

# The Boosted Difference of Convex functions Algorithm

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School of Mathematical Sciences  
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joint work with **Francisco J. Aragón Artacho**

Variational Analysis and Optimisation Webinar

9th June 2021

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# Outline

- 1 Introduction
- 2 The Boosted DC Algorithm
  - The algorithm: Adding a line search step to DCA
  - Convergence under the Kurdyka–Łojasiewicz property
- 3 Numerical experiments
  - A DC problem in biochemistry
  - The Minimum Sum-of-Squares Clustering Problem
  - The Multidimensional Scaling Problem
- 4 References

# A nonconvex optimization problem

We will focus on the **nonconvex** optimization problem

$$(\mathcal{P}) \underset{x \in \mathbb{R}^m}{\text{minimize}} \quad g(x) - h(x) =: \phi(x),$$

where  $g, h : \mathbb{R}^m \rightarrow \mathbb{R} \cup \{+\infty\}$  are **convex** functions with

$$\inf_{x \in \mathbb{R}^m} \phi(x) > -\infty.$$

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The following assumptions are made:

- WLOG  $g$  and  $h$  are **strongly convex** with modulus  $\rho > 0$   
(otherwise, take  $\tilde{g}(x) := g(x) + \frac{\rho}{2}\|x\|^2$  and  $\tilde{h}(x) := h(x) + \frac{\rho}{2}\|x\|^2$ ).

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- $g$  is **continuously differentiable** on an open set containing  $\text{dom } h$ .
- $h$  is **subdifferentiable** at every point in  $\text{dom } h$ ; i.e.,  $\partial h(x) \neq \emptyset$  for all  $x \in \text{dom } h$ .

# First-order necessary optimality condition and critical points

( $\mathcal{P}$ ) minimize  $\phi(x) := g(x) - h(x)$ , with  $g$  smooth and  $h$  convex  
 $x \in \mathbb{R}^m$

Fact (First-order necessary optimality condition)

If  $x^* \in \text{dom } \phi$  is an optimal solution of ( $\mathcal{P}$ )  $\Rightarrow \partial h(x^*) = \{\nabla g(x^*)\}$ .



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We say that  $\bar{x}$  is a **critical point** of  $(\mathcal{P})$  if  $\nabla g(\bar{x}) \in \partial h(\bar{x})$ .

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$$\phi(x) := \left( \|x\|^2 + \sum_{i=1}^m x_i \right) - \left( \sum_{i=1}^m |x_i| \right).$$

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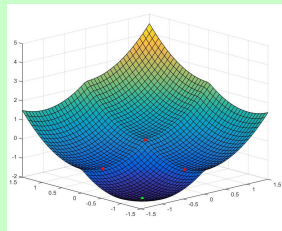
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Then,  $\phi$  has  $2^m$  critical points (any  $x \in \{-1, 0\}^m$ ), and only one point  $x^* := (-1, \dots, -1)$  satisfying  $\partial h(x^*) = \{\nabla g(x^*)\}$ , which is the global minimum of  $\phi$ .



# Previous works: linearizing the nonconvex part

Fukushima–Mine'81

$$(\mathcal{P}) \underset{x \in \mathbb{R}^m}{\text{minimize}} \quad \phi(x) := g(x) - h(x)$$

- In 1981 Fukushima and Mine introduced two algorithms to minimize a **composite function**  $g - h$ , where  $g$  is **(strictly) convex** (possibly nonsmooth) and  $h$  is **smooth** (possibly nonconvex).

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**ALGORITHM 1 (FM'81):** Fix some parameters  $\alpha > 0$  and  $0 < \beta < 1$ . Let  $x_0$  be any initial point and set  $k := 0$ .

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- In 1986 Pham Dinh and Souad introduced an algorithm to minimize a **DC functions**  $g - h$ , where  $g$  and  $h$  are **both convex** (*possibly nonsmooth*). This was further developed by Pham Dinh, Le Thi and their collaborators.

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**ALGORITHM 2 (DCA):** Let  $x_0$  be any initial point and set  $k := 0$ .

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## Proposition

If  $g$  and  $h$  are strongly convex with constant  $\rho > 0$ , then

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$\Rightarrow$  If  $0 < \alpha \leq \rho$ , the iterations of FM'81 and DCA coincide.

# FM'81 and DCA

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- FM'81 is based on the fact that  $d_k := y_k - x_k$  is a descent direction at  $x_k$ : it holds  $\phi'(x_k; d_k) \leq -\rho \|d_k\|^2$ .
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Yes, if  $g$  is **smooth**, thanks to the fact that

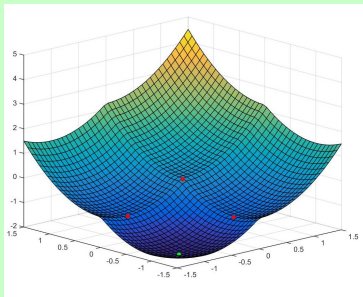
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# DCA can be slow and get easily trapped by critical points

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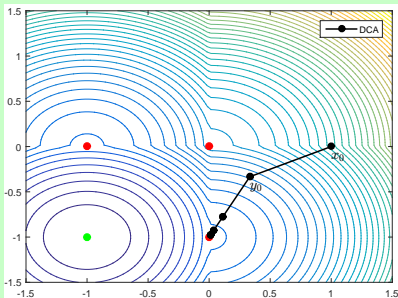


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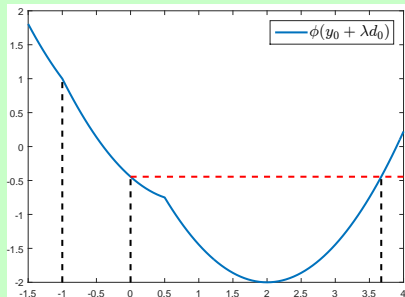
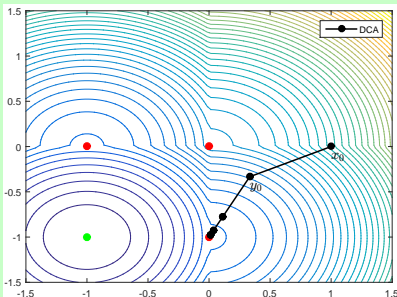


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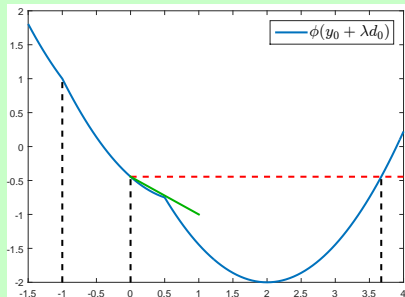
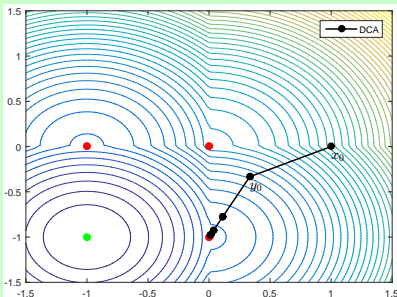


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# Outline

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- 2 **The Boosted DC Algorithm**
  - The algorithm: Adding a line search step to DCA
  - Convergence under the Kurdyka–Łojasiewicz property
- 3 Numerical experiments
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$$\phi(x) := g(x) - h(x), u_k \in \partial h(x_k), y_k \in \partial g^*(u_k)$$

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Hence

$$\phi'(y_k; d_k) \leq \langle \nabla g(y_k) - v, d_k \rangle = \langle u_k - v, y_k - x_k \rangle \leq -\rho \|d_k\|^2. \quad \blacksquare$$

# The Boosted DC Algorithm

## BDCA (*Boosted DC Algorithm*)

Fix  $\alpha > 0$  and  $0 < \beta < 1$ . Let  $x_0$  be any initial point and set  $k := 0$ .

