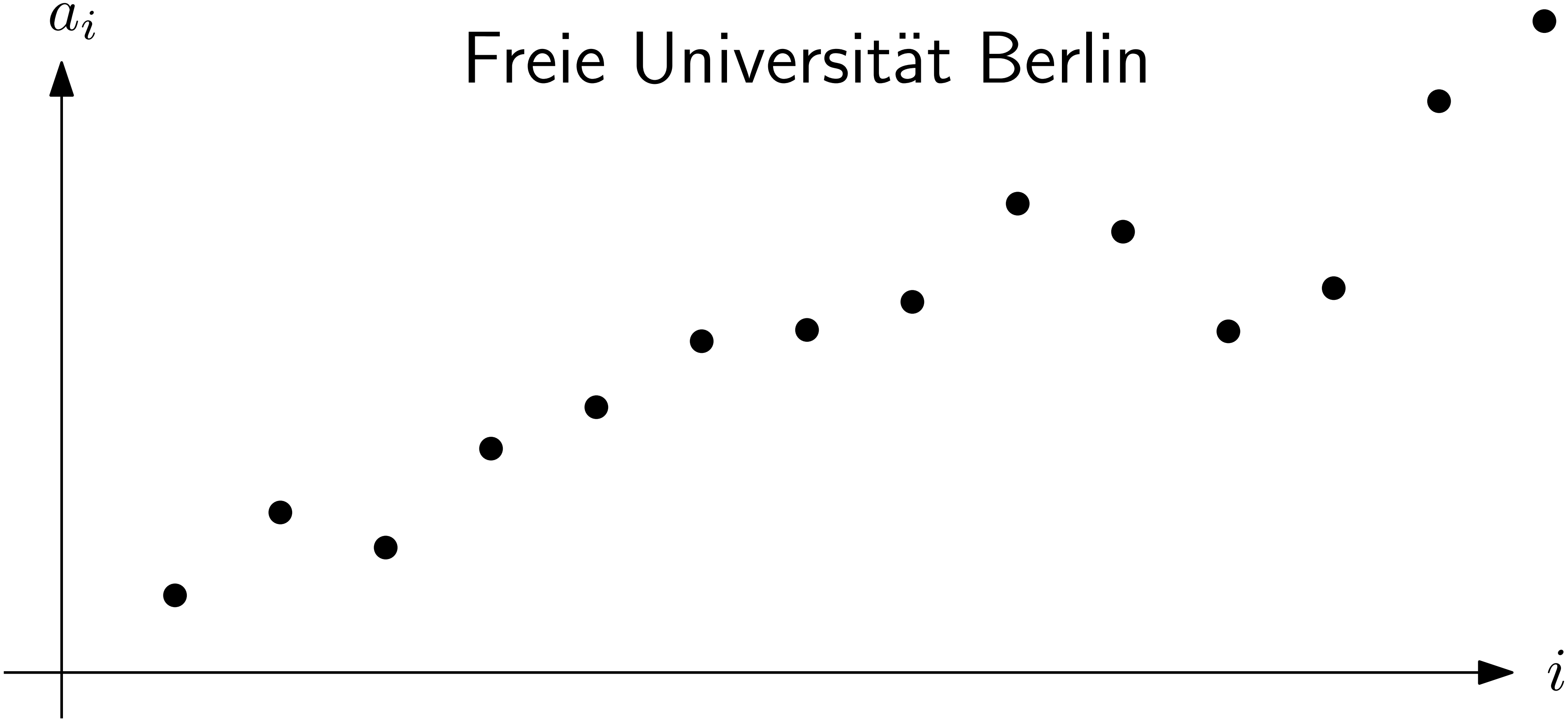
Algorithms for Isotonic Regression

Günter Rote

Freie Universität Berlin



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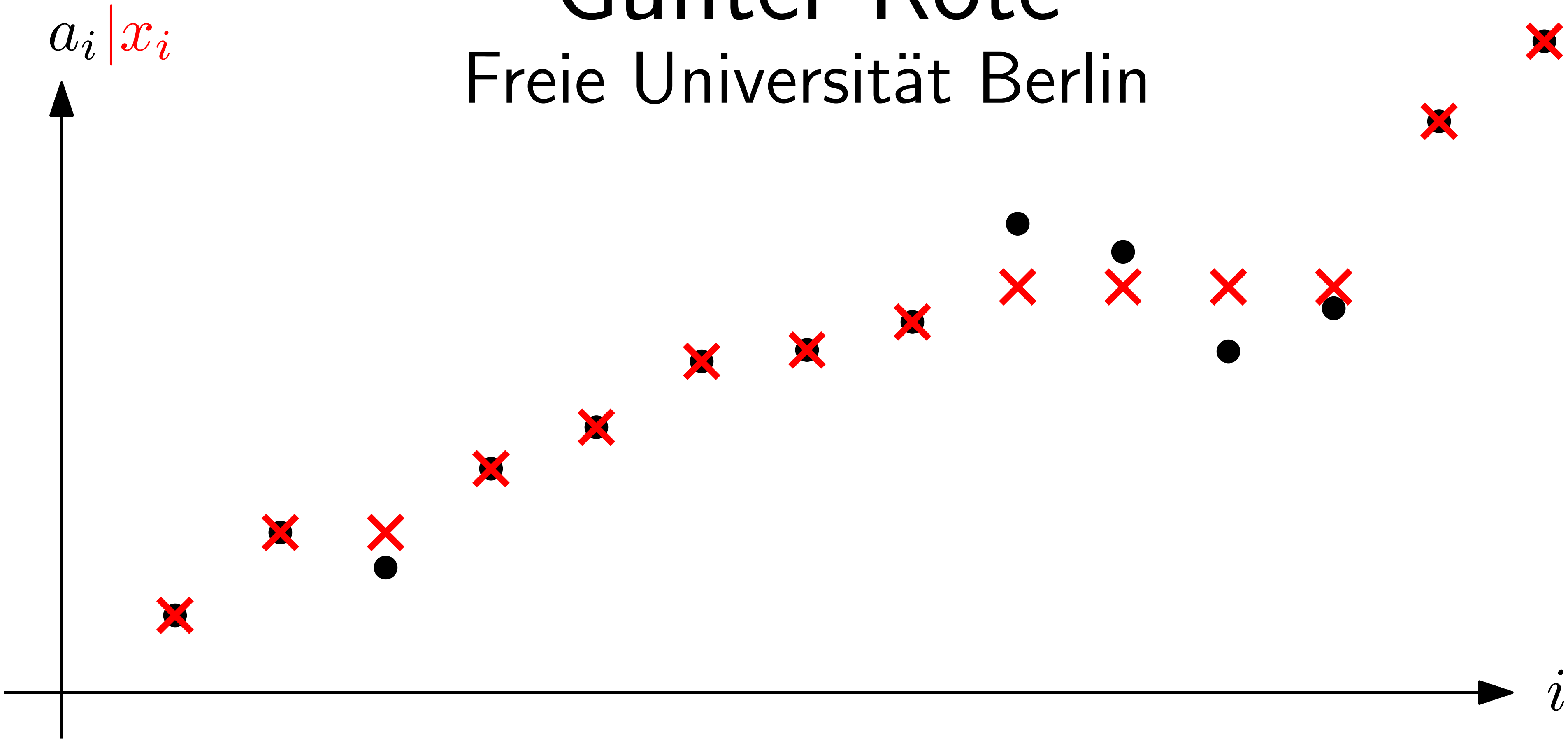

$$\text{Minimize} \sum_{i=1}^{n} h(|x_i - a_i|) \text{ subject to } x_1 \leq \cdots \leq x_n$$

Objective functions

Minimize $\sum_{i=1}^{n} h(|x_i - a_i|)$ subject to $x_1 \le \cdots \le x_n$

- $h(z) = z$: L_1-regression $\quad \sum_{i=1}^{n} |x_i - a_i| \to \min$
- $h(z) = z^2$: L_2-regression $\quad \sum_{i=1}^{n} (x_i - a_i)^2 \to \min$
- $h(z) = z^p$, $p \to \infty$: L_∞-regression $\quad \max_{1 \le i \le n} |x_i - a_i| \to \min$

versions with weights $w_i > 0$:

$$\sum_{i=1}^{n} w_i |x_i - a_i|, \qquad \sum_{i=1}^{n} w_i (x_i - a_i)^2, \qquad \max_{1 \le i \le n} w_i |x_i - a_i|,$$

General form: $\sum_{i=1}^{n} h_i(x_i) \to \min \;\Big/\; \max_{1 \le i \le n} h_i(x_i) \to \min$

$(*)$ h_i convex and piecewise “simple”

Overview

- The classical *Pool Adjacent Violators* (PAV) algorithm
- dynamic programming
- More general constraints:

$$x_i \le x_j \text{ for } i \prec j$$

  with a given partial order $\prec$

  - In particular, $L_{\max}$ regression with a d-dimensional partial order
  - Randomized optimization technique of Timothy Chan (1998)

Pool Adjacent Violators (PAV)

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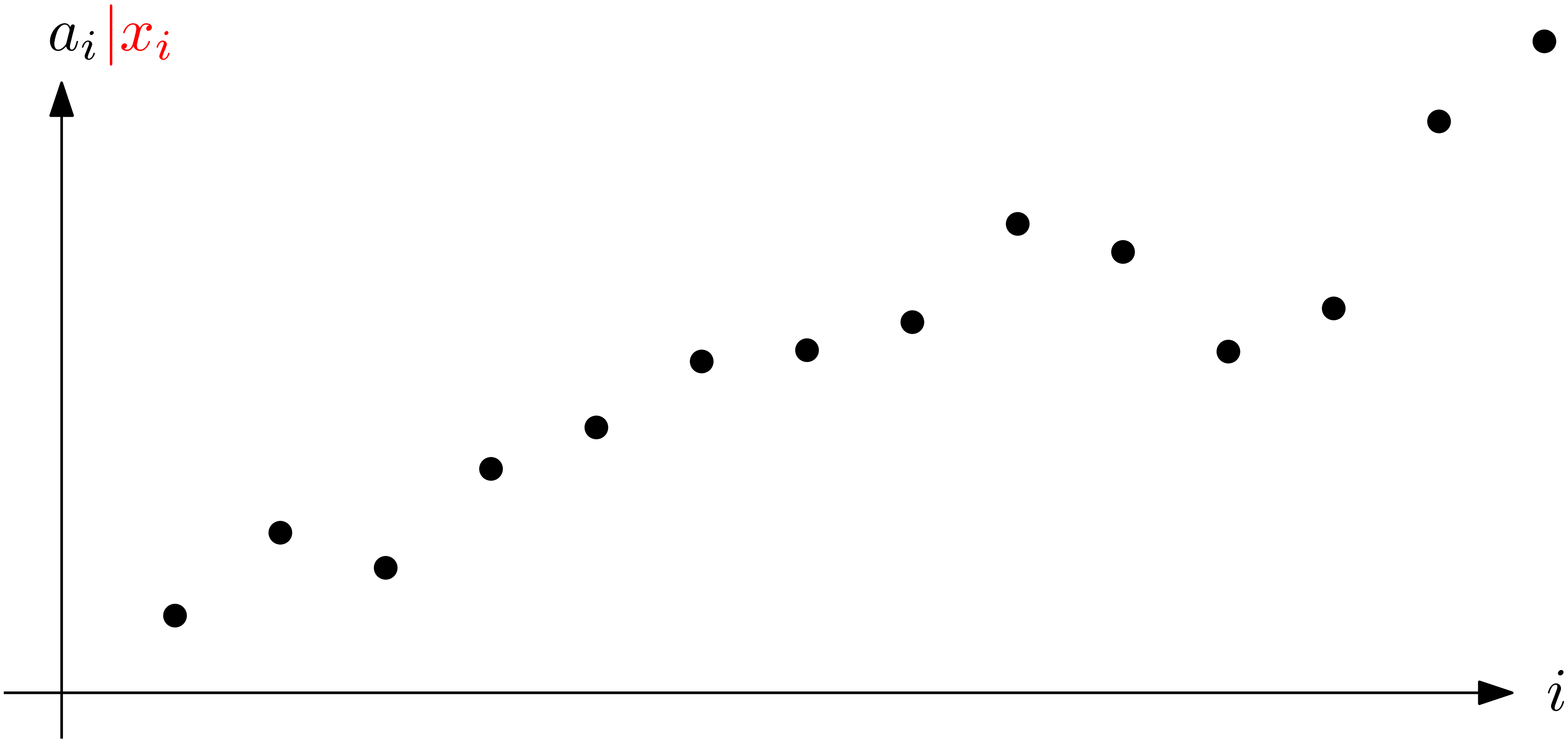

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$$\text{Minimize } \sum_{i=1}^{n} h(|x_i - a_i|) \text{ subject to } x_1 \le \cdots \le x_n$$

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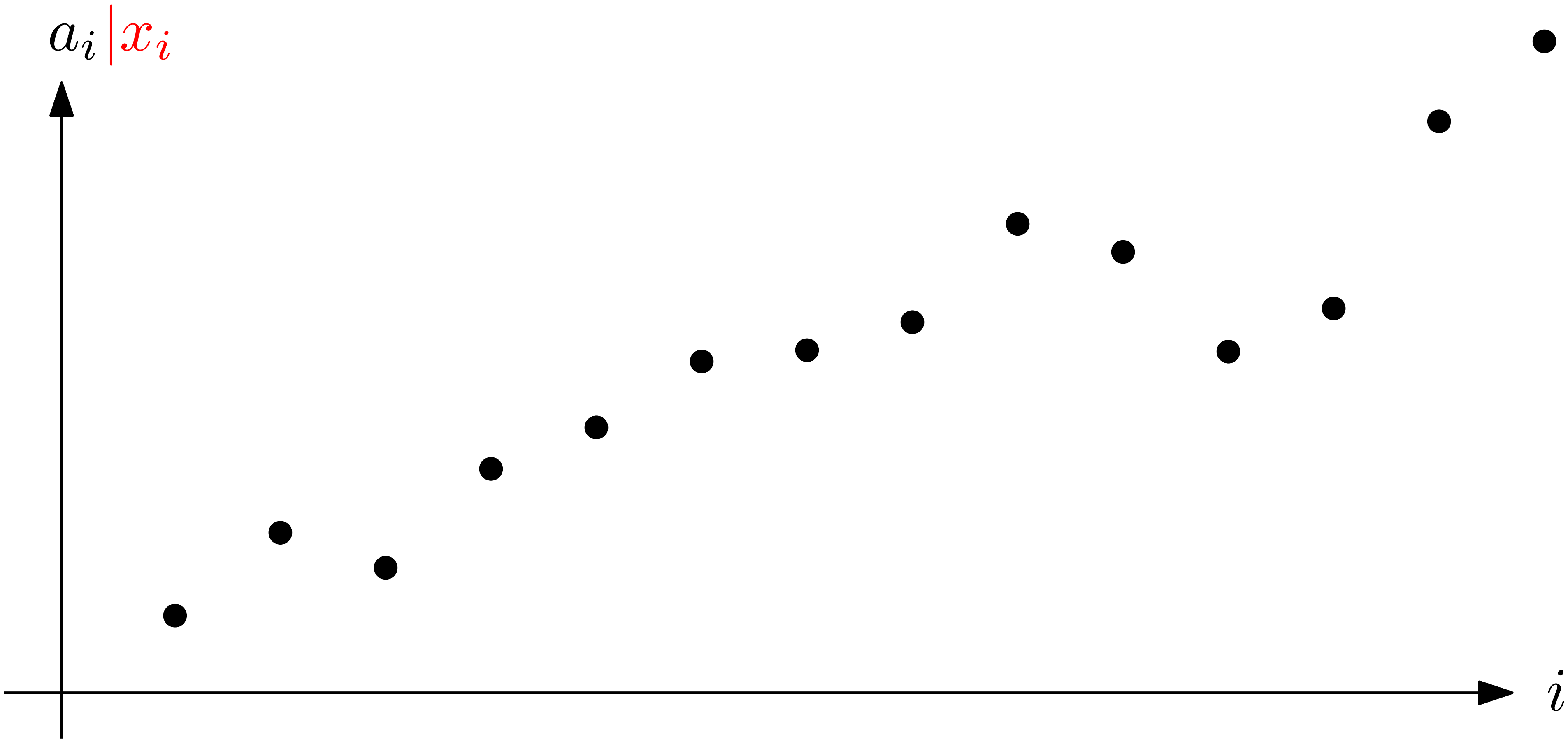

