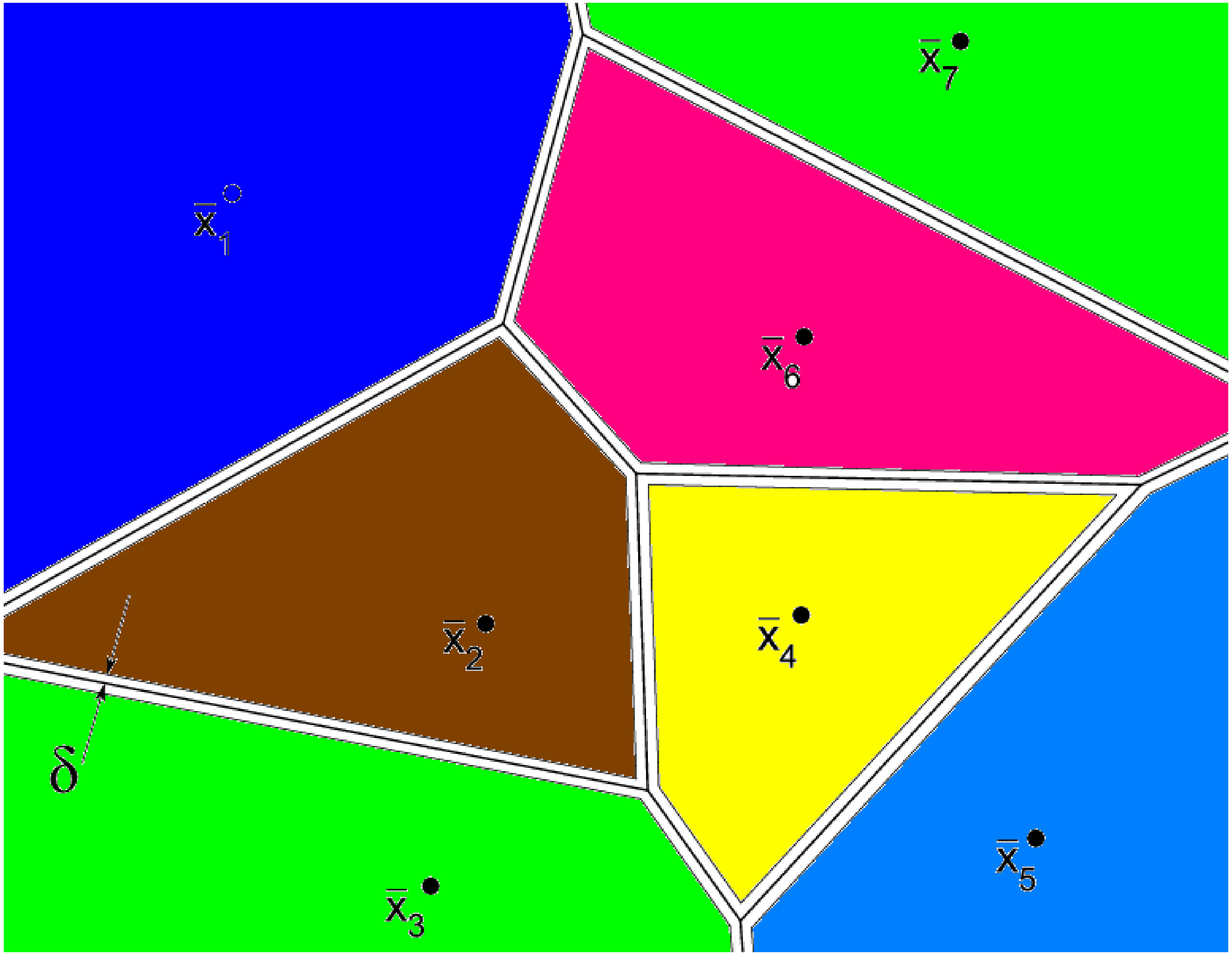
The Boundary Band Zone



Gravitational Region => $\overline{x}_2$



Gravitational Regions



Hyperbolic Smoothing Clustering Method JUMBO

General Problem Formulation:

$S = \{S_1, \dots, S_m\}$ Set of m observations

$x_i \; , \; i = 1, \dots, q$ Centroides of the clusters

$z_j = \min_{i=1,\dots,q} \left\| s_j - x_i \right\|$ Distance of the observation j to nearest centroide

Objective function specification

$$Minimize \quad \sum_{j=1}^{m} f(z_j)$$

where $f(z_j)$ is **an arbitrary monotonic increasing function of the distance** z_j

Hyperbolic Smoothing Clustering Method JUMBO

General Problem Formulation:

$$\mathit{Minimize} \quad \sum_{j=1}^{m} f(z_j)$$

$$z_j = \min_{i=1,\dots,q} \left\| s_j - x_i \right\|, \; j = 1,\dots,m$$

Trivial Examples of monotonic increasing functions:

$$\sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j^2 \qquad \sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j$$

Possible Distance Metrics:

L_2 (Euclidean) L_1 (Manhattan) L_∞ (Chebychev) L_p (Minkowshi)

Hyperbolic Smoothing Clustering Method
JUMBO - 2 casos importantes

Minimum Sum-of- Squares Clustering Problem:

$$\sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j^2$$

Minimum Sum-of-Distance Clustering Problem

Multisource Fermat-Weber Location Problem

p-Median Location Problem:

$$\sum_{j=1}^{m} f(z_j) = \sum_{j=1}^{m} Z_j$$

First Component of the Objective Function Tratamento caso geral

The component associated with the set of boundary observations, can be calculated by using the previous presented smoothing approach:

$$Minimize \;\; F_B(x) = \sum_{j \in J_B} f(z_j)$$

where each z_j results from the calculation of a zero of each equation:

$$h(x, z_j) = \sum_{i=1}^{q} \phi\big(z_j - \theta(s_j, x_i, \gamma), \tau\big) - \varepsilon = 0, \; j \in J_B$$

Second Component of the Objective Function Tratamento caso geral

The component associated with the gravitational regions, can be calculated in a simpler form:

$$Minimize\ \ F_G(x) = \sum_{i=1}^{q} \sum_{j \in J_i} f(\|s_j - x_i\|)$$

where J_i is the set of observations associated to cluster i .