- 1 Select  $u_k \in \partial h(x_k)$  and find the unique solution  $y_k$  of the problem

$$(\mathcal{P}_k) \underset{x \in \mathbb{R}^m}{\text{minimize}} \quad g(x) - \langle u_k, x \rangle.$$

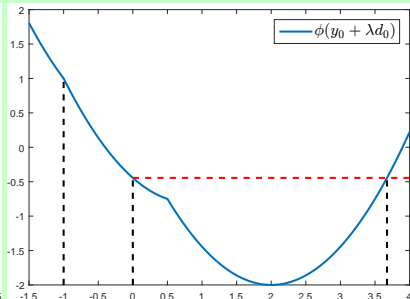
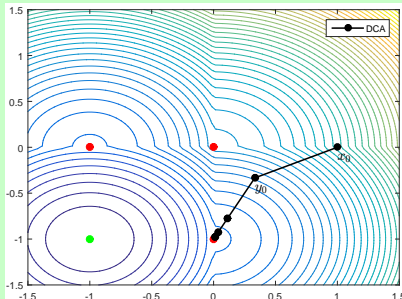
- 2 Set  $d_k := y_k - x_k$ . If  $d_k = 0 \Rightarrow$  **stop** and **return**  $x_k$ .
- 3 Choose **any**  $\bar{\lambda}_k \geq 0$ . Set  $\lambda_k := \bar{\lambda}_k$ .  
**while**  $\phi(y_k + \lambda_k d_k) > \phi(y_k) - \alpha \lambda_k^2 \|d_k\|^2$  **do**  $\lambda_k := \beta \lambda_k$ .
- 4 Set  $x_{k+1} := y_k + \lambda_k d_k$ ,  $k := k + 1$ , and **go to** Step 1.

# DCA vs BDCA

## Example (Revisited)

Consider the DC function  $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}$  defined as  $\phi := g - h$ , where

$$g(x) = \frac{3}{2} (x_1^2 + x_2^2) + x_1 + x_2 \quad \text{and} \quad h(x) = |x_1| + |x_2| + \frac{1}{2} (x_1^2 + x_2^2).$$

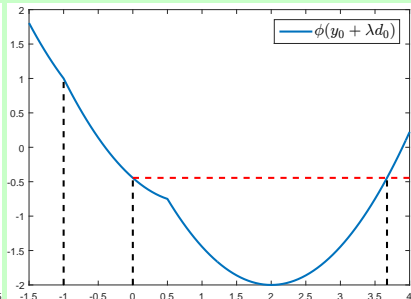
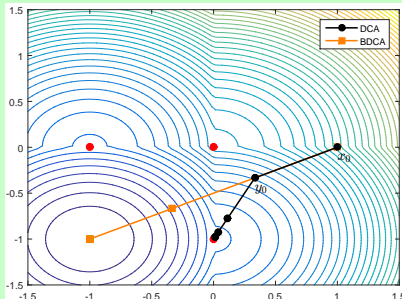


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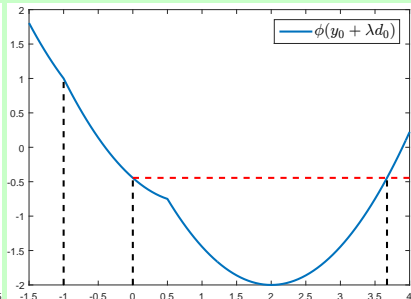
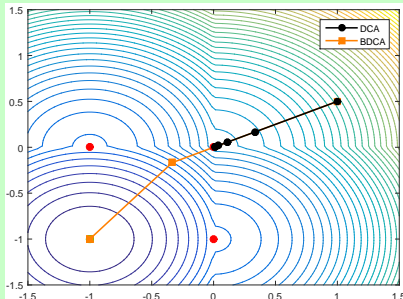


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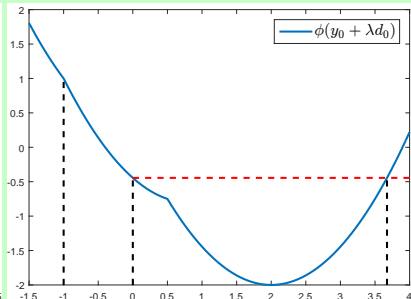
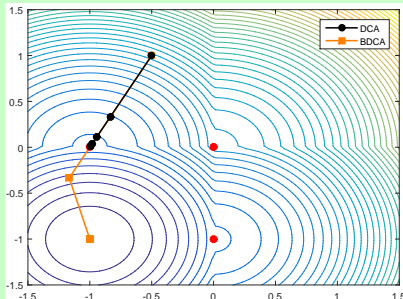


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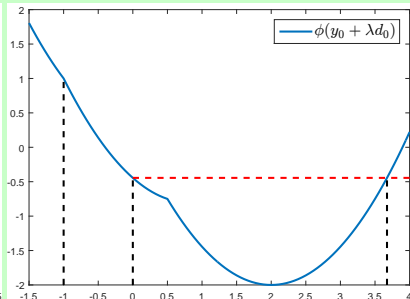
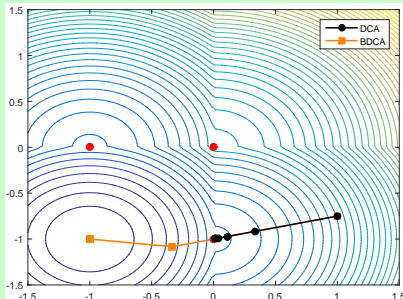


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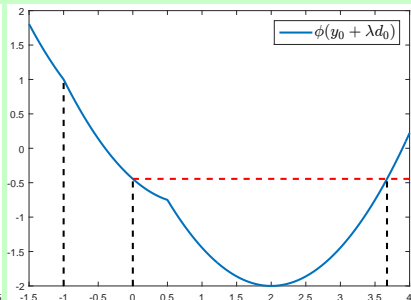
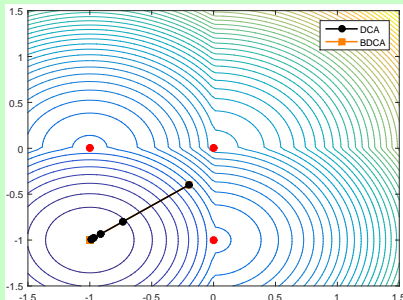


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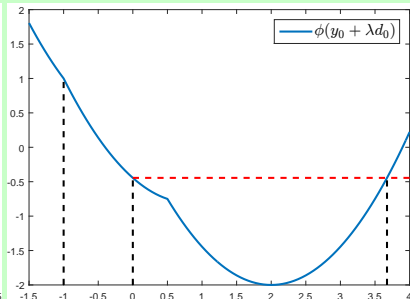
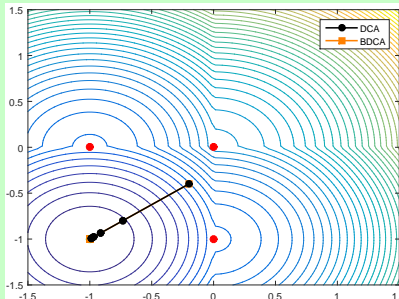


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	$(-1, -1)$	$(-1, 0)$	$(0, -1)$	$(0, 0)$
DCA	249,763	249,841	250,204	250,192
BDCA	996,104	1,922	1,974	0

**Table:** For one million random starting points in  $[-1.5, 1.5]^2$ , we count the sequences converging to each of the four stationary points.