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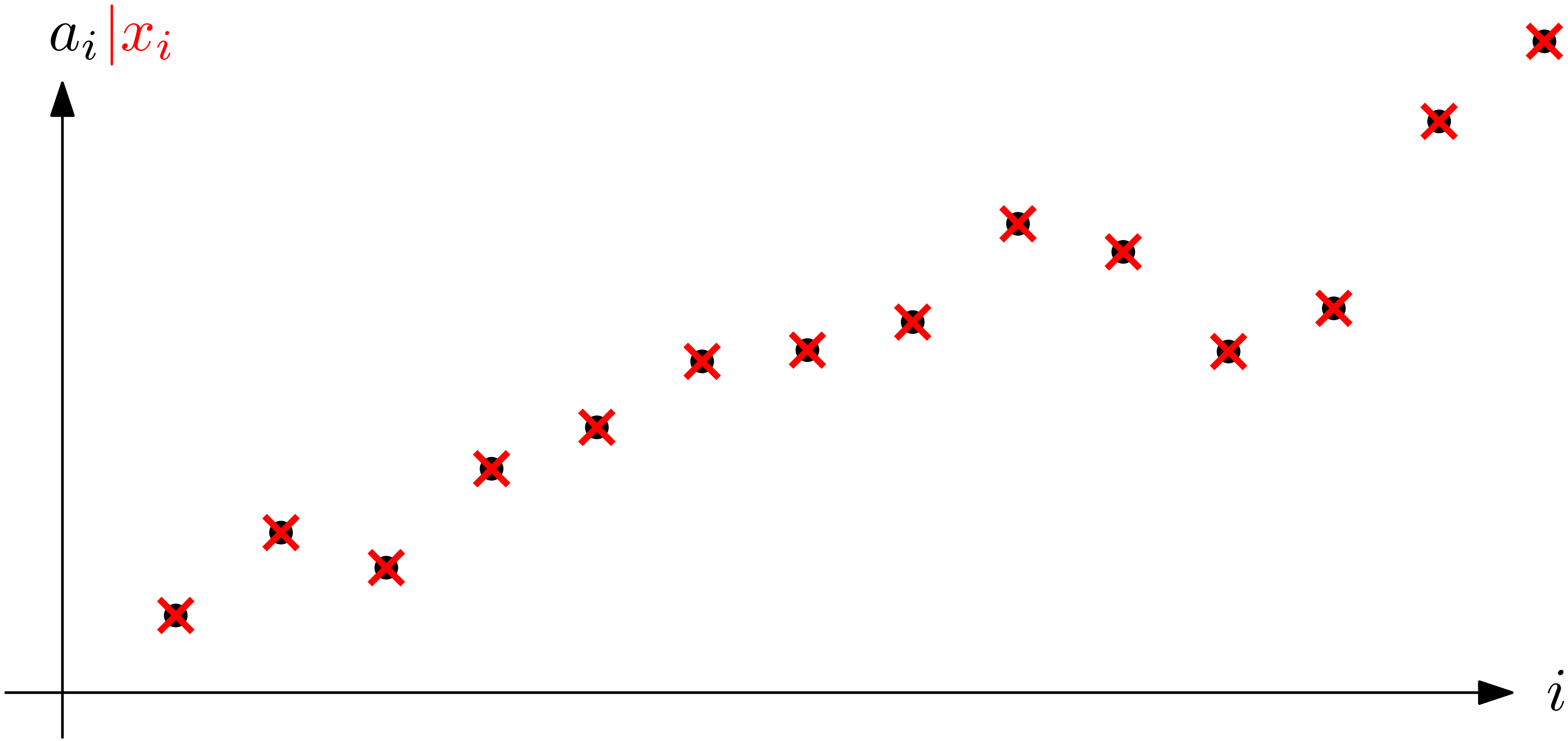

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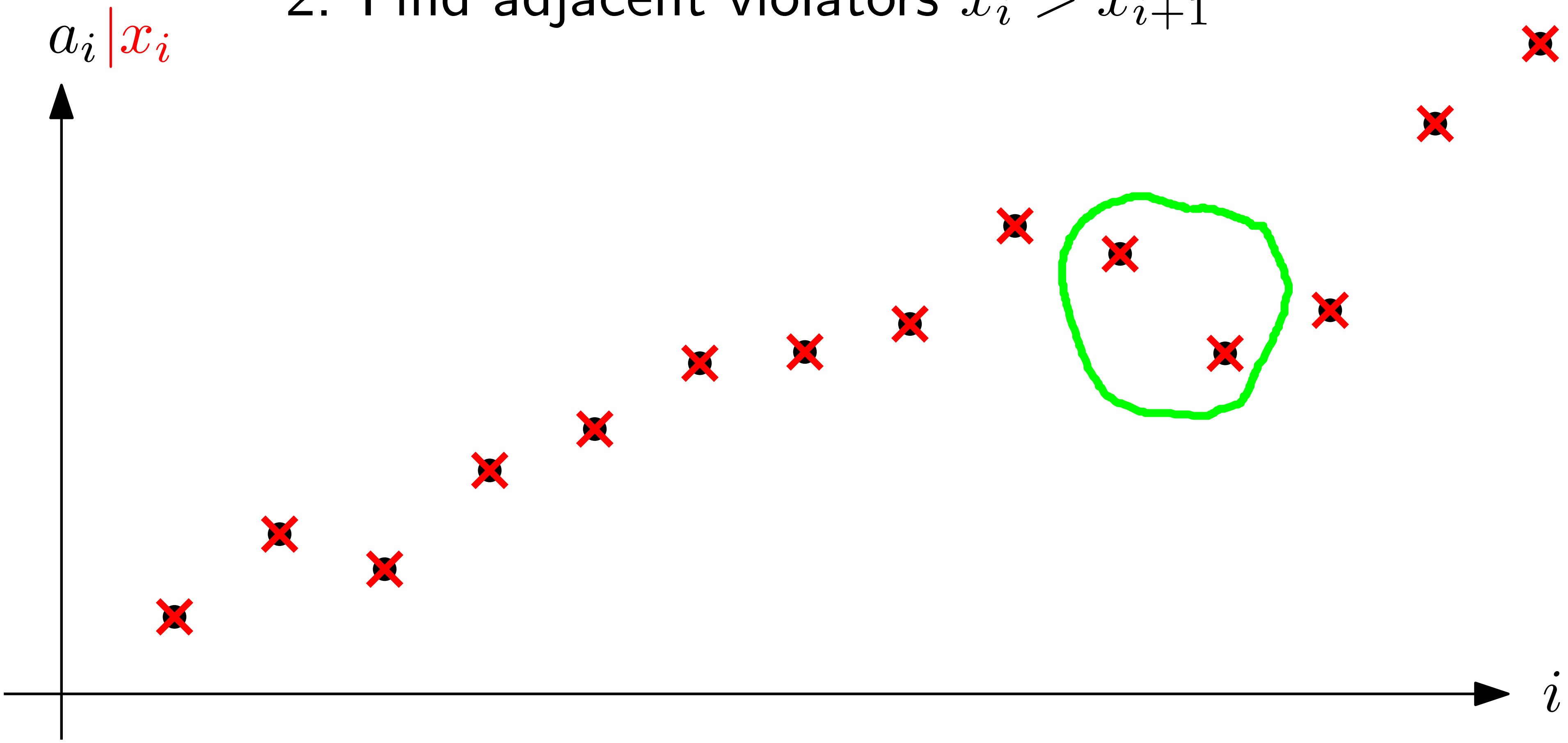

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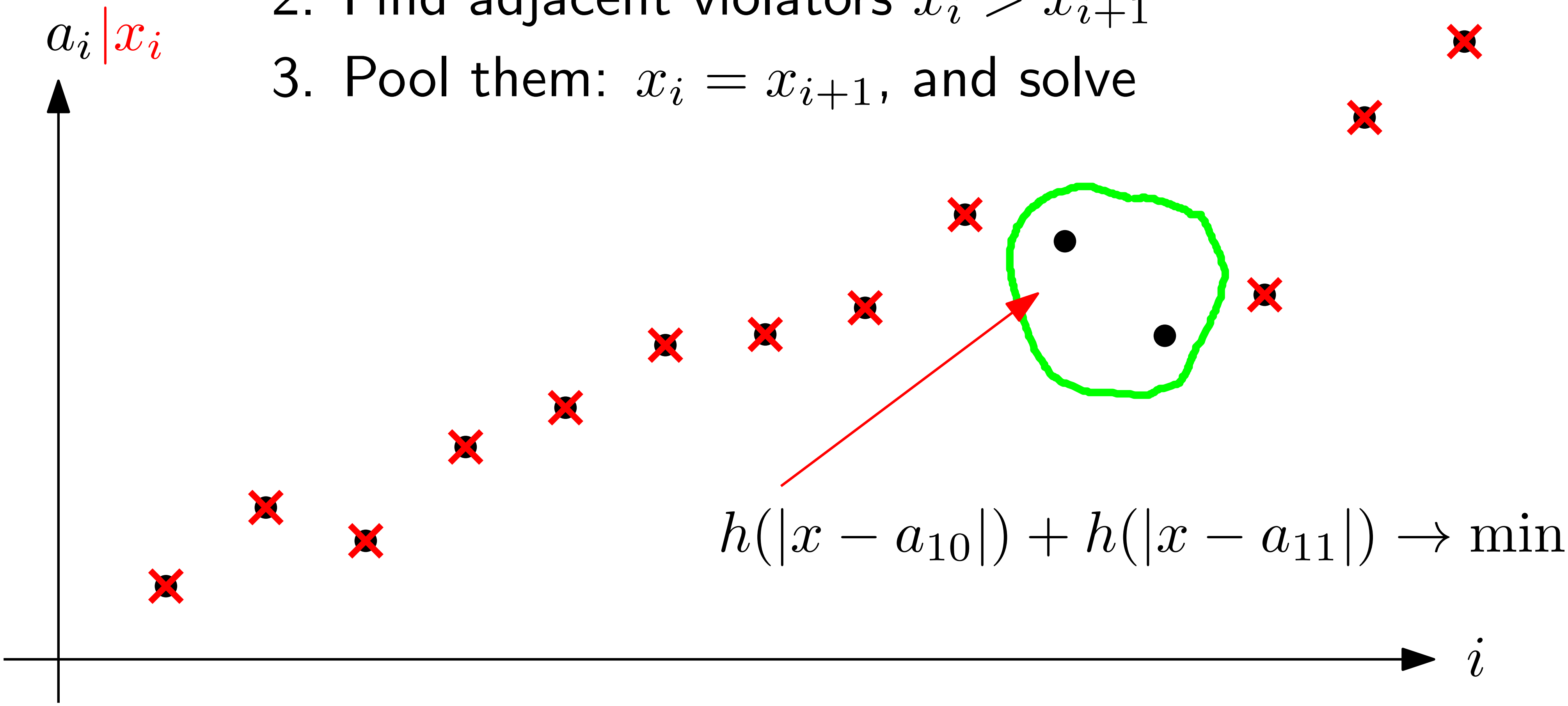

$h(|x - a_{10}|) + h(|x - a_{11}|) \rightarrow \min$

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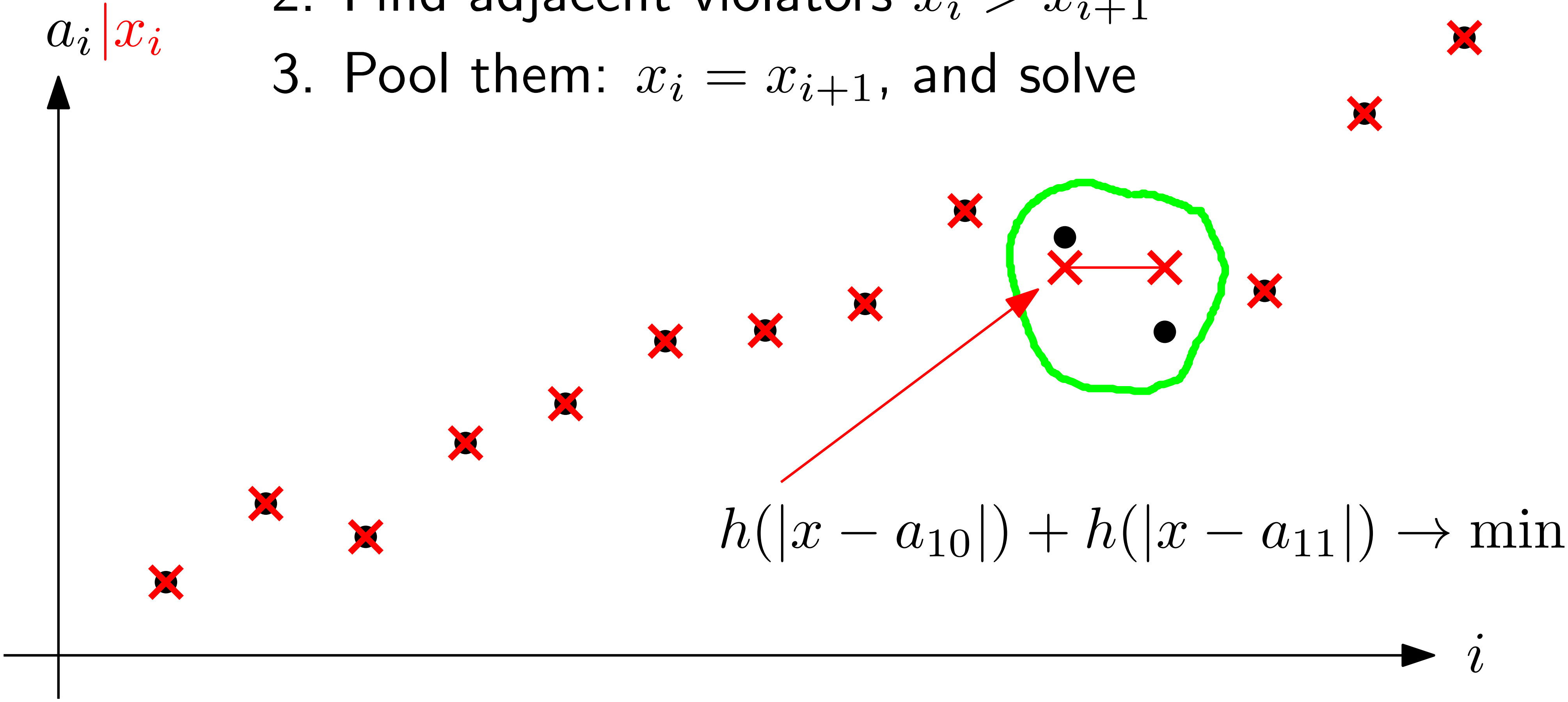