Remark:

For each gravitational observation, it is a priori known its associated centroid.

Hyperbolic Smoothing Clustering Method JUMBO Casos Especiais

Além do problema geral para Clustering a patente contempla 2 formulações particulares com ganhos diferenciados:

- Minimum Sum-of-Squares Euclidean Norm

  (mais natural e mais amplamente usada, como pelo **algoritmo k-means)**

- Minimum Sum-of-Distances Manhattan Norm

IEEE - International Conference on Data Mining (ICDM) 2006
Votação Pesquisadores em Data Mining

Knowl Inf Syst (2008) 14:1–37
DOI 10.1007/s10115-007-0114-2

SURVEY PAPER

Top 10 algorithms in data mining

Xindong Wu · Vipin Kumar · J. Ross Quinlan · Joydeep Ghosh · Qiang Yang · Hiroshi Motoda · Geoffrey J. McLachlan · Angus Ng · Bing Liu · Philip S. Yu · Zhi-Hua Zhou · Michael Steinbach · David J. Hand · Dan Steinberg

Received: 9 July 2007 / Revised: 28 September 2007 / Accepted: 8 October 2007
Published online: 4 December 2007

Abstract This paper presents the top 10 data mining algorithms identified by the IEEE International Conference on Data Mining (ICDM) in December 2006: C4.5, *k*-Means, SVM, Apriori, EM, PageRank, AdaBoost, *k*NN, Naive Bayes, and CART. These top 10 algorithms are among the most influential data mining algorithms in the research community. With each algorithm, we provide a description of the algorithm, discuss the impact of the algorithm, and review current and further research on the algorithm. These 10 algorithms cover classification,

IEEE - International Conference on Data Mining (ICDM) 2006
Votação Pesquisadores em Data Mining

- C4.5
- k-Means Algorithm
- SVM
- Apriori
- EM
- PageRank
- AdaBoost
- kNN
- Naive Bayes
- CART

Second Component for the MSSC
Tratamento específico
Minimum Sum-of-Squares Euclidean

Second Component for the MSSC

Tratamento específico

Minimum Sum-of-Squares Euclidean

Relação entre Momentos

Relação entre os momentos

Existem as seguintes relações entre os momentos centrados na média, m_r, e os referidos a uma origem arbitrária m_r.

$$\begin{cases} m_2 = m_2' - m_2'^2 \\ m_3 = m_3' - 3m_1'm_2' + 2m_1'^3 \\ m_4 = m_4' - 4m_1'm_3' + 6m_1'^2m_2' - 3m_1'^4 \end{cases} \tag{7}$$

etc. (veja o Probl. 5). Note-se que $m_1' = \bar{X} - A$.

Second Component for the MSSC
Tratamento específico
Minimum Sum-of-Squares Euclidean

Demostração Relação entre Momentos

5. Provar que: (a) $m_2 = m_2' - m_1'^2$; (b) $m_3 = m_3' - 3\,m_1'm_2' + 2m_1'^3$; (c) $m_4 = m_4' - 4m_1'm_3' + 6m_1'^2m_2' - 3m_1'^4$.

Solução:

(a) Se $d = X - A$, então $X = A + d$, $\bar{X} = A + \bar{d}$ e $X - \bar{X} = d - \bar{d}$.

$$m_2 = \overline{(X-\bar{X})^2} = \overline{(d-\bar{d})^2} = \overline{d^2 - 2\,\bar{d}d + \bar{d}^2} =$$
$$= \overline{d^2} - 2\bar{d}^2 + \bar{d}^2 = \overline{d^2} - \bar{d}^2 = m_2' - m_1'^2.$$

(b)
$$m_3 = \overline{(X-\bar{X})^3} = \overline{(d-\bar{d})^3} = \overline{(d^3 - 3d^2\bar{d} + 3d\bar{d}^2 - \bar{d}^3)} =$$
$$= \overline{d^3} - 3\bar{d}\,\overline{d^2} + 3\bar{d}^3 - \bar{d}^3 = \overline{d^3} - 3\bar{d}\,\overline{d^2} + 2\bar{d}^3 = m_3' - 3\,m_1'm_2' + 2\,m_1'^3.$$

(c)
$$m_4 = \overline{(X-\bar{X})^4} = \overline{(d-\bar{d})^4} = \overline{(d^4 - 4d^3\bar{d} + 6d^2\bar{d}^2 - 4d\bar{d}^3 + \bar{d}^4)} =$$
$$= \overline{d^4} - 4\bar{d}\,\overline{d^3} + 6\bar{d}\,\overline{d^2} - 4\bar{d}^4 + \bar{d}^4 = \overline{d^4} - 4\bar{d}\,\overline{d^3} + 6\bar{d}^2\,\overline{d^2} - 3\bar{d}^4 =$$
$$= m_4' - 4m_1'\,m_3' + 6m_1'^2\,m_2' - 3m_1'^4.$$

Por extensão dêste método, podem ser deduzidos resultados semelhantes para m_5, m_6, etc.