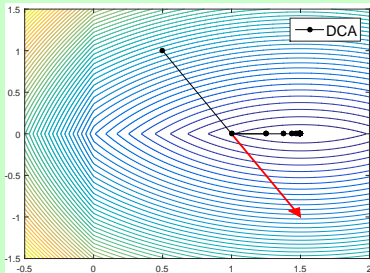
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## Example (Failure of BDCA when $g$ is not differentiable)

Consider the following modification of the previous example

$$g(x) = -\frac{5}{2}x_1 + x_1^2 + x_2^2 + |x_1| + |x_2| \quad \text{and} \quad h(x) = \frac{1}{2}(x_1^2 + x_2^2),$$

so  $h$  is differentiable but  $g$  is not. Let  $x_0 = (0.5, 1)$ . The point generated by DCA is  $y_0 = (1, 0)$  and  $d_0 = y_0 - x_0 = (0.5, -1)$  is not a descent direction for  $\phi$  at  $y_0$ :



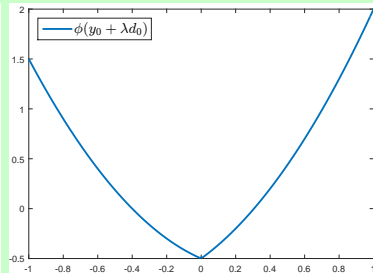
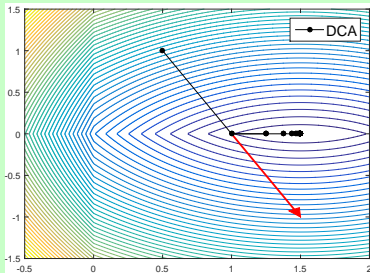
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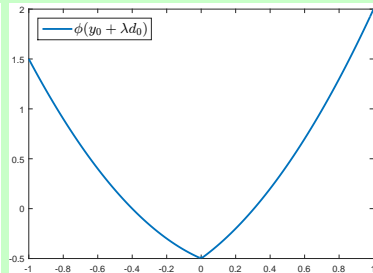
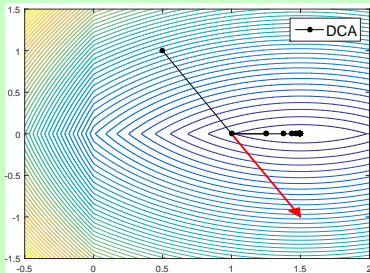
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## Proposition

Let  $\phi = g - h$ , where  $g : \mathbb{R} \rightarrow \mathbb{R}$  and  $h : \mathbb{R} \rightarrow \mathbb{R}$  are convex and  $h$  is differentiable. If  $0 \notin \partial_C \phi(y_k)$ , then  $\phi'(y_k; y_k - x_k) < 0$ .

# Convergence of BDCA

$$(\mathcal{P}) \underset{x \in \mathbb{R}^m}{\text{minimize}} \phi(x) := g(x) - h(x)$$

Our convergence results follow the ideas from



[H. Attouch, J. Bolte](#): On the convergence of the proximal algorithm for nonsmooth functions involving analytic features. *Math. Program.* 116 (2009), 5–16.

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- 3  $\sum_{k=0}^{+\infty} \|d_k\|^2 < +\infty$ . Further, if there is some  $\bar{\lambda}$  such that  $\lambda_k \leq \bar{\lambda}$  for all  $k$ , then  $\sum_{k=0}^{+\infty} \|x_{k+1} - x_k\|^2 < +\infty$ .



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# The Kurdyka–Łojasiewicz property

## Definition

Let  $f : \mathbb{R}^m \rightarrow \mathbb{R}$  be a locally Lipschitz function. We say that  $f$  satisfies the **strong Kurdyka–Łojasiewicz inequality** at  $x^* \in \mathbb{R}^m$  if there exist  $\eta \in ]0, +\infty[$ , a neighborhood  $U$  of  $x^*$ , and a concave function  $\varphi : [0, \eta] \rightarrow [0, +\infty[$  such that:

- 1  $\varphi(0) = 0$ ;
- 2  $\varphi$  is of class  $\mathcal{C}^1$  on  $]0, \eta[$ ;
- 3  $\varphi' > 0$  on  $]0, \eta[$ ;
- 4 for all  $x \in U$  with  $f(x^*) < f(x) < f(x^*) + \eta$  we have
 
$$\varphi'(f(x) - f(x^*)) \operatorname{dist}(0, \partial_C f(x)) \geq 1.$$

Here  $\partial_C f$  stands for the **Clarke subdifferential**

$$\partial_C f(\bar{x}) = \operatorname{co} \left\{ \lim_{x \rightarrow \bar{x}, x \notin \Omega_f} \nabla f(x) \right\},$$

where  $\operatorname{co}$  stands for the convex hull and  $\Omega_f$  denotes the set of Lebesgue measure zero where  $f$  fails to be differentiable.

# Convergence under the Kurdyka–Łojasiewicz property

$$(\mathcal{P}) \underset{x \in \mathbb{R}^m}{\text{minimize}} \quad \phi(x) := g(x) - h(x)$$

## Theorem (Convergence)

Let  $\{x_k\}$  be the sequence generated by the BDCA. Suppose that  $\{x_k\}$  has a **cluster point**  $x^*$ , that  $\nabla g$  is **locally Lipschitz** around  $x^*$  and that  $\phi$  satisfies the **strong Kurdyka–Łojasiewicz** inequality at  $x^*$ . Then  $\{x_k\}$  **converges** to  $x^*$ , which is a **critical point** of  $(\mathcal{P})$ .

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## Proof

- Technical but “standard”.
- $\lambda_k$  can be zero or unbounded!
- We either need Clarke’s subdifferential or to assume that  $-\phi$  satisfies the Kurdyka–Łojasiewicz inequality:

$$\nabla g(y_k) - \nabla g(x_k) \in \partial h(x_k) - \nabla g(x_k) = \boxed{\partial_C(-\phi(x_k)) = -\partial_C\phi(x_k)}$$

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## Theorem (Rate)

Suppose that the sequence  $\{x_k\}$  generated by the BDCA has the limit point  $x^*$ , that  $\nabla g$  is **locally Lipschitz** continuous around  $x^*$  and  $\phi$  satisfies the **strong Kurdyka–Łojasiewicz** inequality at  $x^*$  with  $\varphi(t) = Mt^{1-\theta}$  for some  $M > 0$  and  $0 \leq \theta < 1$ . Then:

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- 3 if  $\theta \in ]\frac{1}{2}, 1[$ , then  $\exists \eta > 0$  s.t.  $\|x_k - x^*\| \leq \eta k^{-\frac{1-\theta}{2\theta-1}}$  for all large  $k$ .

# How to choose the trial step size $\bar{\lambda}_k$ ?

## BDCA (*Boosted DC Algorithm*)

Fix  $\alpha > 0$  and  $0 < \beta < 1$ . Let  $x_0$  be any initial point and set  $k := 0$ .

- 1 Select  $u_k \in \partial h(x_k)$  and  $y_k \in \partial g^*(u_k)$ .
- 2 Set  $d_k := y_k - x_k$ . If  $d_k = 0 \Rightarrow$  **stop** and **return**  $x_k$ .
- 3 Choose **any**  $\bar{\lambda}_k \geq 0$ . Set  $\lambda_k := \bar{\lambda}_k$ .  
**while**  $\phi(y_k + \lambda_k d_k) > \phi(y_k) - \alpha \lambda_k^2 \|d_k\|^2$  **do**  $\lambda_k := \beta \lambda_k$ .
- 4 Set  $x_{k+1} := y_k + \lambda_k d_k$ ,  $k := k + 1$ , and **go to** Step 1.