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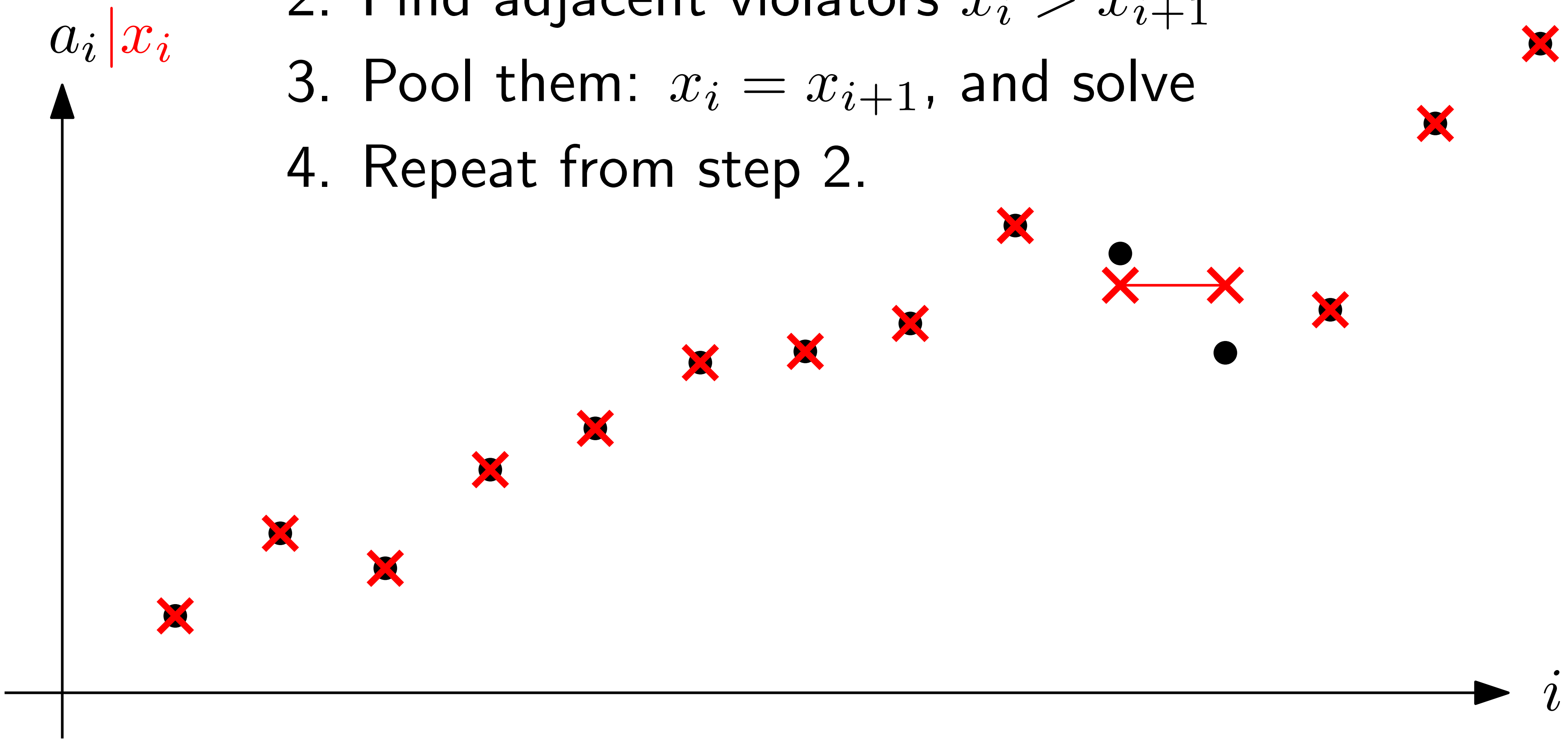

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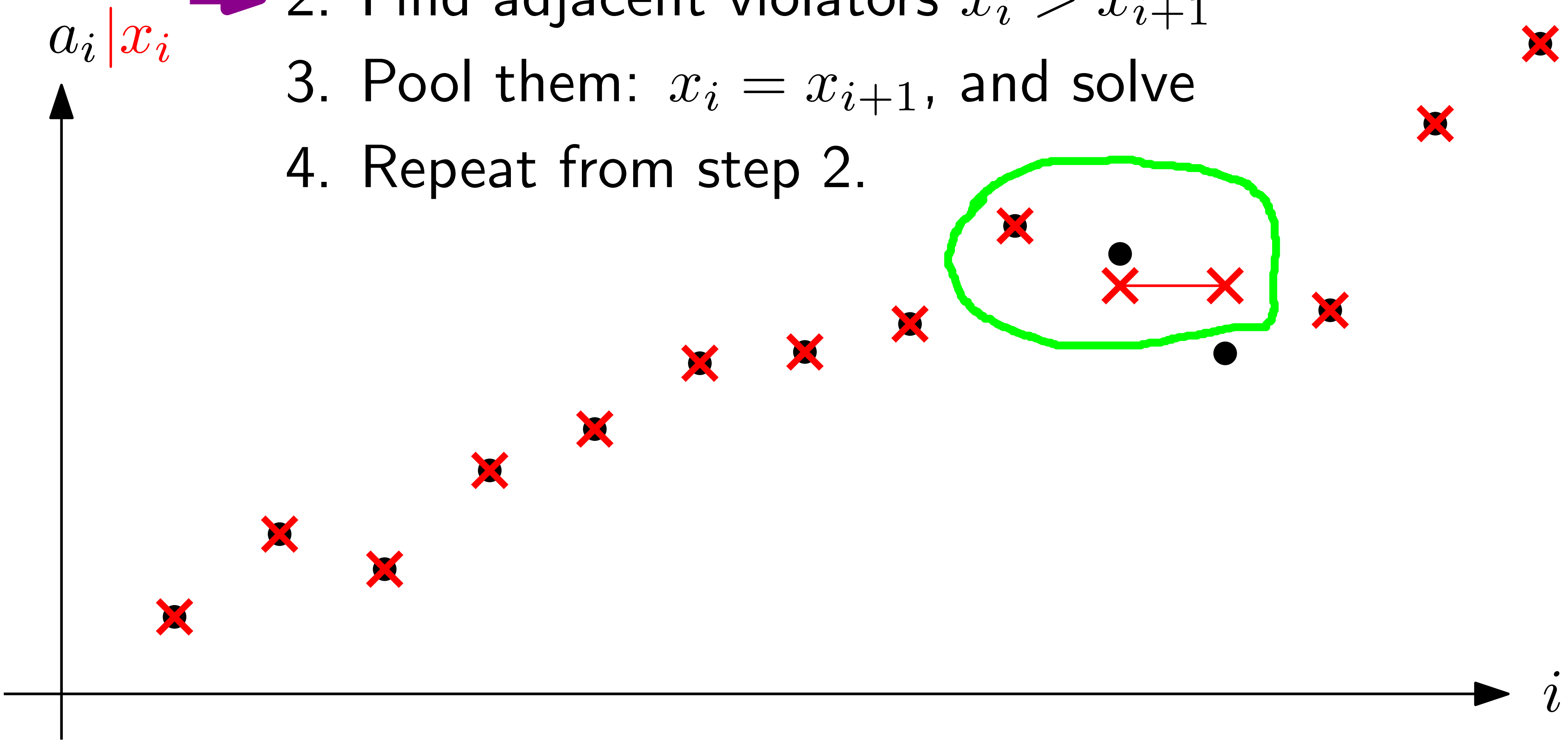

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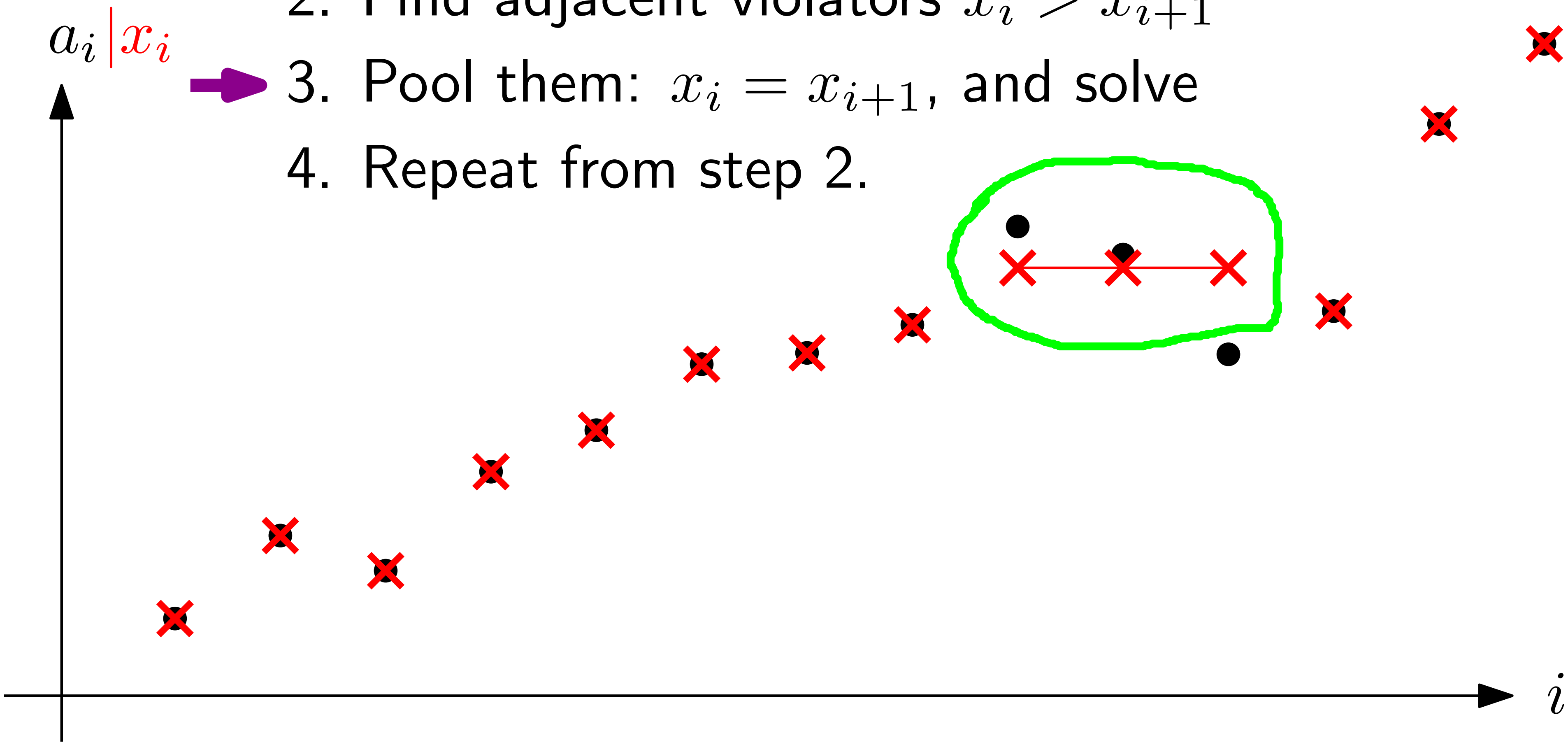

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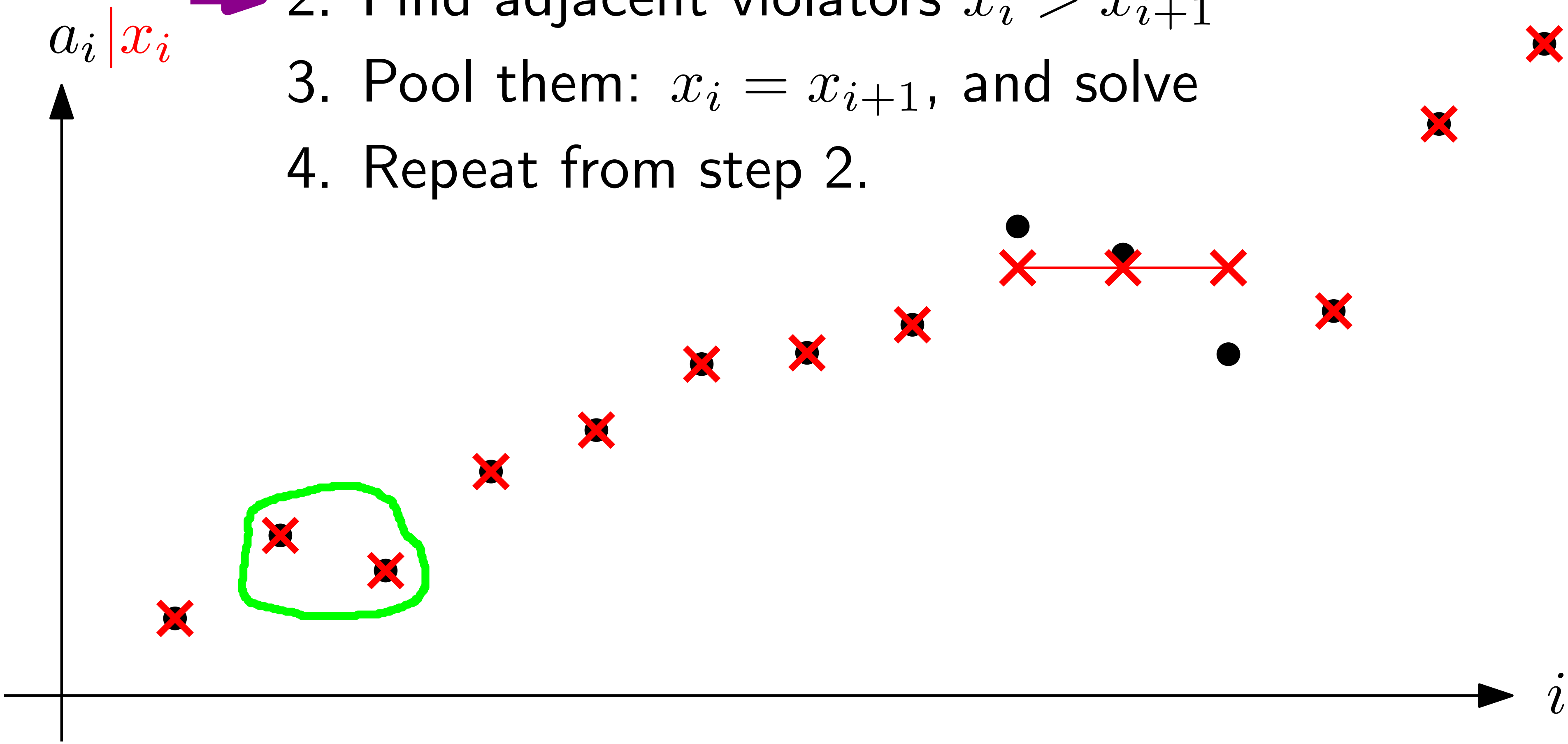