Second Component for the MSSC
Tratamento específico

For The Minimum Sum-of-Squares Clustering formulation, the second component, associated with the gravitational regions, can be calculated in a direct form:

$$Minimize \;\; F_G(x) = \sum_{i=1}^{q} \sum_{j \in J_i} \left\| s_j - v_i \right\|_2^2 + \sum_{i=1}^{q} \left| J_i \right| \left\| x_i - v_i \right\|_2^2$$

where J_i is the set of observations associated to centroid i

v_i is the gravity center of cluster i.

Gradient of the Second Component for the MSSC Tratamento específico

The gradient of the second component, associated with the gravitational regions, can be calculated in an easy way:

$$\nabla F_G(x) = \sum_{\iota=1}^{q} 2\left|J_i\right| \left(x_i - v_i\right)$$

where J_i is the number the of observations associated to centroid i

Hyperbolic Smoothing Clustering Method
JUMBO – Additional Feature

Finally, the HSCM methodology has as a differentiated feature the capability to produce results following the traditional ***hard focus,*** as well as the ***fuzzy one***, a fact that is also unprecedented in the literature as well as in software offered in the market.

Eventos Precedentes 3

1. Dean Webb, aluno doutorado de Bagirov, relatava o processo e o sucesso de suas experiências na utilização do software HSCM que lhes enviara.
2. Terminei a nova submissão para a Pattern Recognition atendendo ao referee com celeridade 26 outubro 2008
3. No dia seguinte comecei a nova versão com inclusão do esquema "*Partition into Boundary Band Zone and Gravitational Regions*"
4. Finalizei: implementação software, produção resultados, confecção tabelas, redação artigo e digitação em LATEX em 02 dez 2008, ou seja, **37 dias.**

Eventos Precedentes 4

1. Relatorio Tecnico PESC ES-724-8 Dezembro 2008 registrando novos resultados da nova versão do Hyperbolic Smoothing Clustering Method com pruning!! Speed-up da ordem de 600 vezes

2. 11th Conference of the International Federation of Classification Societes (IFCS 2009), March 13-18, 2009, Dresden, Germany, divulgação pública do Pruning

3. Finalmente, tomamos decisão de submeter patente ao USPTO

Dificuldades para Preparação da Patente

1. Apesar de empenho reiterado, constatei absoluta falta de suporte para a confecção do pedido da patente ao USPTO no âmbito da UFRJ
2. Unanimidade da proclamação pela comunidade: Algoritmo não é patenteável (síndrome de Karmakar!)
3. Corrida contra o tempo: 02 dezembro de 2009, deadline da originalidade
4. Dificuldades de natureza familiar

Depósito da Patente

1. Mergulhei nos sites do USPTO, baixei cerca de 25 patentes aprovadas sobre temas similares e as perscrutei em detalhes.
2. Selecionei cerca de 8 patentes mais pertinentes e fiz pequeno resumo
3. Desenvolvi estrutura da petição
4. Preenchi a estrutura com material dos 2 artigos prontos
5. Depositei patente em 02 dezembro de 2009 (último dia da originalidade)

Escopo da Patente

Problemas com resultados prévios exitosos:

- **Covering of Planar Regions with Equal Circles**
- **Minimum Sum-of-Squares Clustering**
- **Multisource Fermat-Weber**

Desenvolvimento Especificação Continente Geral contemplando, além dos 3 problemas acima, uma amplitude de formulações

Articulação com qualquer métrica de distâncias:

Euclidiana, Manhattan, Minkowski e Chebychev.

Problemas da Literatura com forte utilização em Data Science Applications

Blum *et. al* (2018) pag. 209:

One assumption commonly made in *clustering analysis* is that clusters are center-based.

Three standard criteria often used are:

- **k-center clustering** **=> Covering**
- **k-median clustering** **=> Fermat Weber**
- **k-means clustering** **=> Clustering**

Dificuldades na Tramitação da Patente no USPTO

Espada de Dâmocles:

Após de cerca de 3 anos de espera, chega o primeiro parecer exarado pelos examinador responsável do USPTO:

Publicação do Relatório Técnico PESC ES-675-5 Abril 2005 viola o necessário requisito de Originalidade!

Dificuldades na Tramitação da Patente no USPTO

Falhas de Natureza Processualística:

Redação da Patente tem que estar em conformidade com os padrões consolidados no USPTO desde o início de seu funcionamento em 1871.

Descrição da “Application” é IMUTÁVEL!

Dificuldades na Tramitação da Patente no USPTO

Descrição das reivindicações *(claims)* devem ser justificadas pelo conteúdo previamente apresentado na “Application”.

Descrição das reivindicações *(claims)* devem ser encadeadas uma a uma baseadas no princípio da veracidade das antecedentes.

Dificuldades na Tramitação da Patente no USPTO

Descrição das reivindicações *(claims)* devem ser encadeadas uma a uma baseadas no princípio da veracidade das antecedentes.