One possibility would be to set  $\bar{\lambda}_k = \bar{\lambda}$  for all  $k$ .



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One possibility would be to set  $\bar{\lambda}_k = \bar{\lambda}$  for all  $k$ . Instead, we propose:

## Self-adaptive trial step size

Fix  $\gamma > 1$ . Set  $\bar{\lambda}_0 := 0$ . Choose some  $\bar{\lambda}_1 > 0$  and obtain  $\lambda_1$  by BDCA. For any  $k \geq 2$ :

- 1 **if**  $\lambda_{k-2} = \bar{\lambda}_{k-2}$  **and**  $\lambda_{k-1} = \bar{\lambda}_{k-1}$  **then** set  $\bar{\lambda}_k := \gamma \lambda_{k-1}$ ;  
**else** set  $\bar{\lambda}_k := \lambda_{k-1}$ .
- 2 Obtain  $\lambda_k$  from  $\bar{\lambda}_k$  by the backtracking step of BDCA.

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# Experiment 1: Finding steady states of biochemical networks

We were interested in finding a solution to the problem

$$\underset{x \in \mathbb{R}^m}{\text{minimize}} \quad \phi(x) := \|p(x) - c(x)\|^2$$

where

$$p(x) := [F, R] \exp\left(p + [F, R]^T x\right) \quad \text{and} \quad c(x) := [R, F] \exp\left(p + [F, R]^T x\right),$$

and  $F, R \in \mathbb{Z}_{\geq 0}^{m \times n}$  ( $m$  molecular species,  $n$  reversible elementary reactions).

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- We can then apply BDCA to the functions

$$g(x) := 2\left(\|p(x)\|^2 + \|c(x)\|^2\right) + \frac{\rho}{2}\|x\|^2 \quad \text{and} \quad h(x) := \|p(x) + c(x)\|^2 + \frac{\rho}{2}\|x\|^2,$$

for any  $\rho > 0$ . Our results **guarantee the convergence** of the sequence generated by BDCA, **as long as the sequence is bounded**.

# Finding steady states of biochemical networks

A boring table of computational results. . .

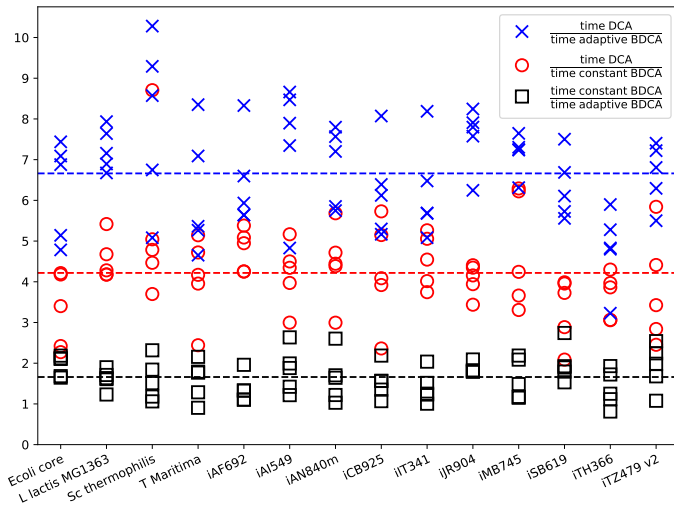
Taking  $\rho := 100$ ,  $\bar{\lambda}_k := 50$  (constant),  $\beta := 0.5$  and  $\alpha := 0.4$ , we obtain:

DATA			ALGORITHMS: Time Spent (seconds)						RATIO (avg.)	
Model Name	m	n	BDCA			DCA			DCA/BDCA	
			min.	max.	avg.	min.	max.	avg.	iter.	time
Ecoli core	72	94	16	26	20	68	105	87	4.9	4.4
L lactis MG1363	486	615	2926	4029	3424	14522	18212	16670	5.2	4.9
Sc thermophilis	349	444	291	553	358	1302	2004	1611	4.9	4.5
T Maritima	434	554	1333	2623	1920	5476	12559	8517	4.7	4.4
iAF692	466	546	1677	2275	1967	8337	11187	9466	5.3	4.8
iAI549	307	355	177	254	209	665	1078	913	4.9	4.4
iAN840m	549	840	3229	6939	4721	16473	28957	21413	5.0	4.5
iCB925	416	584	1831	2450	2133	7358	11465	9887	5.0	4.6
iIT341	425	504	1925	2883	2302	9434	20310	12262	5.7	5.3
iJR904	597	915	6363	9836	7623	24988	43640	33621	4.4	4.8
iMB745	528	652	2629	5091	4252	16438	25172	20269	5.0	4.8
iSB619	462	598	2407	5972	3323	8346	25468	13967	4.3	4.2
iTH366	587	713	3310	5707	4464	13613	30044	20715	5.0	4.6
iTZ479 v2	435	560	1211	2656	2216	7368	12592	10120	4.9	4.6

For each model, we selected a random kinetic parameter  $p \in [-1, 1]^{2n}$  and 10 initial random points  $x_0 \in [-2, 2]^m$ . BDCA was run 1000 iterations, DCA was run until it reached the same value obtained by BDCA.

# Finding steady states of biochemical networks

Comparison of the constant and self-adaptive trial step size strategy for BDCA





# Applications to Biochemistry

Nature Protocols (2019)

## The COBRA Toolbox

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## The COntstraint-Based Reconstruction and Analysis Toolbox

View The COBRA Toolbox source code on [GitHub](#).



The COntstraint-Based Reconstruction and Analysis Toolbox is a MATLAB software suite for quantitative prediction of cellular and multicellular biochemical networks with constraint-based modelling. It implements a comprehensive collection of basic and advanced modelling methods, including reconstruction and model generation as well as biased and unbiased model-driven analysis methods.

It is widely used for modelling, analysing and predicting a variety of metabolic phenotypes using genome-scale biochemical networks.

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# The Minimum Sum-of-Squares Clustering Problem

**Clustering** is an unsupervised technique for data analysis whose objective is to **group** a collection of objects **into clusters** based on similarity.

- Let  $A = \{a^1, \dots, a^n\}$  be a finite set of points in  $\mathbb{R}^m$ , which represent the data points to be grouped.
- The goal is to partition  $A$  into  $k$  disjoint subsets  $A^1, \dots, A^k$ , called clusters, such that a clustering criterion is optimized.