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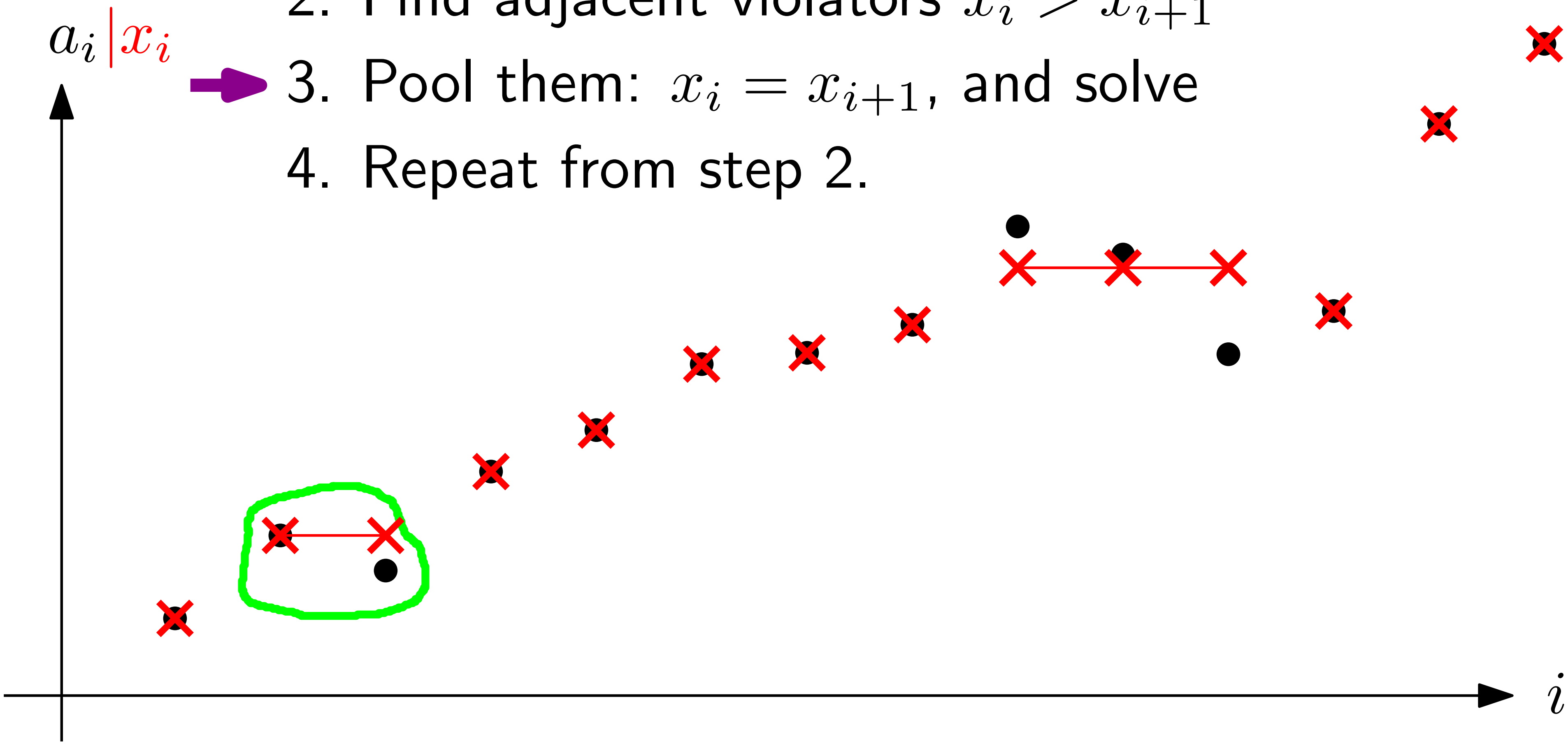

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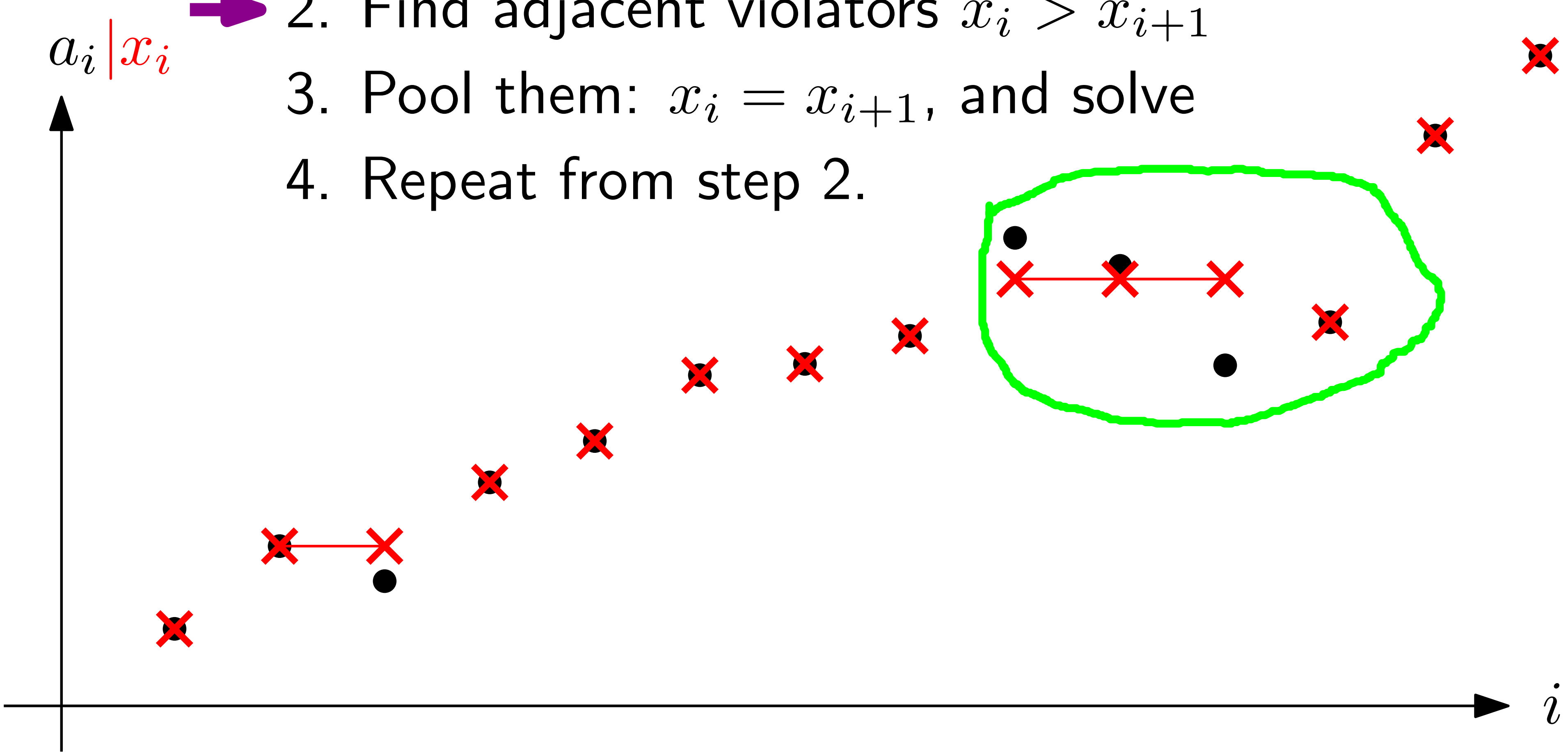

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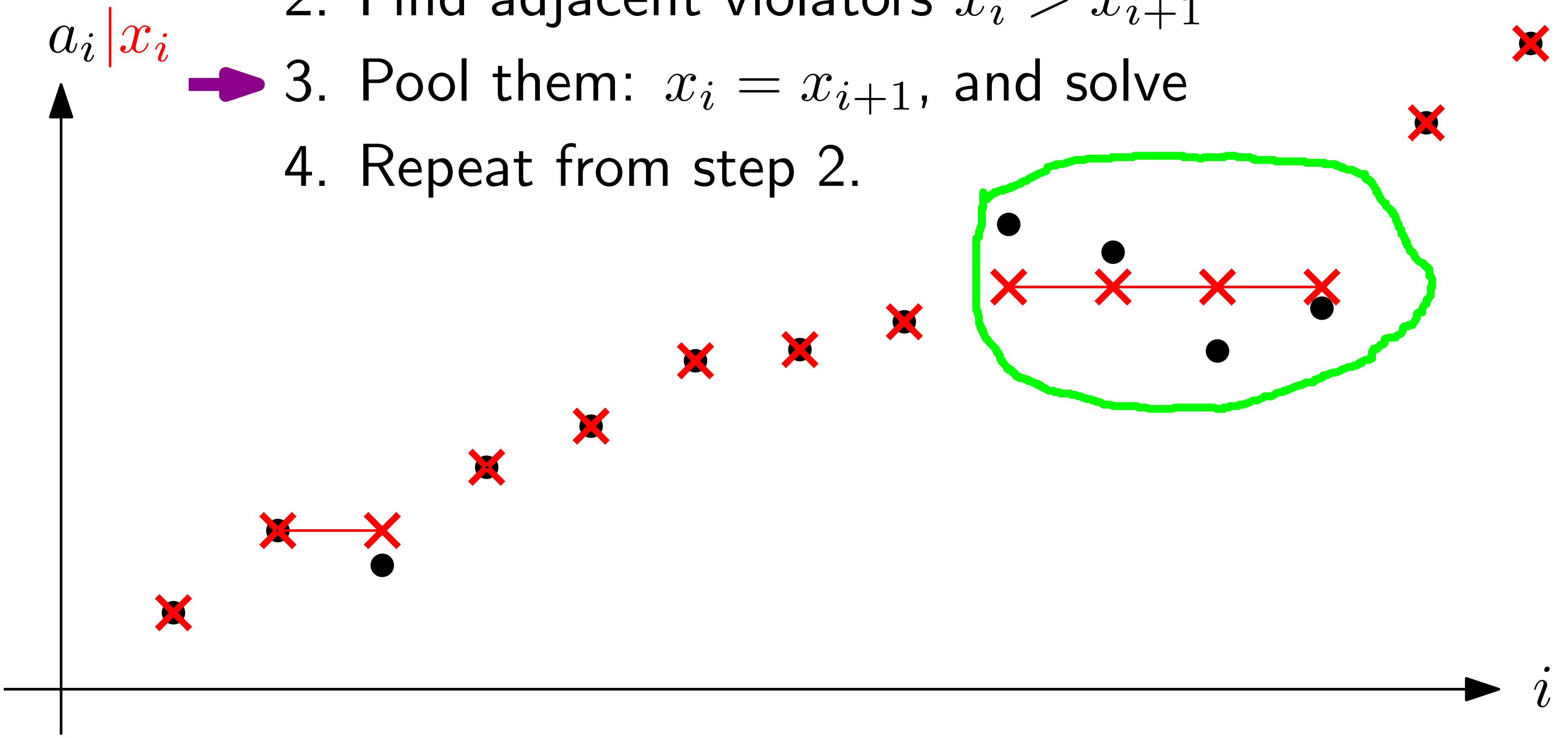

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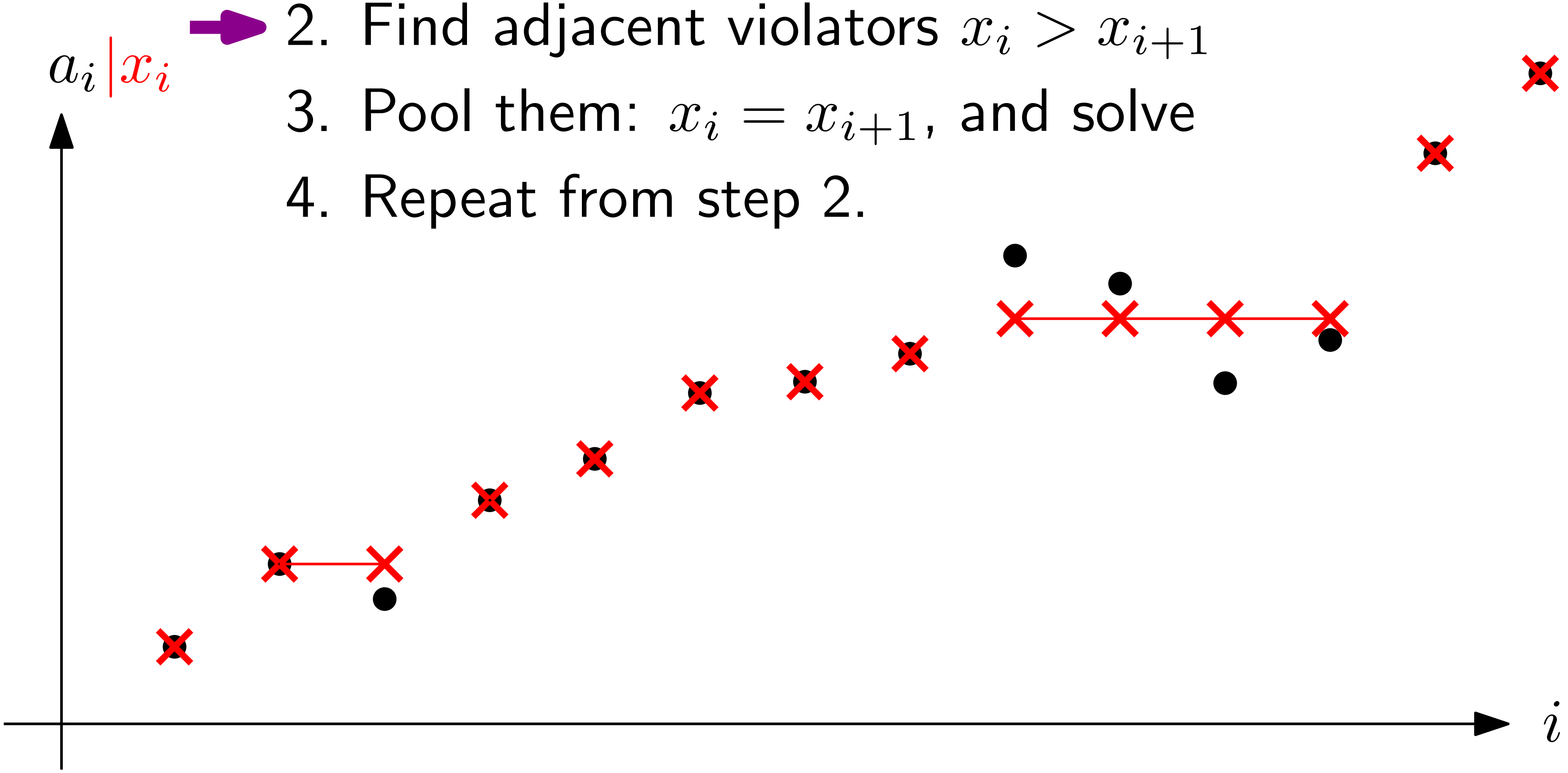

Subproblems

$$\min \sum_{s \le i \le t} w_i |x - a_i| \implies x^* = \text{weighted median of } a_s, \ldots, a_t$$

$$\min \sum_{s \le i \le t} w_i (x - a_i)^2 \implies x^* = \text{weighted mean of } a_s, \ldots, a_t$$

$$x^* = \frac{\sum_{s \le i \le t} w_i a_i}{\sum_{s \le i \le t} w_i} \text{ in } O(1) \text{ time, after } O(n) \text{ preprocessing}$$

Weighted isotonic L_2 regression is solvable in $O(n)$ time.

Subproblems

$$\min \sum_{s \le i \le t} w_i |x - a_i| \implies x^* = \text{weighted median of } a_s, \dots, a_t$$

Ahuja and Orlin [2001]:
$O(n \log n)$ algorithm based on PAV and *scaling*:

- Solve the problem for scaled (integer) data $\bar{a}_i := 2\lfloor a_i/2 \rfloor$.
- Solution for original data a_i can be recovered in $O(n)$ time.
- We can assume $a_i \in \{1, 2, \dots, n\}$, after sorting.