Falha Incorrigível:

Falta da Especificação de um Computador

Hyperbolic Smoothing Minimum Distance

(FALHA: Sem justificativas no conteúdo na "Application")

- A short list of such problems involving minimum distance or minimum value calculations is presented below:
- Min-max problems;
- Min-max-min problems;
- Min-sum-min problems;
- Covering a plane region by circles;
- Covering a tridimensional body by spheres;
  - Gamma knife problem
- Location problems;
  - Facilities location problems;
  - Hub and spike location problems;
  - Steiner problems;
  - Minisum and minimax location problems;
- Districting problems;
- Packing problems;
- Scheduling problems;
- Geometric distance problems;
  - Protein folding problems;
- Spherical point arrangements problems;
  - Elliptic Fekete problem;
  - Fekete problem;
  - Power sum problem;
  - Tammes (Hard-spheres) problem.

Cancelamento do Pedido Original da Patente

Em face da presença de Contradições Inconciliáveis na Especificação do Pedido Original da Patente, restou-nos a decisão de:

- Cancelamento do mesmo
- Abertura de novo Pedido com Modificações Marginais saneando Falhas existentes nesse Pedido Original.

Abertura de Pedido Reformulado da Patente

- Abertura de novo Pedido Reformulado com Modificações Marginais saneando Falhas
- Especificação de Presença de Computador
- Redução de 5 para 3 Grupos de Reivindições (claims):

1. **Formulação Geral Açambarcadora**
2. **Minimum sum-of-squares clustering – Euclidean norm**
3. **Minimum sum-of-distances clustering – Manhattan norm**

Dificuldades na Tramitação da Reformulação Pedido

Várias iterações dedicadas à Construção de Redação precisa e fundamentada das Reivindicações

"Alice case" era dificuldade intransponível para patente de software!!

2019 Revised Patent Subject Matter Eligibility Guidance, issued on January 7, 2019 🡐= Salvação da Lavoura

?????????

Aprovação do Pedido da Patente: US10,217,056

Final e surpreendentemente o nosso Pedido de Patente foi PUBLICADO em 26 Fevereiro de 2019!

Patente no USPTO, Capa - Parte Superior

US010217056B2

(12) **United States Patent**
Xavier et al.

(10) **Patent No.:** **US 10,217,056 B2**
(45) **Date of Patent:** **Feb. 26, 2019**

(54) **HYPERBOLIC SMOOTHING CLUSTERING AND MINIMUM DISTANCE METHODS**

(71) Applicants: **Adilson Elias Xavier**, Rio de Janeiro (BR); **Vinicius Layter Xavier**, Rio de Janeiro (BR)

(72) Inventors: **Adilson Elias Xavier**, Rio de Janeiro (BR); **Vinicius Layter Xavier**, Rio de Janeiro (BR)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 804 days.

(21) Appl. No.: **14/717,568**

(22) Filed: **May 20, 2015**

(65) **Prior Publication Data**

US 2016/0019467 A1 Jan. 21, 2016

Related U.S. Application Data

(63) Continuation-in-part of application No. 13/513,296, filed as application No. PCT/BR2009/000400 on Dec. 2, 2009.

(51) **Int. Cl.**
G06F 15/18 (2006.01)
G06N 7/02 (2006.01)

(52) **U.S. Cl.**
CPC ***G06N 7/02*** (2013.01)

(58) **Field of Classification Search**
CPC G06F 19/24; G06N 7/02
USPC 706/12, 15, 20, 45
See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

2005/0209785 A1 * 9/2005 Wells G06F 19/24 702/19
2006/0208870 A1 * 9/2006 Dousson G05B 23/027 340/506

OTHER PUBLICATIONS

Demyanov, Alexei. "On the Solution of Min-sum-min Problems." Journal of Global Optimization 31.3 (2005): 437-453.
Xavier, A. et al. "Optimal covering of plane domains by circles via hyperbolic smoothing." Journal of Global Optimization 31.3 (2005): 493-504.
Xavier, A. et al. "A novel contribution to the tammes problem by the hyperbolic smoothing method." EURO Mini Conference: EurOPT-2008, Lituania. May 2008.

* cited by examiner

Primary Examiner — David R Vincent
(74) *Attorney, Agent, or Firm* — Fildes & Outland, P.C.

(57) **ABSTRACT**

The invention concerns four methodologies regarding the unsupervised clustering of a set of observations in multidimensional space, considering a defined number of clusters. The invention comprises a special procedure for calculating the minimum distance of a given point to a set of points in a multidimensional space, the main component of the first methodology.

21 Claims, 3 Drawing Sheets

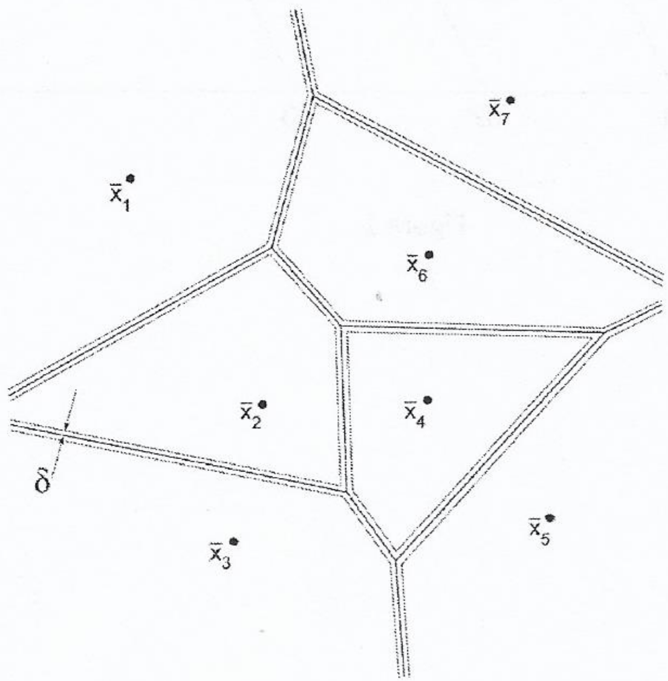
Patente no USPTO, Capa - Parte Inferior

unsupervised clustering of a set of observations in multidi-mensional space, considering a defined number of clusters. The invention comprises a special procedure for calculating the minimum distance of a given point to a set of points in a multidimensional space, the main component of the first methodology.