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The *Minimum Sum-of-Squares Clustering* criterion, one tries to minimize the Euclidean distance of each data point to the centroid of its clusters, denoted by  $X := (x^1, \dots, x^k) \in \mathbb{R}^{m \times k}$ :

$$\underset{X \in \mathbb{R}^{m \times k}}{\text{minimize}} \phi(X) := \frac{1}{n} \sum_{i=1}^n \min_{j=1, \dots, k} \|x^j - a^i\|^2$$

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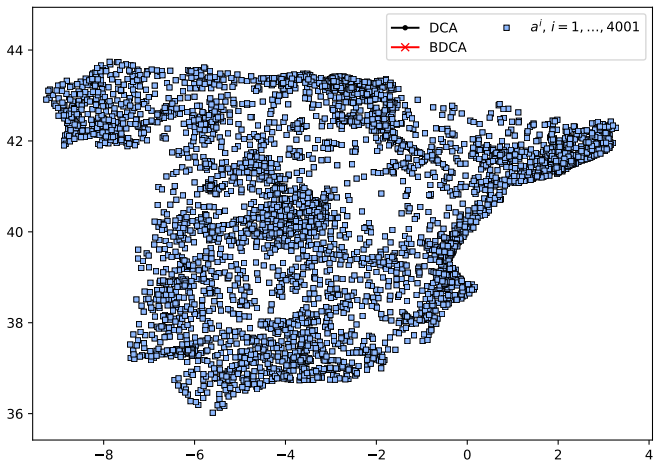
where

$$g(X) := \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^k \|x^j - a^i\|^2 + \frac{\rho}{2} \|X\|^2, \quad (\text{strongly convex and smooth})$$

$$h(X) := \frac{1}{n} \sum_{i=1}^n \max_{j=1, \dots, k} \sum_{t=1, t \neq j}^k \|x^t - a^i\|^2 + \frac{\rho}{2} \|X\|^2. \quad (\text{strongly convex but nonsmooth}).$$

## Experiment 2: Clustering the Spanish cities in the peninsula

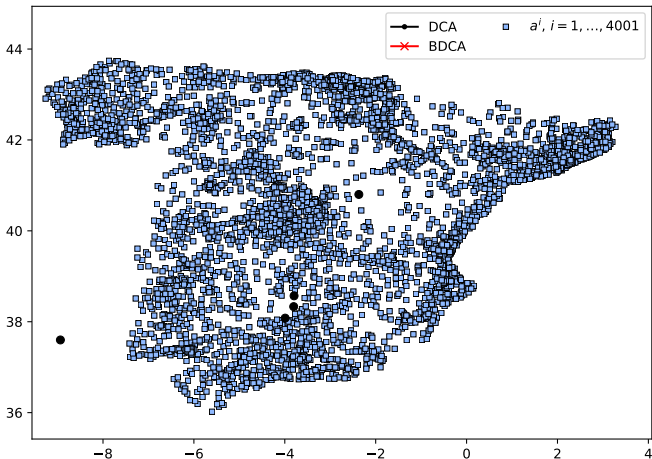
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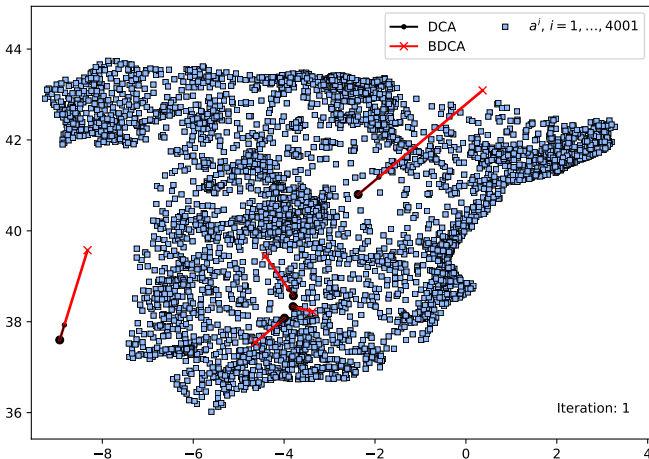
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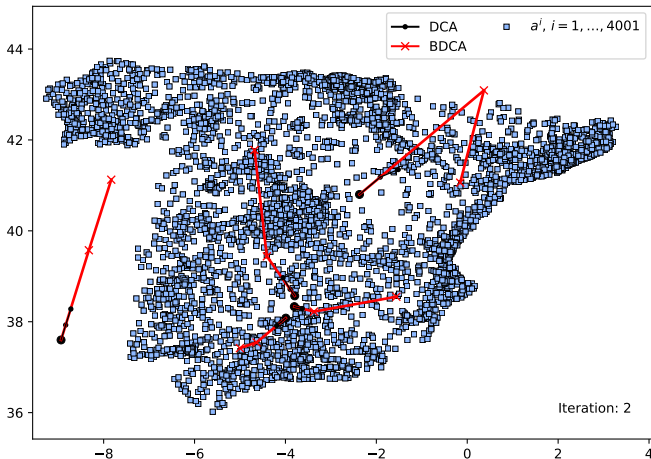