Quentin Stout [2008]: $O(n \log n)$ PAV implementation

- median queries by mergeable trees (2-3-trees, AVL trees) extended with weight information

Rote [2012]: $O(n \log n)$ by dynamic programming.

- A priority queue is sufficient

Dynamic programming

$$f_k(z) := \min\Big\{ \sum_{i=1}^{k} w_i \cdot |x_i - a_i| : x_1 \le x_2 \le \dots \le x_k = z \Big\}$$

$$k = 0, 1, \dots, n; \quad z \in \mathbb{R}$$

Rekursion:

$$f_k(z) := \min\{ f_{k-1}(x) : x \le z \} + w_k \cdot |z - a_k|$$

Dynamic programming

$$f_k(z) := \min\Big\{ \sum_{i=1}^{k} w_i \cdot |x_i - a_i| : x_1 \le x_2 \le \cdots \le x_k = z \Big\}$$

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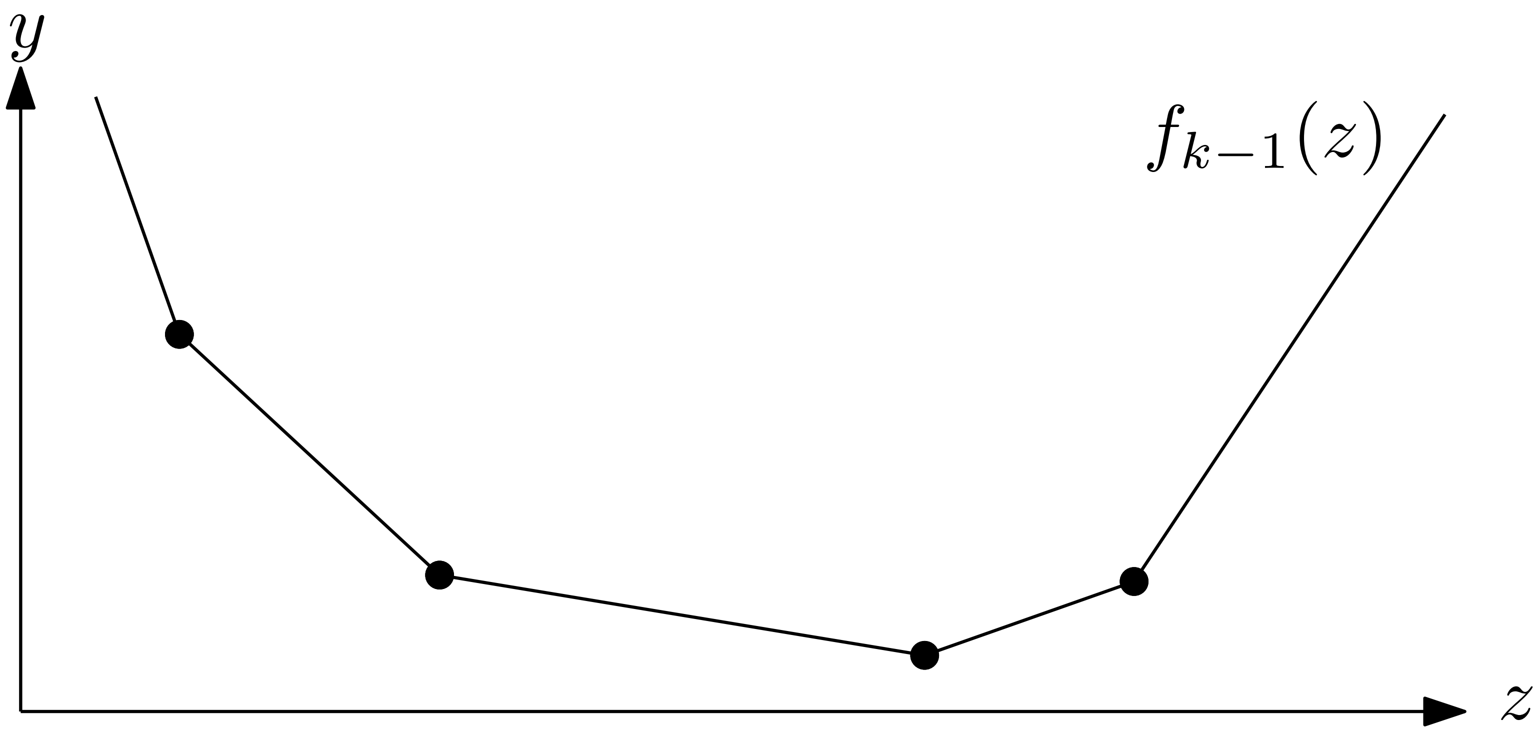
Rekursion:

$$f_k(z) := \underbrace{\min\{\, f_{k-1}(x) : x \le z \,\}}_{g_{k-1}(z)} + w_k \cdot |z - a_k|$$

Transform $f_{k-1} \to g_{k-1} \to f_k$

Recursion step 1

Transform f_{k-1} to $g_{k-1}(z) := \min\{\, f_{k-1}(x) : x \le z \,\}$



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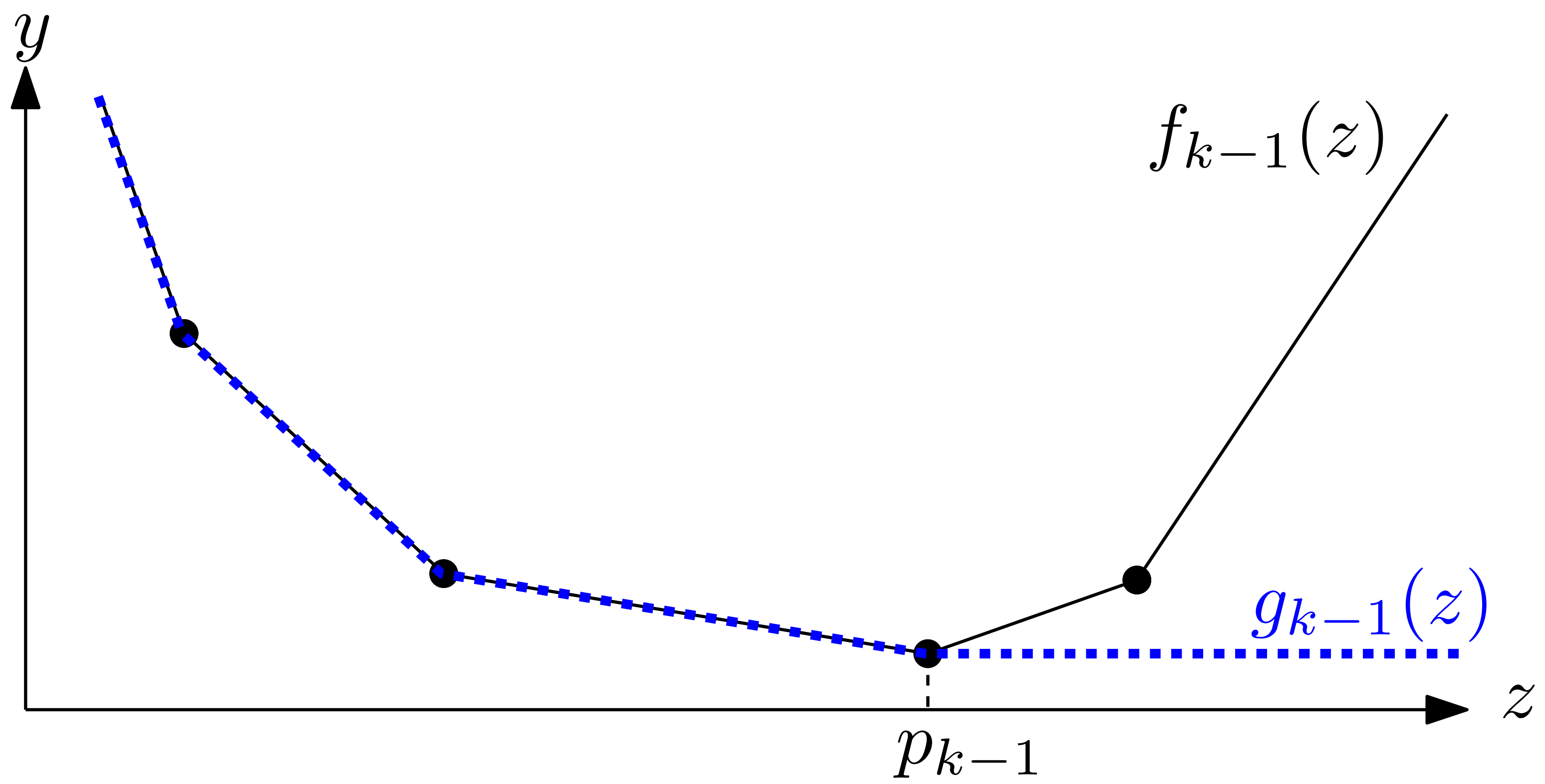


Remove the increasing parts right of the minimum p_{k-1} and replace them by a horizontal part.

Recursion step 2

Transform g_{k-1} to $f_k(z) = g_{k-1}(z) + w_k \cdot |z - a_k|$

- Add two convex piecewise-linear functions

Recursion step 2

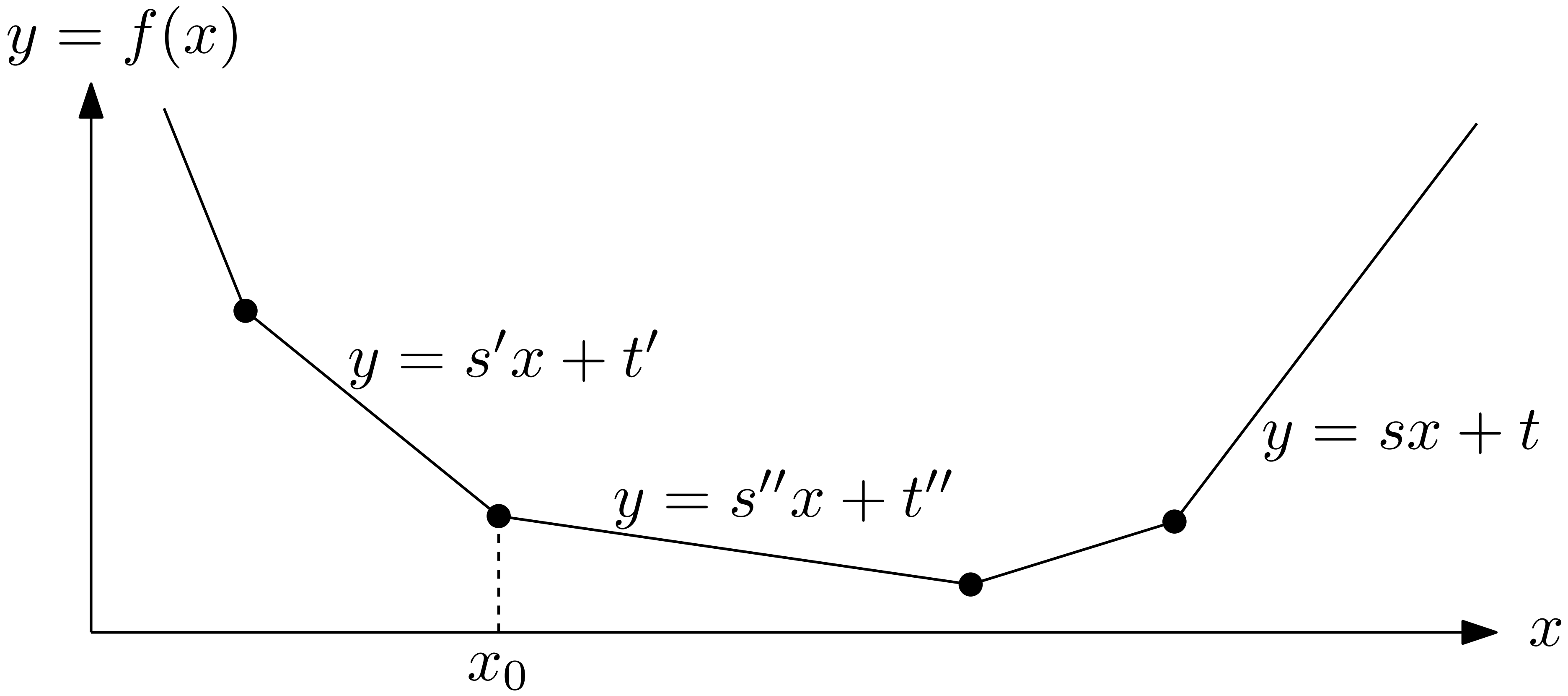
Transform g_{k-1} to $f_k(z) = g_{k-1}(z) + w_k \cdot |z - a_k|$

- Add two convex piecewise-linear functions

Lemma.

- f_k is a piecewise-linear convex function.
- The breakpoints are located at a subset of the points a_i.
- The leftmost piece has slope $-\sum_{i=1}^{k} w_i$.
  The rightmost piece has slope w_k.

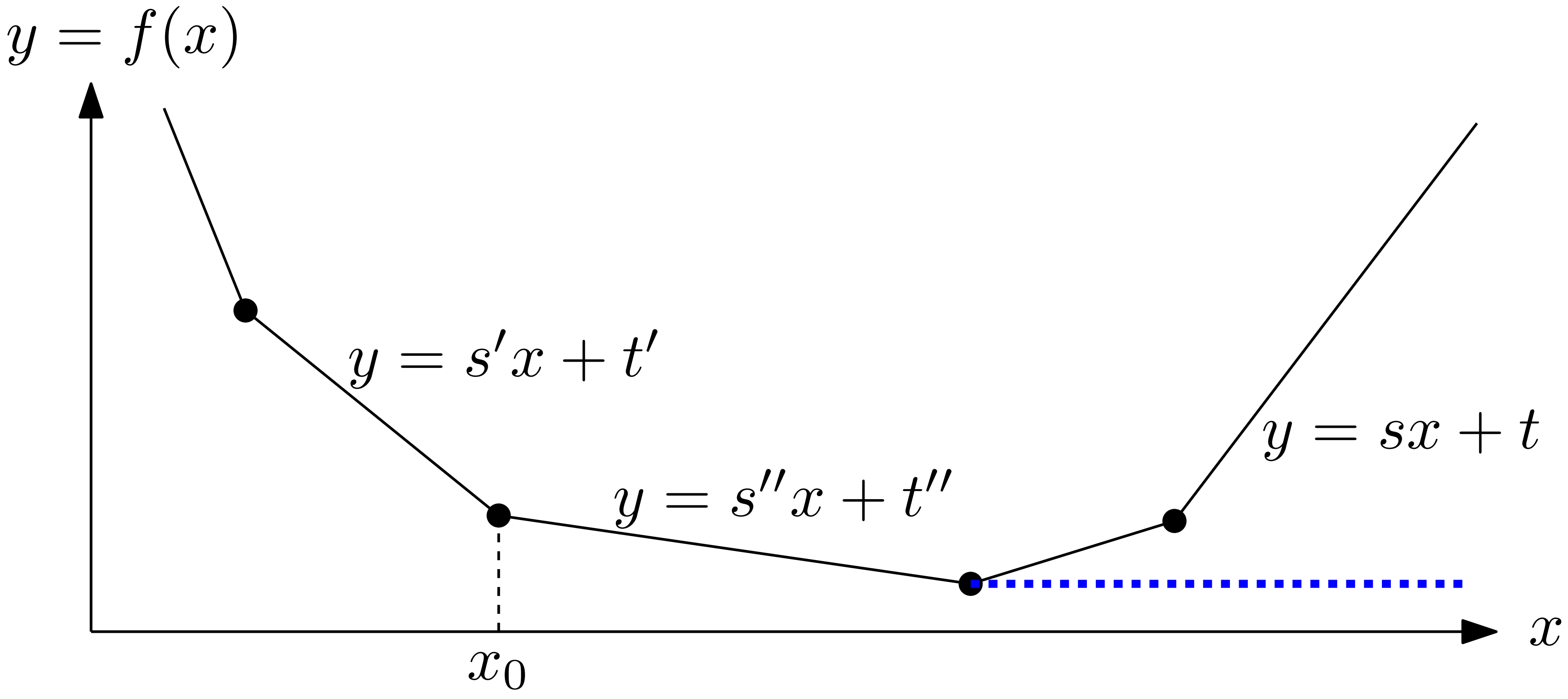
Piecewise-linear functions



f has a breakpoint at *position* x_0 with *value* $s'' - s'$.