(51) **Int. Cl.**
G06F 15/18 (2006.01)
G06N 7/02 (2006.01)

(52) **U.S. Cl.**
CPC ***G06N 7/02*** (2013.01)

21 Claims, 3 Drawing Sheets



Patente:
Acervo de Módulos
Prontos

Problemas da Literatura com forte utilização em Data Science Applications

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One assumption commonly made in *clustering analysis* is that clusters are center-based.

Three standard criteria often used are:

- **k-center clustering => Covering**
- **k-median clustering => Fermat Weber**
- **k-means clustering => HSCM**

k-means clustering

Minimum Sum-of-Squares
Clustering
Concorrente:
Algoritmo k-means

Pump 1 - Part 1/2

460573 observations with 32 components

Clusters	F MIN	Ocor.	Desvio %	CPU (s)	Difference K-means %
2	0.618374E11	10	0.00	4.69	0
3	0.245662E11	4	55.27	3.87	0
4	0.990098E10	9	34.82	5.23	0
5	0.706583E10	1	8.34	7.13	0
6	0.489400E10	7	7.13	7.27	0
7	0.388975E10	6	4.08	8.63	-10.2
8	0.331142E10	5	2.74	9.86	-5.7

Difference between Solutions = 100 (AHSCM – k-means provided by R) / AHSCM

Pump 1 - Part 2/2

460573 observations with 32 components

Clusters	F MIN	Ocor.	Desvio %	CPU (s)	Diference K-means %
7	0.388975E10	6	4.08	8.63	- 10.2
8	0.331142E10	5	2.74	9.86	- 5.7
9	0.285338E10	2	5.36	11.62	- 2.4
10	0.246583E10	1	6.99	15.41	- 11.1
11	0.221496E10	1	7.13	11.37	- 13.5
12	0.198981E10	2	4.65	13.46	-21.6
13	0.180565E10	1	7.48	12.33	- 31.7
14	0.160330E10	1	8.12	16.96	- 40.1

Difference between Solutions = 100 (AHSCM – k-means provided by R) / AHSCM

Four Pumps - 1 to 4

1842292 observations with **32** components

Clusters	F MIN	Ocor.	Desvio %	CPU Time (s)
2	0.299271E12	10	0.00	13.21
3	0.111334E12	10	0.00	16.31
4	0.478524E11	8	35.17	18.99
5	0.379019E11	10	0.00	24.61
6	0.264045E11	8	4.50	31.80
8	0.199645E11	8	1.79	45.80
10	0.164836E11	1	2.18	60.33
12	0.131286E11	2	5.09	73.70
14	0.112396E11	1	4.91	93.67

k-median clustering

Minimum Sum-of-Distances Clustering

Fermat-Weber Location

k-medians Location

Multisource Fermat-Weber Problem
Minimum Sum-of-Distances Clustering Problem
Pump 1 - 460573 observations with 32 components

Clusters	F MIN	Ocor.	Desvio %	CPU (s)
2	0.885528E08	10	0.00	76.93
3	0.475015E08	10	0.00	99.32
4	0.389218E08	10	0.00	116.32
5	0.333147E08	7	2.08	138.29
6	0.299548E08	3	1.37	159.97
8	0.242166E08	1	1.75	200.58
10	0.201629E08	3	1.81	222.49
12	0.183258E08	1	2.18	252.00
14	0.168898E08	1	0.90	281.85

Multisource Fermat-Weber Problem
Minimum Sum-of-Distances Clustering Problem

All Pumps **1842292** observations with **32** components

Clusters	F MIN	Ocor.	Desvio %	CPU (s)
2	0.498733E9	10	0.00	384.65
3	0.226730E9	6	40.45	448.07
4	0.189407E9	6	36.34	616.20
5	0.152422E9	10	0.00	574.99
6	0.138617E9	7	0.54	628.25
8	0.121730E9	1	0.31	760.48
10	0.111810E9	1	1.87	920.41
12	0.103909E9	1	2.70	1074.60
14	0.963093E8	1	4.14	1345.27

Multisource Fermat-Weber Problem
Minimum Sum-of-Distances Clustering Problem

Largest instance usually presented by the literature:

TSP1060: 1060 cities with 2 components

Our largest instance:

All Pumps: 1842292 observ. with **32** components

This instance is 27808 times greater!!!!