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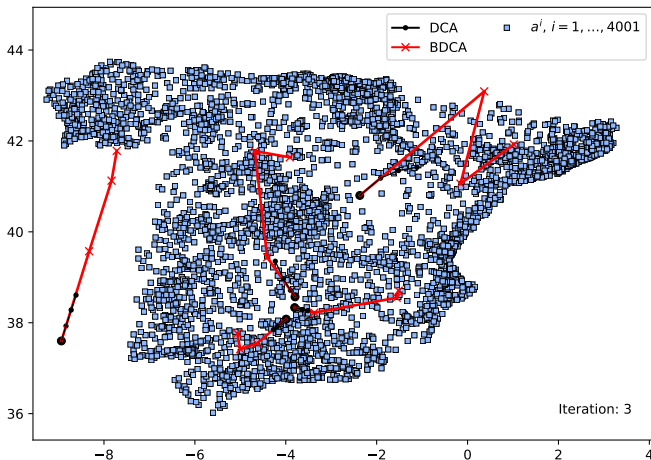
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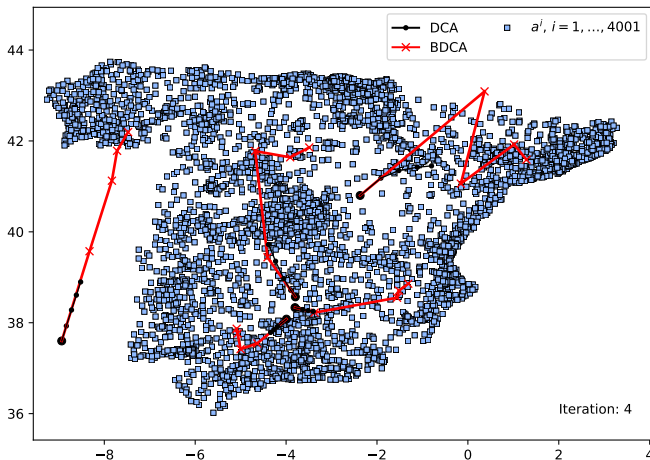
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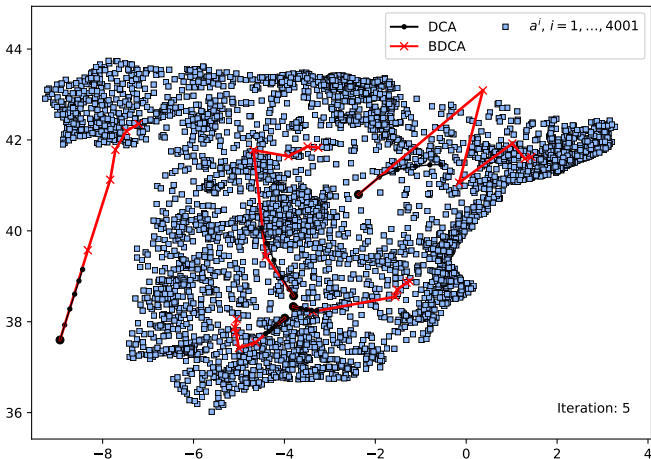
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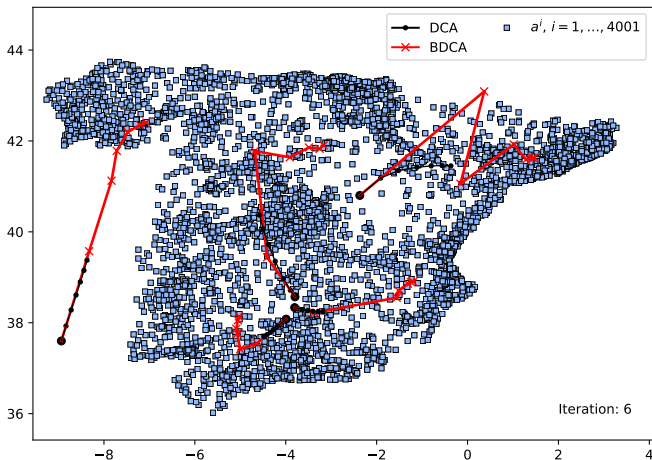
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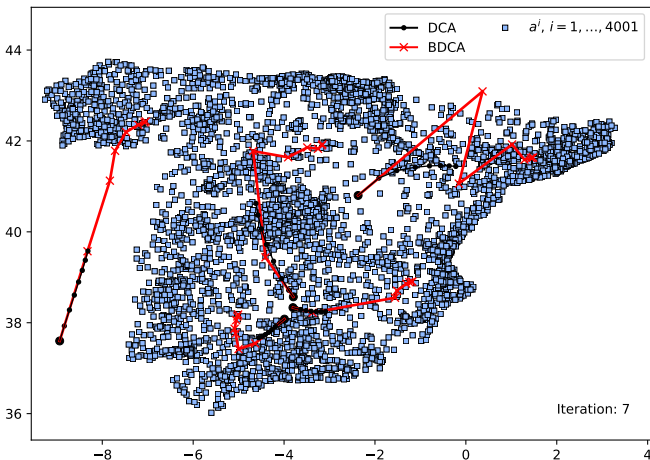
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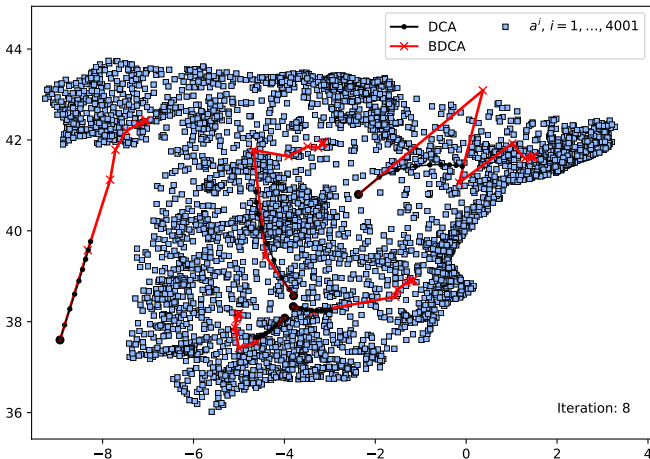
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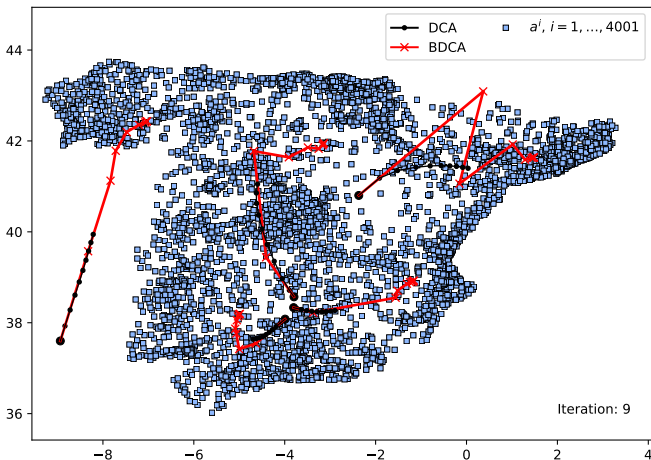
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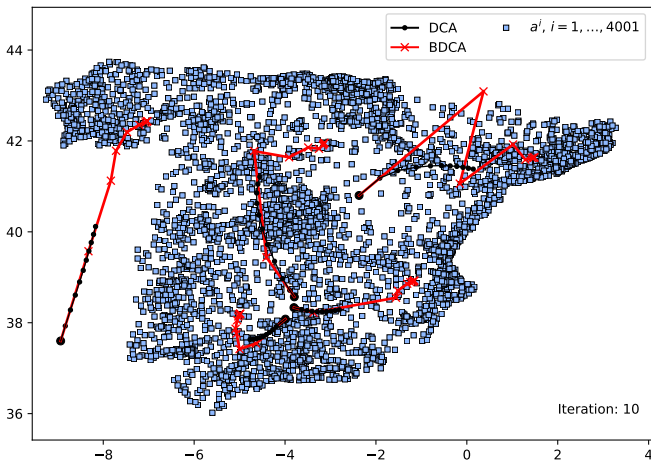


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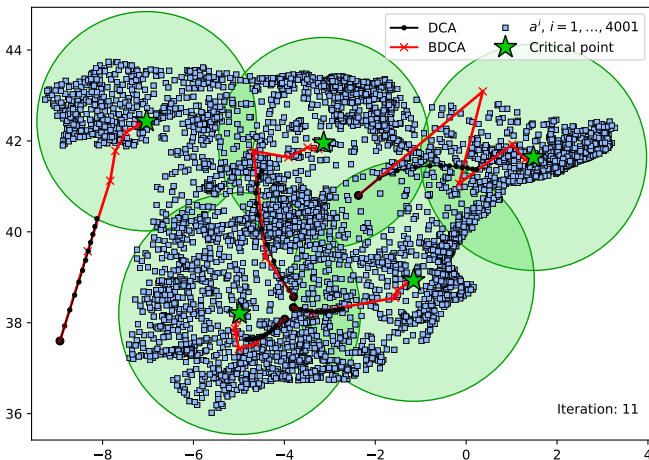
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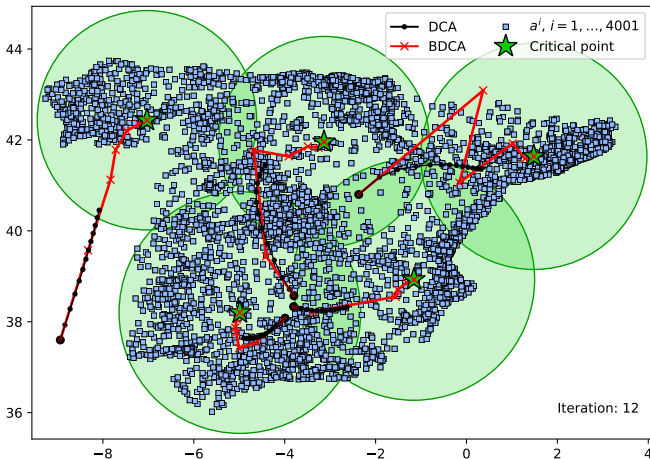
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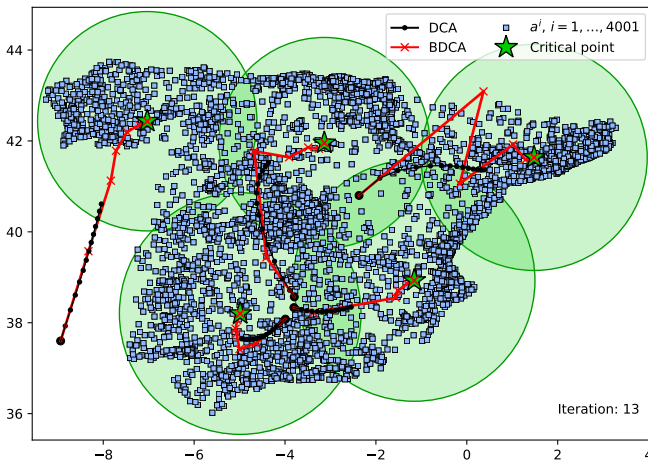
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## Experiment 2: Clustering the Spanish cities in the peninsula