Represent f by the rightmost slope s and the set of breakpoints (position+value). (The rightmost intercept t is not needed.)

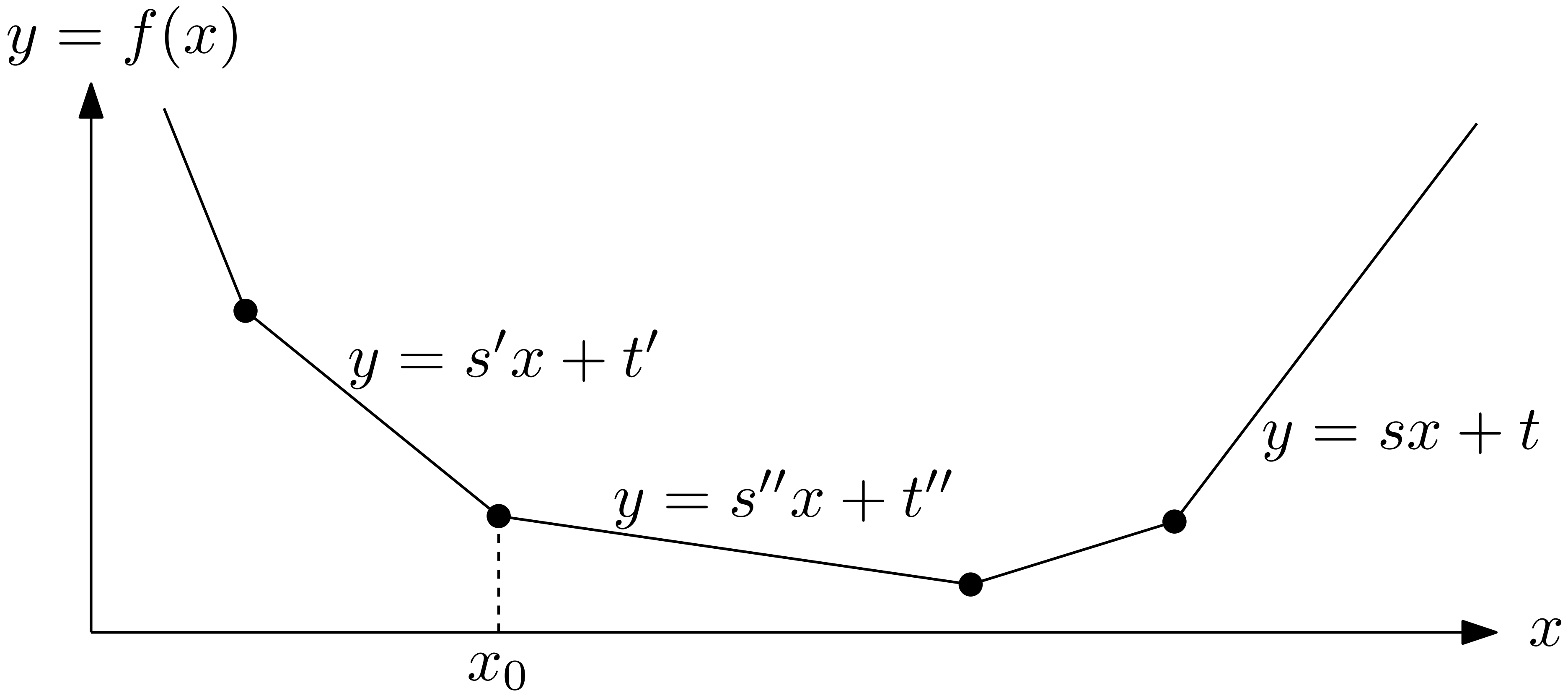
Piecewise-linear functions



Transformation $f_{k-1} \to g_{k-1}$:

```
while $s -$ (value of rightmost breakpoint) $\geq 0$:
    remove rightmost breakpoint
    update $s$
update $s$ to $0$
```

Piecewise-linear functions

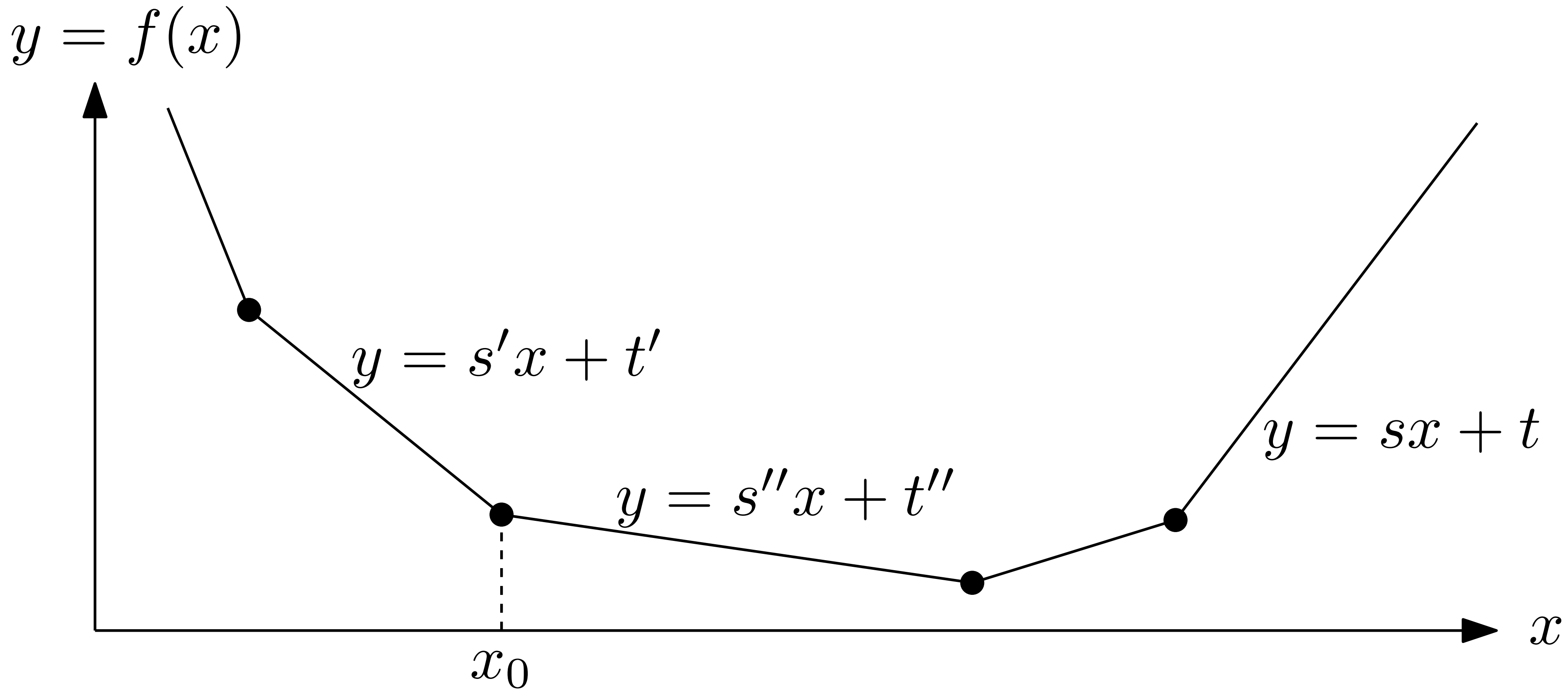


Transformation $g_{k-1} \to f_k(z) = g_{k-1}(z) + w_k \cdot |z - a_k|$

add w_k to s.

add a breakpoint at position a_k with value $2w_k$.

Piecewise-linear functions



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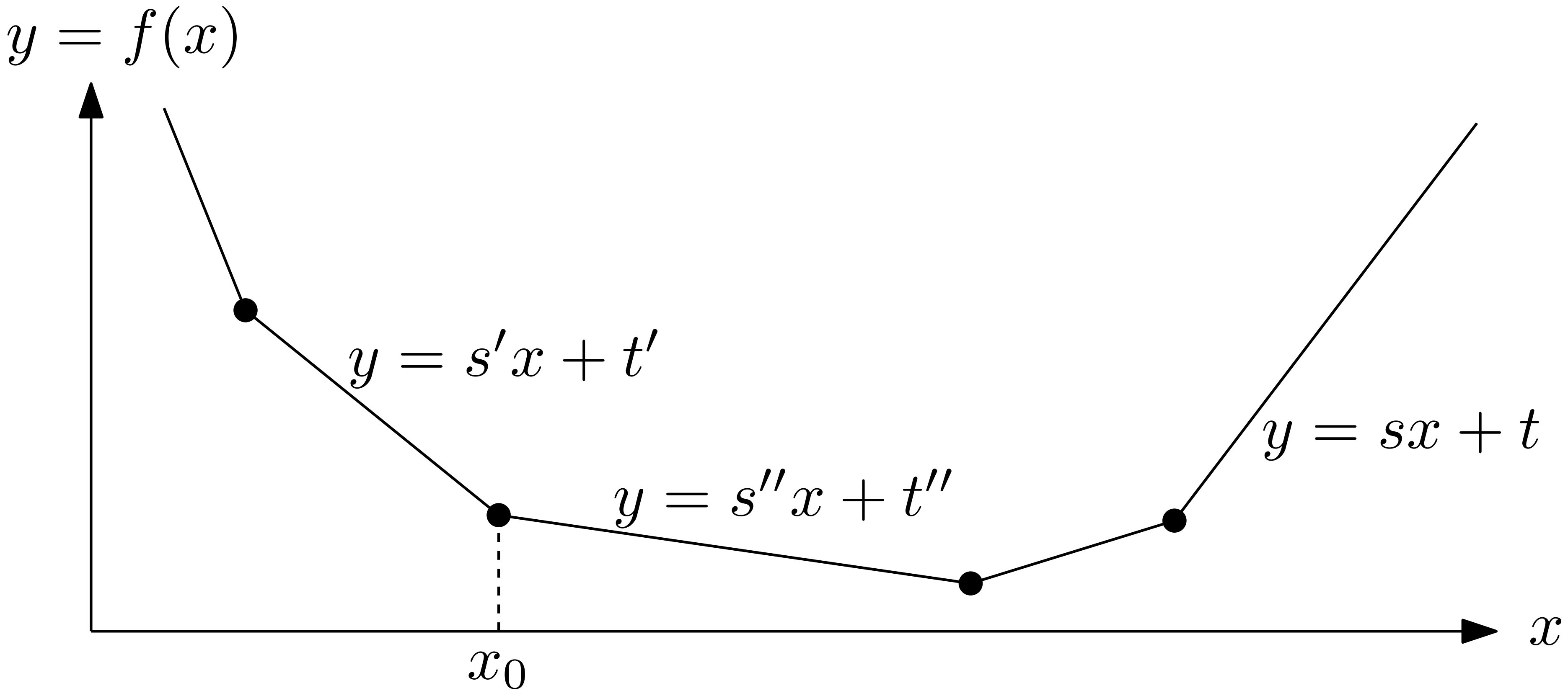

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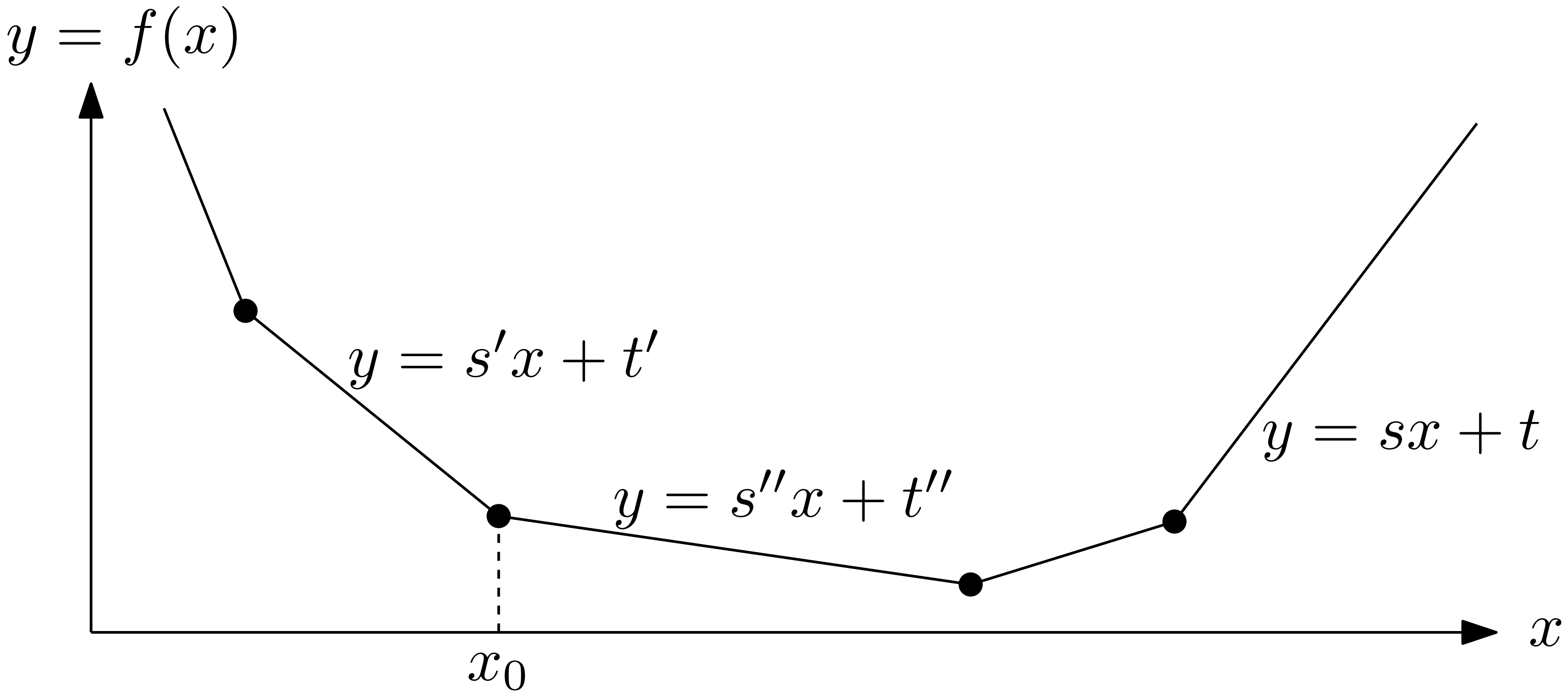