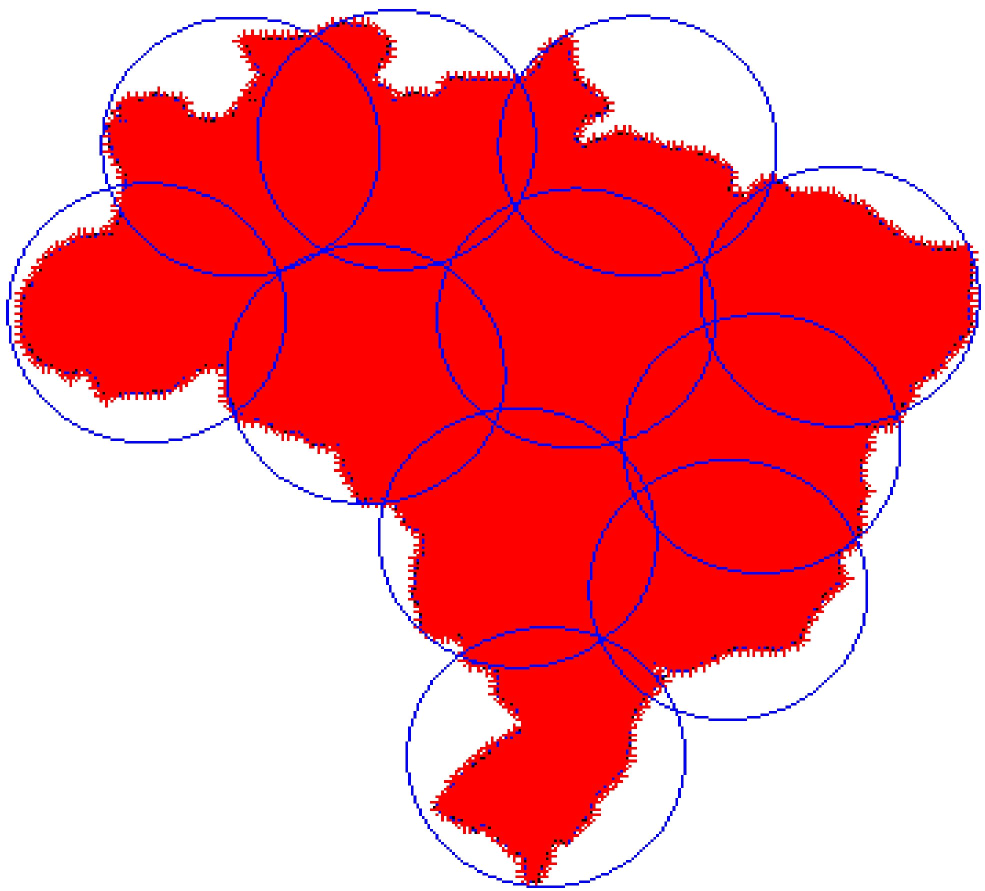
k-center clustering

Covering of Planar Regions

Covering of Solid Bodies

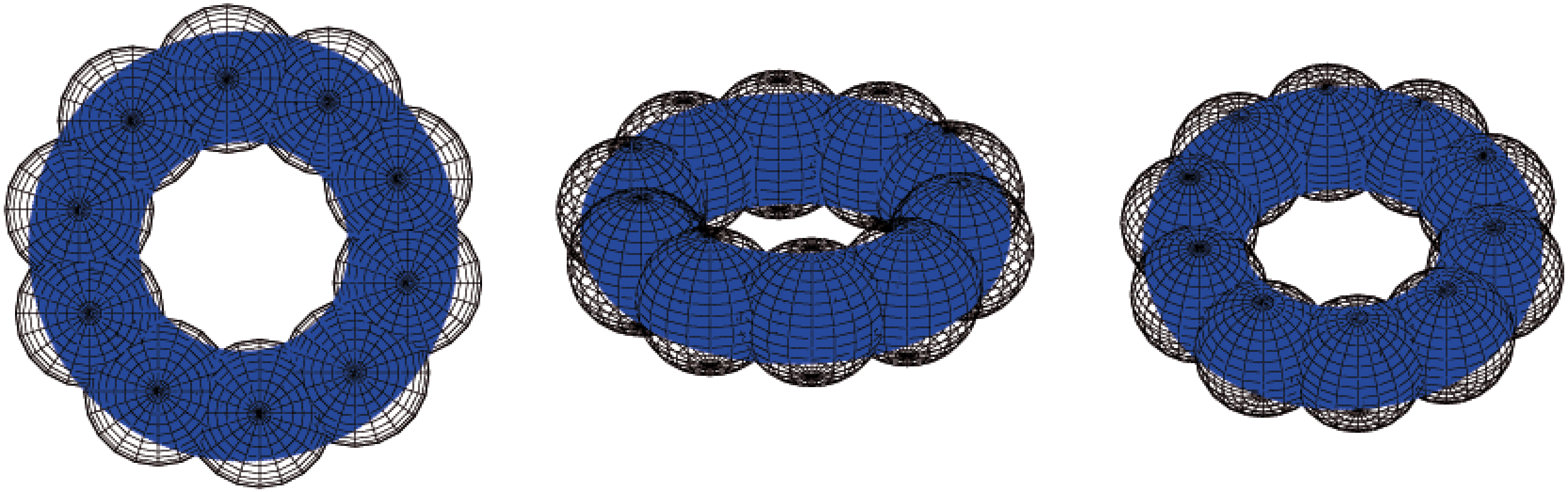
(min-max-min problem)