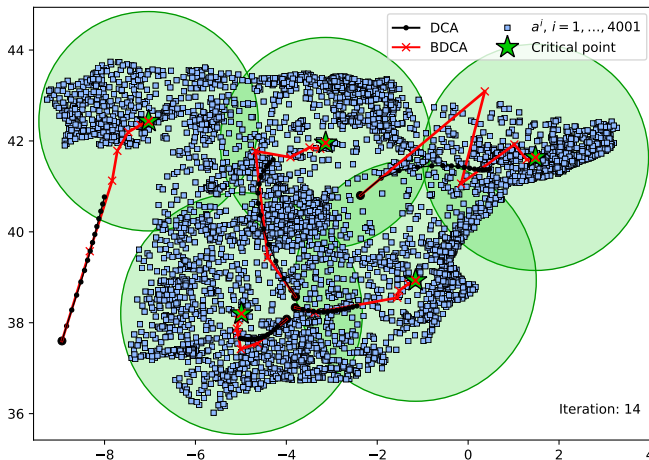
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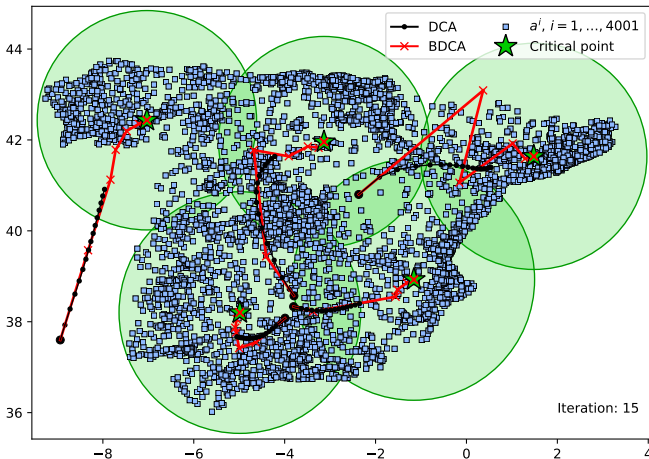
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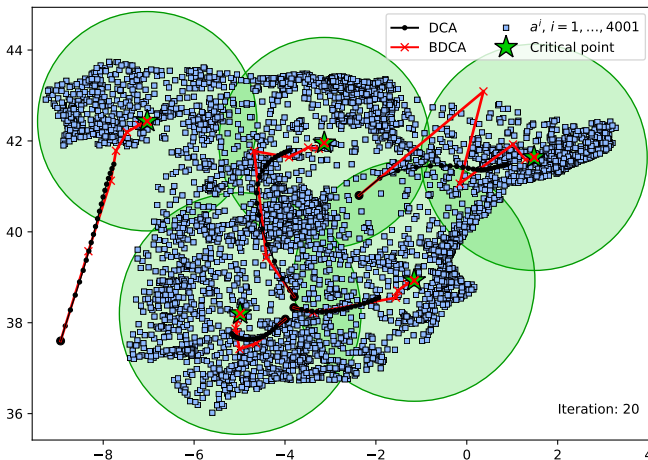
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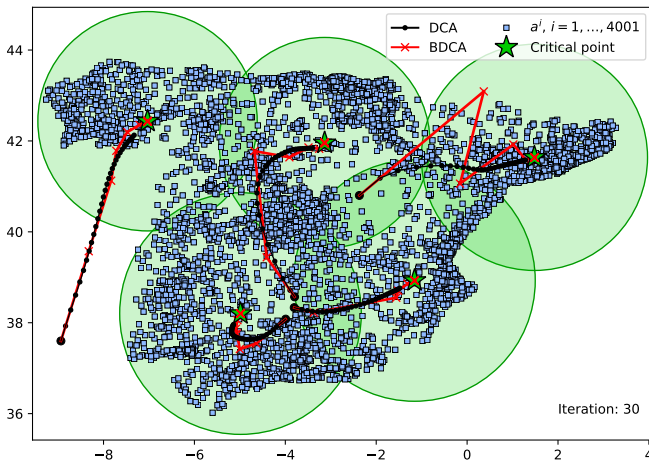
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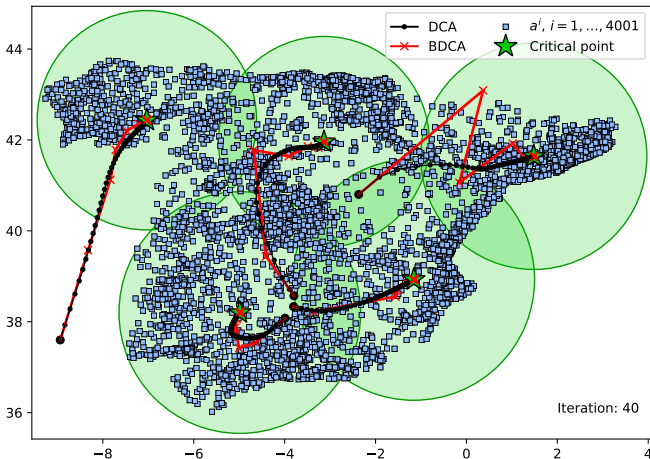


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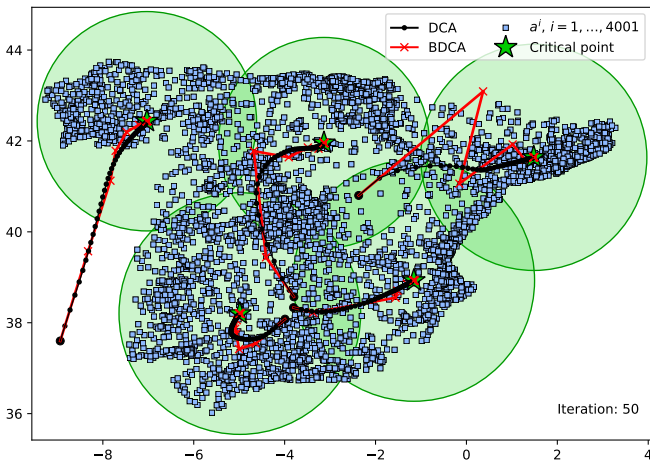
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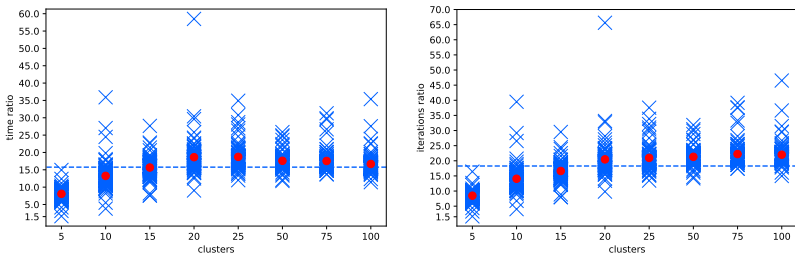
**PROBLEM:** Find a partition into  $k$  clusters of the 4001 Spanish cities in the peninsula with more than 500 residents, with  $k \in \{5, 10, 15, 20, 25, 50, 75, 100\}$ .