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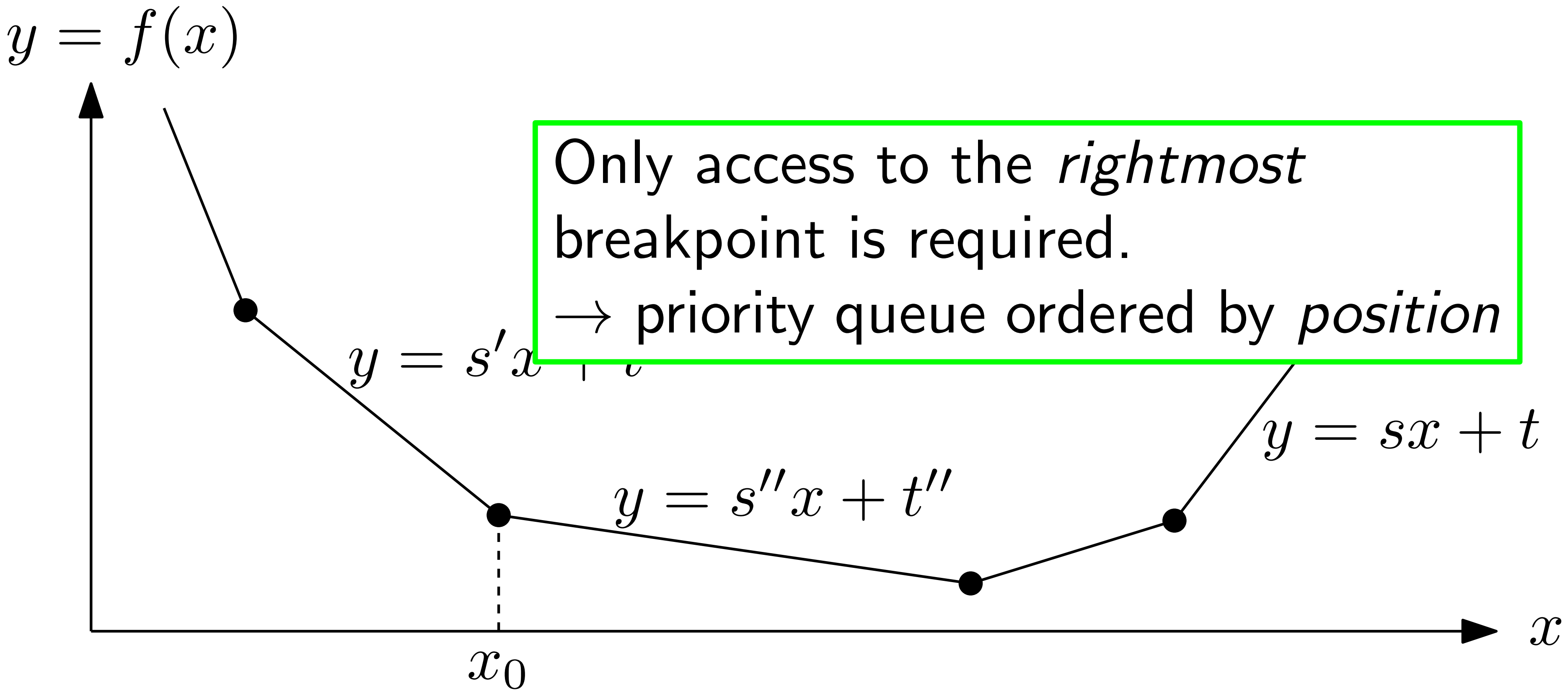


Only access to the *rightmost* breakpoint is required.
→ priority queue ordered by *position*

Transformation $f_{k-1} \to g_{k-1}$:

```
while $s -$ (value of rightmost breakpoint) $\geq 0$:
    remove rightmost breakpoint
    update $s$
update $s$ to $0$
```

The algorithm

```
$Q := \emptyset$; // priority queue of breakpoints ordered by the key position;
$s := 0$;
for $k = 1, \dots, n$ do                                                    $g_{k-1}$
    $Q$.add(new breakpoint with position $:= a_k$, value $:= 2w_k$);
    $s := s + w_k$;                                                          $f_k$
    loop
        $B := Q$.findmax; // rightmost breakpoint $B$
        if $s - B$.value $< 0$ then exit loop;
        ;
        $s := s - B$.value;
        $Q$.deletemax;
    $p_k := B$.position;
    $B$.value                                                                $g_k$
    $s := 0$; // We have computed $g_k$.
// Compute the optimal solution $x_1, \dots, x_n$ backwards:
$x_n := p_n$;
for $k = n-1, n-2, \dots, 1$ do $x_k := \min\{x_{k+1}, p_k\}$;
.
```

General objective functions

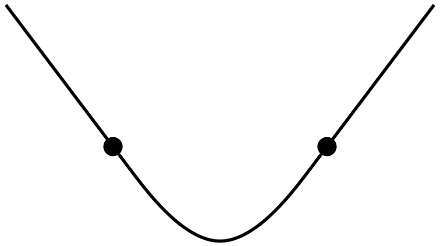
$$\text{Minimize } \sum_{i=1}^{n} h_i(x_i)$$

Each h_i is convex and piecewise “simple”:

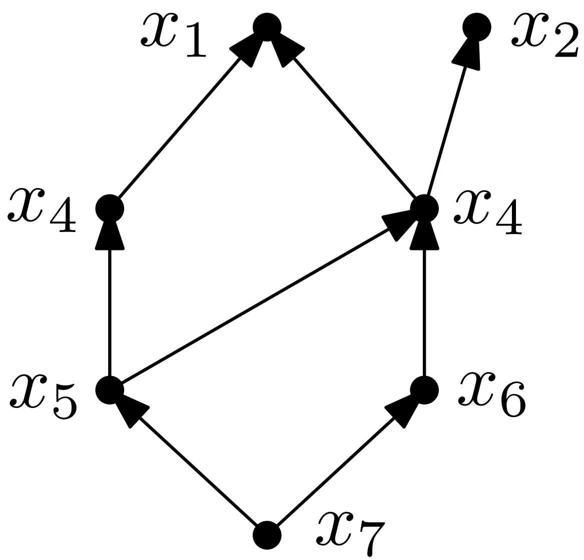
- Summation of pieces in constant time
- Minimum on a sum of pieces in constant time

Examples:

- L_3 norm: $h_i(x) = \begin{cases} (x-a_i)^3, & x \ge a_i \\ -(x-a_i)^3, & x \le a_i \end{cases} \Rightarrow O(n \log n)$ time
- L_4 norm: $h_i(x) = (x-a_i)^4 \Rightarrow O(n)$ time
  (no breakpoints! A stack suffices.)
- Linear + sinusoidal pieces: $-w_i \cos(x - a_i)$



General partial orders



Minimize $\sum_{i=1}^{n} h_i(x_i)$ or $\max_{1\le i\le n} h_i(x_i)$

subject to

$$x_i \le x_j \text{ for } i \prec j$$

for a given partial order $\prec$.

PAV can be extended to tree-like partial orders.

weighted L_1-regression for a DAG with m edges in $O(nm + n^2 \log n)$ time.

[Angelov, Harb, Kannan, and Wang, SODA'2006]

. . . and many other results

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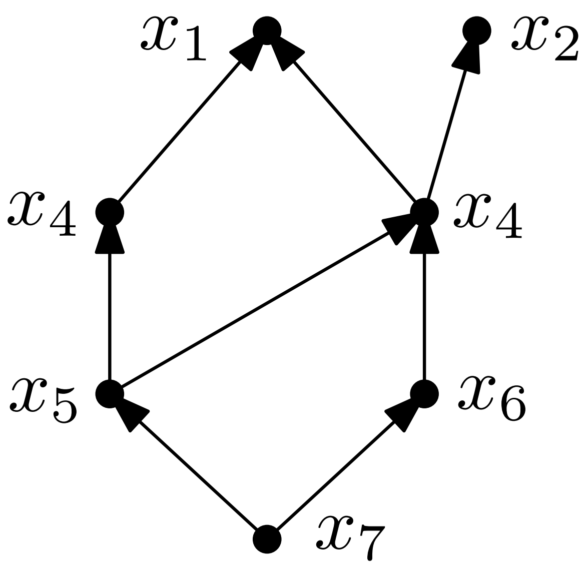

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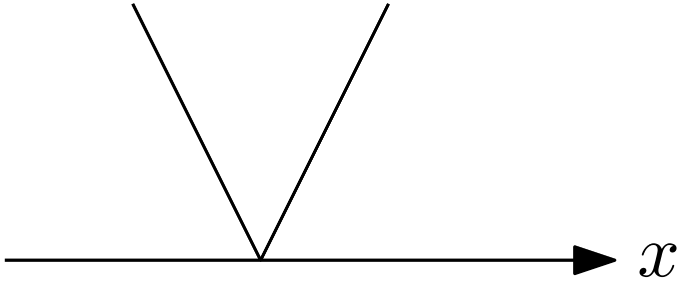
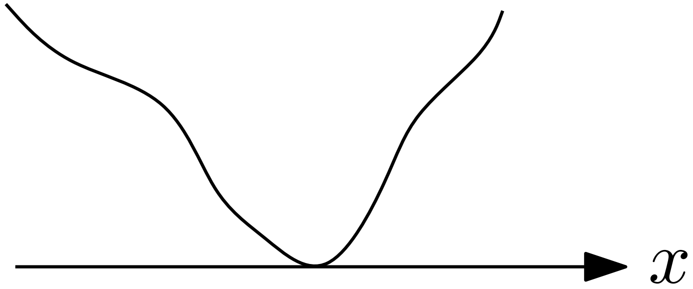
Weighted L_∞ regression

Minimize $z := \max_{1 \le i \le n} h_i(x_i)$ subject to $x_i \le x_j$ for $i \prec j$.

$$h_i(x) = w_i |x - a_i|$$



or $h_i(x) =$ any function which increases from a minimum into both directions



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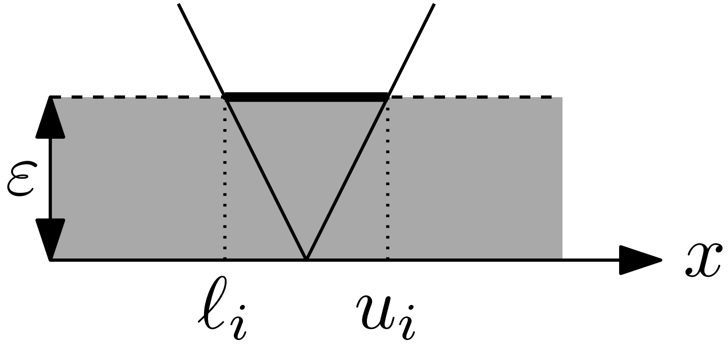

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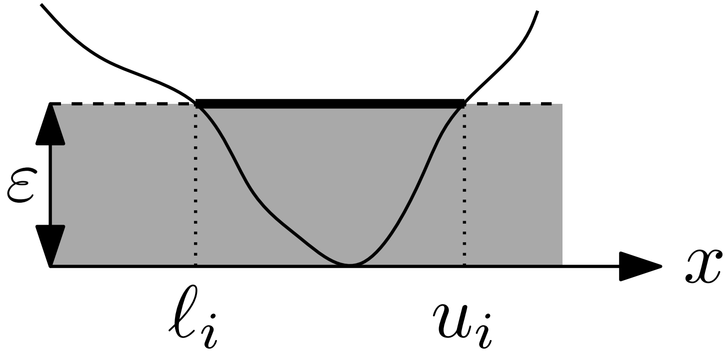


$$h_i(x) \le \varepsilon \iff \ell_i(\varepsilon) \le x \le u_i(\varepsilon)$$

Checking feasibility

Is the optimum value $z^* \le \varepsilon$? [$z = \max_i h_i(x_i)$]

Find values x_i with

$$\ell_i(\varepsilon) \le x_i \le u_i(\varepsilon) \text{ for all } i, \text{ and} \tag{1}$$

$$x_i \le x_j \text{ for } i \prec j. \tag{2}$$

Find the smallest values $x_i = x_i^{\mathrm{low}}$ with

$$\ell_i(\varepsilon) \le x_i \text{ for all } i, \text{ and}$$

$$x_i \le x_j \text{ for } i \prec j.$$

Result: $x_j^{\mathrm{low}} = \max\{\ell_j, \max\{\, \ell_i \mid i \prec j \,\}\}$

Calculate in topological order:

$$x_j^{\mathrm{low}} := \max\{\ell_i, \max\{\, x_i^{\mathrm{low}} \mid i \text{ predecessor of } j \,\}\}$$

$z^* \le \varepsilon$ iff $x_i^{\mathrm{low}} \le u_i$ for all i $\implies O(m+n)$ time

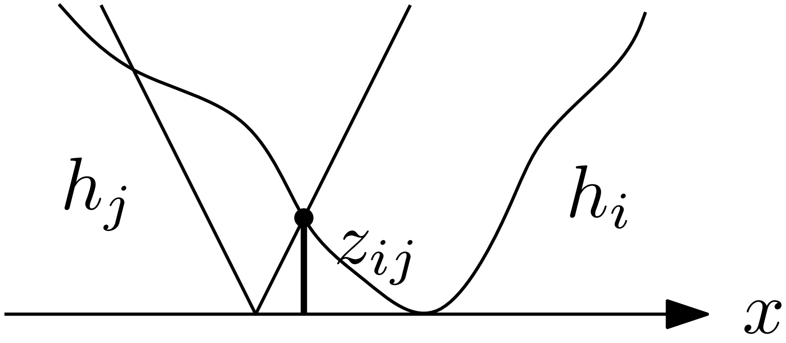
Characterizing feasibility

$z^* \le \varepsilon$ iff for every pair i, j with $i \prec j$:

$$\ell_i(\varepsilon) \le u_j(\varepsilon)$$

Theorem.
Define for every pair i, j:

$$z_{ij} := \min\{\, \varepsilon \mid \ell_i(\varepsilon) \le u_j(\varepsilon) \,\}$$



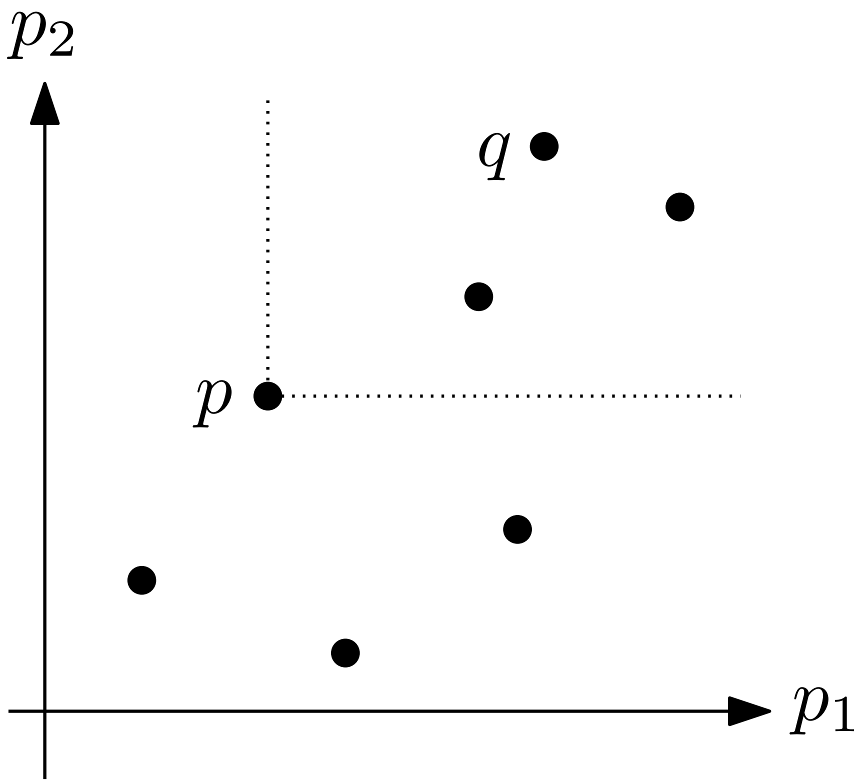
Then $z^* = \max\{\, z_{ij} \mid i \prec j \,\}$.