Covering of a planar region by 11 Circles - 8986 pixels

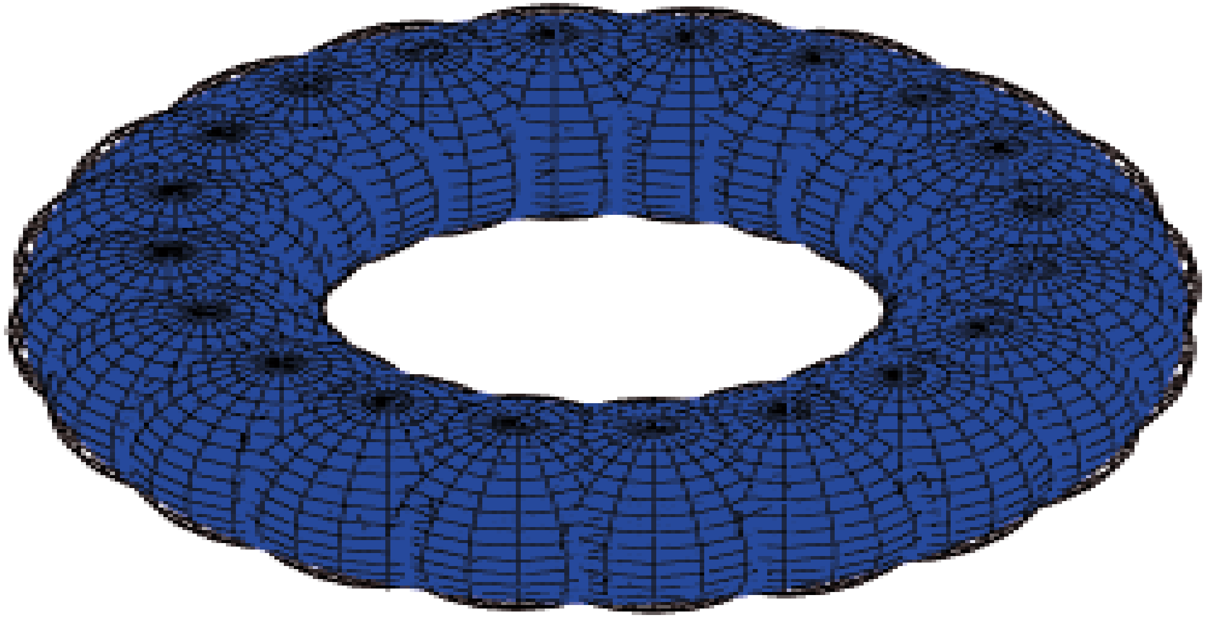


Covering of solid bodies – 3D

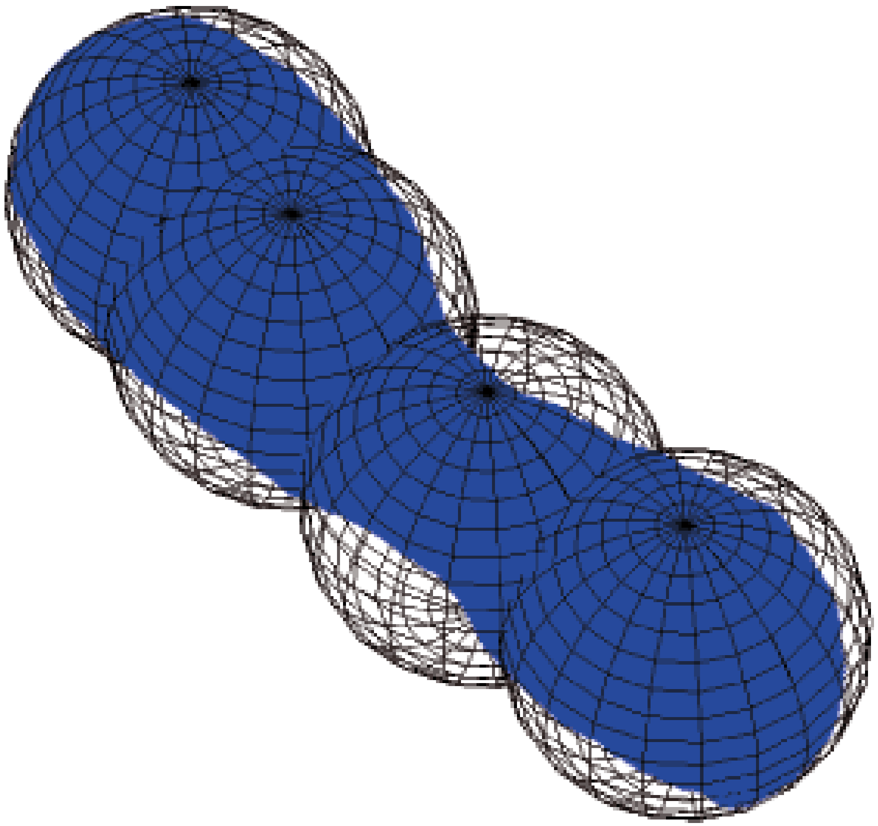
Toro – 224080 Voxels = Cobertura com 10 Esferas



Covering of a toro with 20 spheres



Covering of a beam with 361904 voxels



END

Petrobras Bombas de Exploração
Minimum Sum-of-Squares Clustering k-means
Observações: 1 842 292 - Componentes: 32

GRUPOS	F Min	OCORRENCIAS	DESVIO MED	T MEDIO (seg.)
2	0.299271E+12	10	0.00	13.21
3	0.111334E+12	10	0.00	16.31
4	0.478524E+11	8	35.17	18.99
5	0.379019E+11	10	0.00	24.61
6	0.264045E+11	8	4.50	31.80
7	0.225402E+11	2	5.72	49.87
8	0.199645E+11	8	1.79	45.80
9	0.178466E+11	1	4.30	52.51
10	0.164836E+11	1	2.18	60.33
11	0.148231E+11	1	2.28	68.78
12	0.131286E+11	2	5.09	73.70
13	0.121717E+11	1	5.51	77.22
14	0.112396E+11	1	4.91	93.67