For 100 random starting points, BDCA was stopped when the relative error of  $\phi$  was smaller than  $10^{-3}$ . Then, DCA was run from the same starting point until the same value of the objective function was reached (which did not happen in 31 instances).

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**Figure:** Comparison between DCA and BDCA. We represent the ratios of running time (left) and number of iterations (right) between DCA and BDCA.

## Experiment 3: Clustering random points in an $m$ -dimensional box

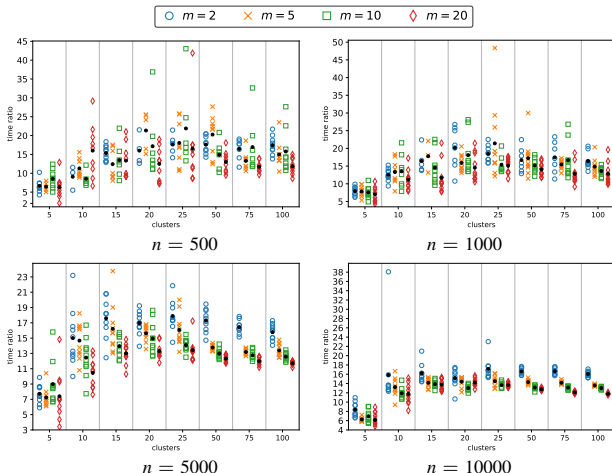
We took  $n$  random points in  $\mathbb{R}^m$  (normal distribution), with  $n \in \{500, 1000, 5000, 10000\}$  and  $m \in \{2, 5, 10, 20\}$ . For each  $(n, m)$ , 10 random starting points were chosen. Then:

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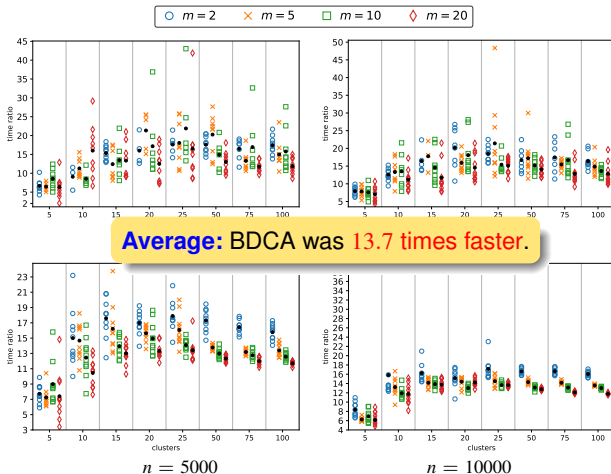
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# Outline

- 1 Introduction
- 2 The Boosted DC Algorithm
  - The algorithm: Adding a line search step to DCA
  - Convergence under the Kurdyka–Łojasiewicz property
- 3 Numerical experiments
  - A DC problem in biochemistry
  - The Minimum Sum-of-Squares Clustering Problem
  - **The Multidimensional Scaling Problem**
- 4 References



# The Multidimensional Scaling Problem

Suppose that we have a table of distances between some objects, known as the **dissimilarity matrix**. If the objects are  $n$  points  $x^1, x^2, \dots, x^n$  in  $\mathbb{R}^q$ , the dissimilarity matrix can be defined by the Euclidean distance between them:

$$\delta_{ij} = \|x^i - x^j\| := \mathbf{d}_{ij}(X),$$

where we denote by  $X$  the  $n \times q$  matrix whose rows are  $x^1, x^2, \dots, x^n$ .

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Given a target dimension  $p \leq q$ , the **MDS problem** consists in finding  $n$  points in  $\mathbb{R}^p$ , which are represented by an  $n \times p$  matrix  $X^*$ , such that

$$\text{Stress}(X^*) := \sum_{i < j} w_{ij} (\mathbf{d}_{ij}(X^*) - \delta_{ij})^2$$

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This can be equivalently formulated as a DC problem by setting

$$g(X) := \frac{1}{2} \sum_{i < j} w_{ij} \mathbf{d}_{ij}^2(X) + \frac{\rho}{2} \|X\|^2,$$

$$h(X) := \sum_{i < j} w_{ij} \delta_{ij} \mathbf{d}_{ij}(X) + \frac{\rho}{2} \|X\|^2,$$

for some  $\rho \geq 0$ . Moreover, it is clear that  $g$  is differentiable while  $h$  is not, but  $\partial h$  can be explicitly computed.

## Experiment 4: MDS for Spanish cities

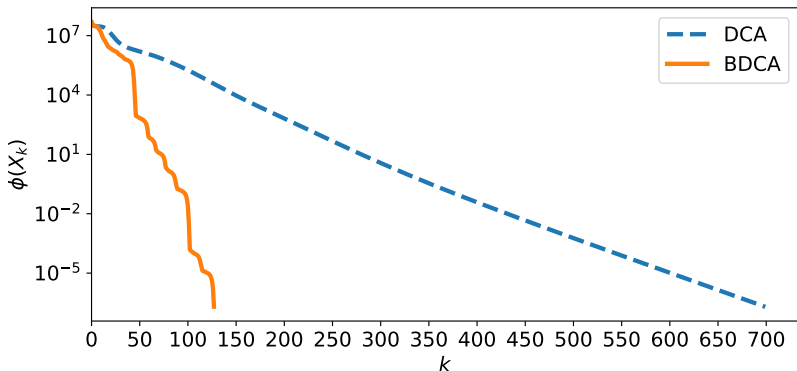
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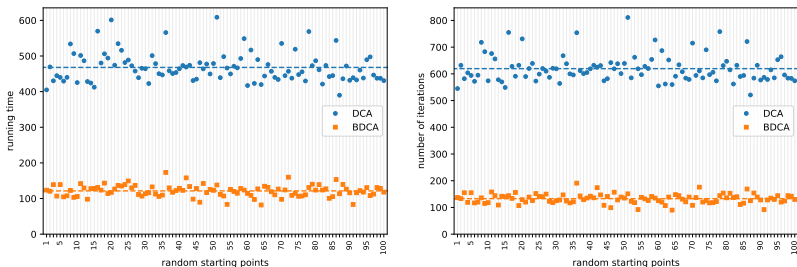
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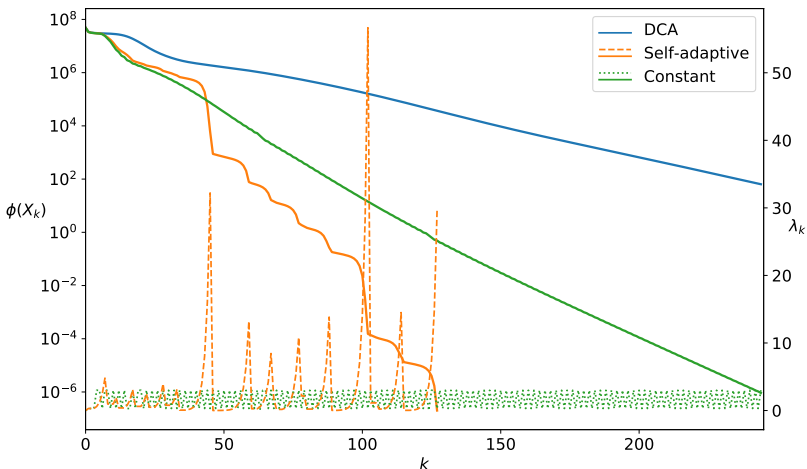
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**Figure:** Running time (left) and number of iterations (right) of DCA and BDCA for 100 random instances.

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# Main References



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