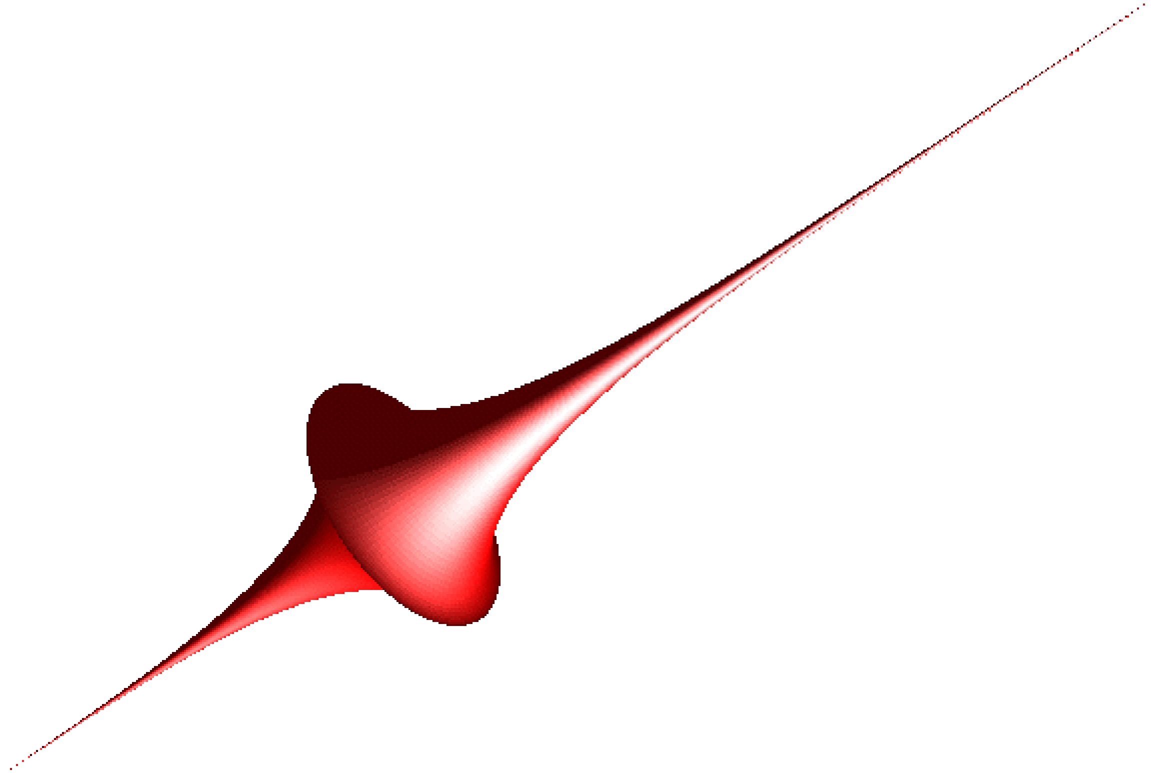
Petrobras Bombas de Exploração

Minimum Sum of Distances Clustering k-median

Observações: 1 842 292 - Componentes: 32

GRUPOS	F Min	OCORRENCIAS	DESVIO MED	T MEDIO (seg.)
2	0.498733D9	10	0.00	384.65
3	0.226730D9	6	40.45	448.07
4	0.189407D9	6	36.34	616.20
5	0.152422D9	10	0.00	574.99
6	0.138617D9	7	0.54	628.25
7	0.127348D9	7	1.56	686.58
8	0.121730D9	1	0.31	760.48
9	0.116238D9	1	1.35	851.12
10	0.111810D9	1	1.87	920.41
11	0.106322D9	1	3.06	1015.11
12	0.103909D9	1	2.70	1074.60
13	0.101445D9	1	2.12	1143.03
14	0.963093D8	1	4.14	1345.27

Logotipo: Pseudo-esfera



Desempenho computacional do HSCM

Os Resultados Computacionais obtidos pelo HSCM, quer no **k-means clustering** ou **k-medians clustering**, oferecem um desempenho diferenciado, segundo critérios de:

- Acurácia
- Consistência
- Escalabilidade
- Velocidade

Computational Optimization and Applications

An incremental clustering algorithm based on hyperbolic smoothing

A.M. Bagirov[1], B. Ordin[2], G. Ozturk[3] and A.E. Xavier[4]

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Bagirov - Prêmio EUROPT 2009

7th EUROPT Workshop on Advances in Continuous Optimization

Remagen, Germany, 3-4 July 2009

Final Report

Traditionally, the EURO working group on continuous optimization – EUROPT – organizes a workshop as a satellite event to the regular EURO conferences. This was the case 2000 in Budapest, 2001 in Rotterdam, 2003 in Istanbul, 2004 in Rhodes, 2006 in Reykjavik, 2007 in Prague, and it was the case this year. On 3-4 July, we organized our 7th EUROPT Workshop on Advances in Continuous Optimization in the German city of Remagen. This place was chosen because of its vicinity to Bonn, the venue of the EURO XXIII conference. EUROPT enjoyed the hospitality of the RheinAhrCampus Remagen, a small but successful University of Applied Sciences, and benefited from their excellent facilities.

Bagirov - Prêmio EUROPT 2009

EUROPT Fellow Adil Bagirov (center) with Marco López (right) and Oliver Stein(left)

1944-
Adilson Elias Xavier

- Brazilian
- Professor COPPE / PESC
- 1982: Proposed the hyperbolic smoothing method for solving non-differentiable problems
- 1982: Proposed the Hyperbolic Smoothing method to solve the general non-linear programming problem