d-dimensional orders

n points $p = (p_1, p_2, \ldots, p_d) \in \mathbb{R}^d$

Product order (domination order):

$$p \prec q \iff (p_1 \le q_1) \wedge (p_2 \le q_2) \wedge \cdots \wedge (p_d \le q_d)$$



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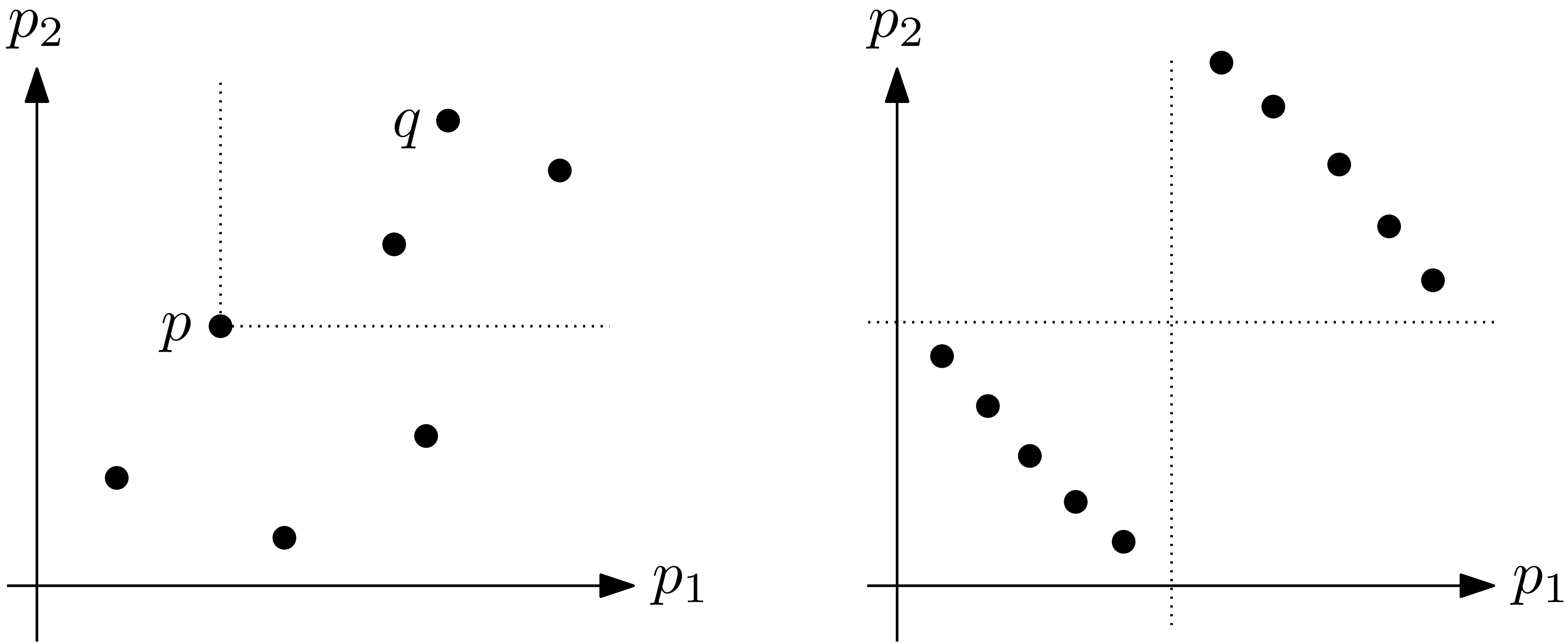

The digraph of the order is not explicitly given.
It might have quadratic size.

L_∞ regression for d-dimensional orders

Stout [2011]: $O(n \log^{d-1} n)$ space and $O(n \log^{d} n)$ time

Embed the order in a DAG with more vertices but fewer edges.

divide-and-conquer strategy, recursive in the dimension.

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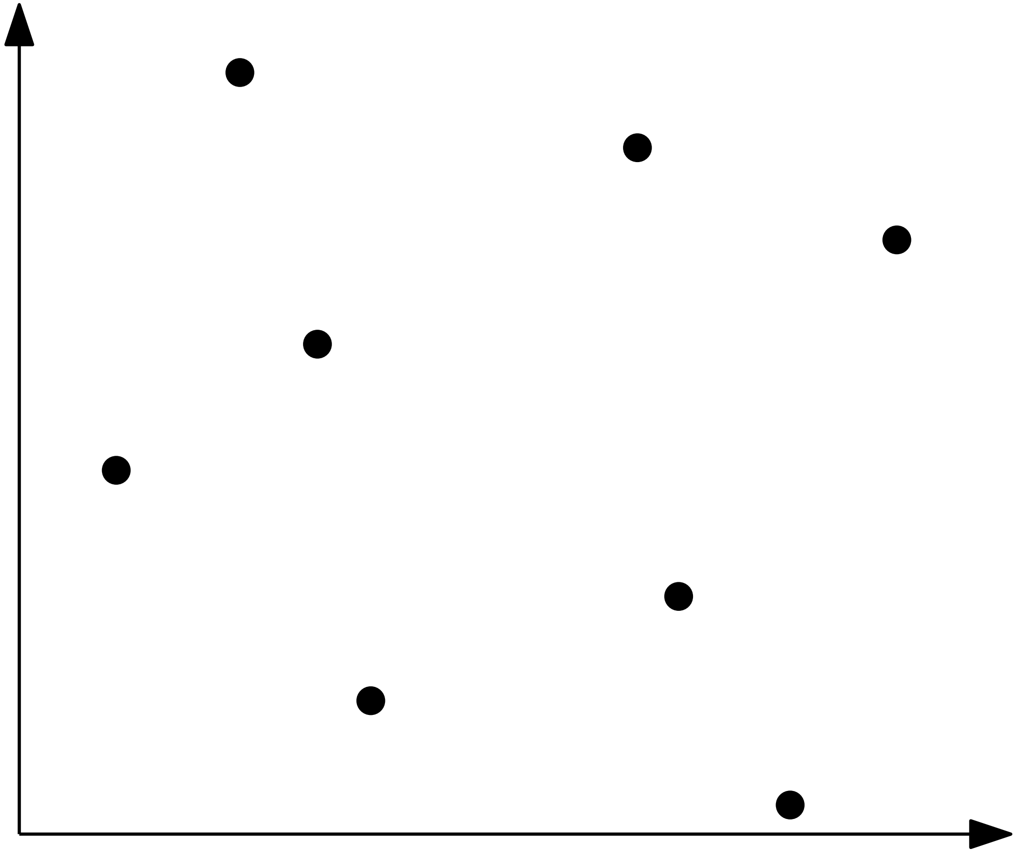

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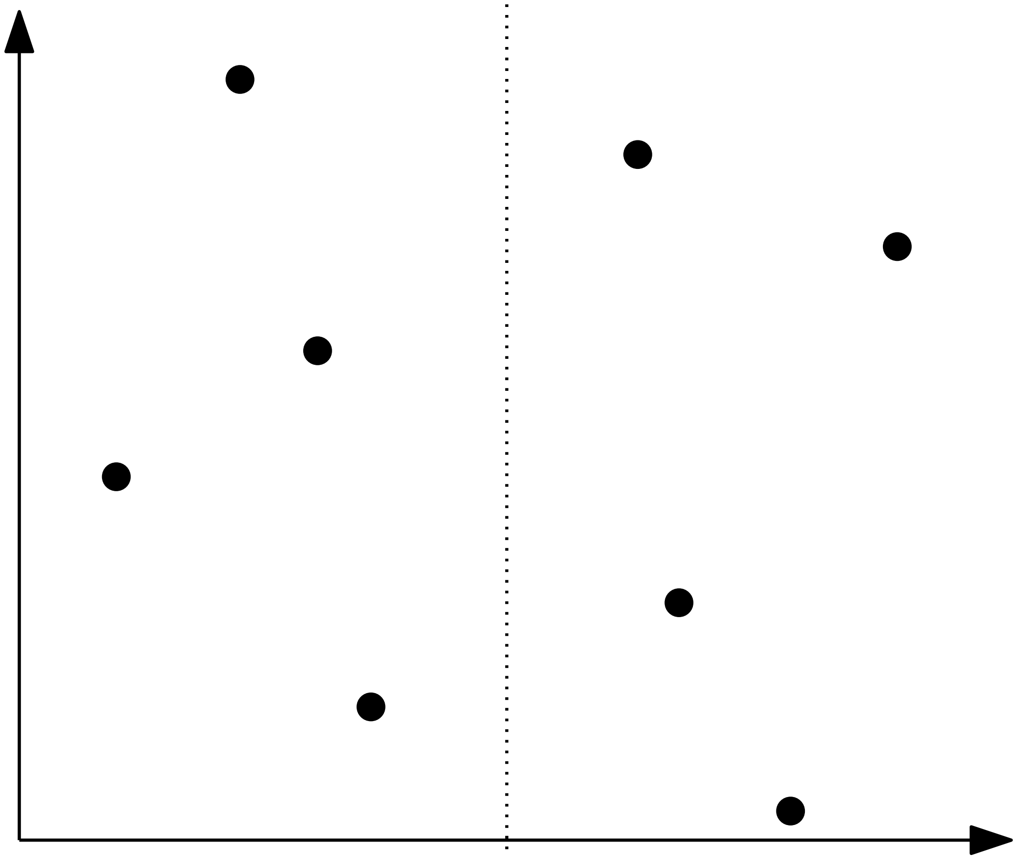

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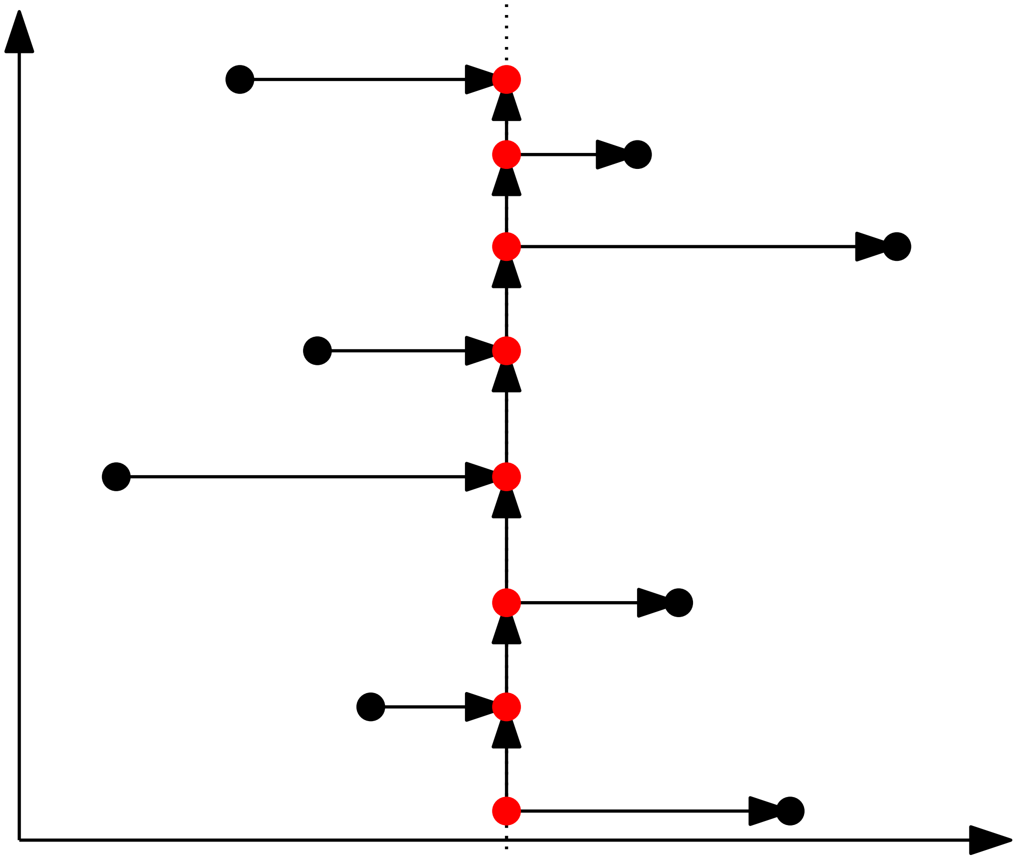

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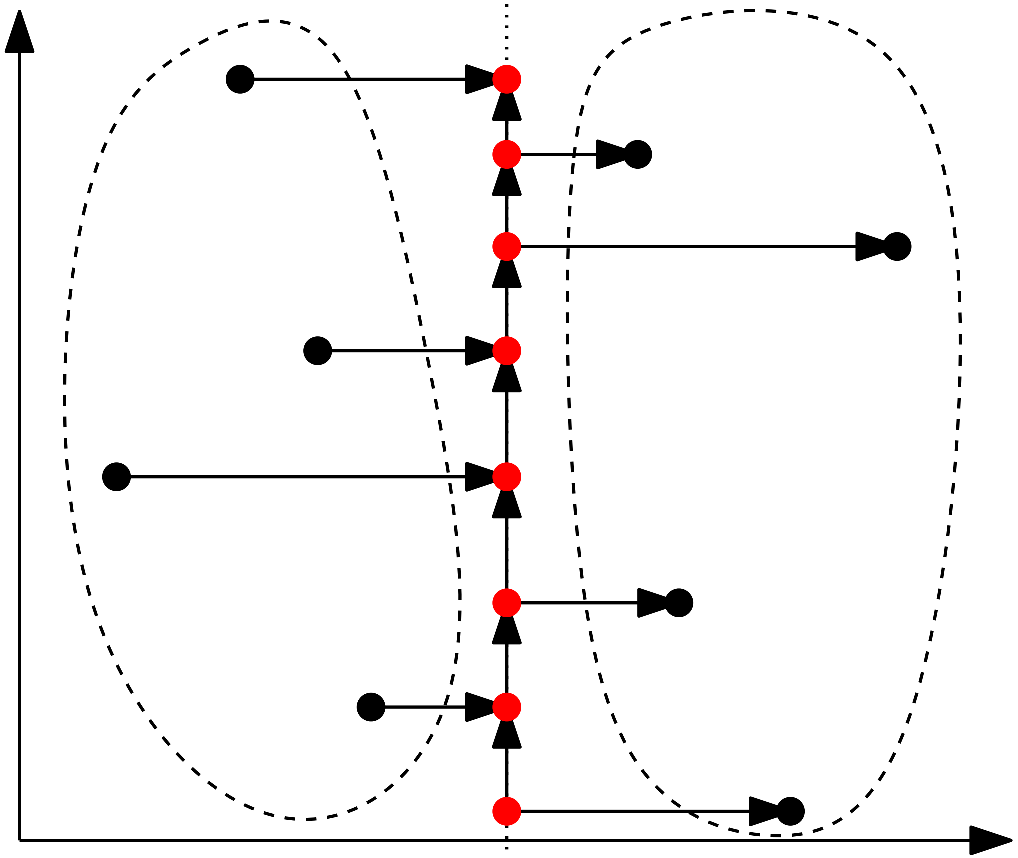

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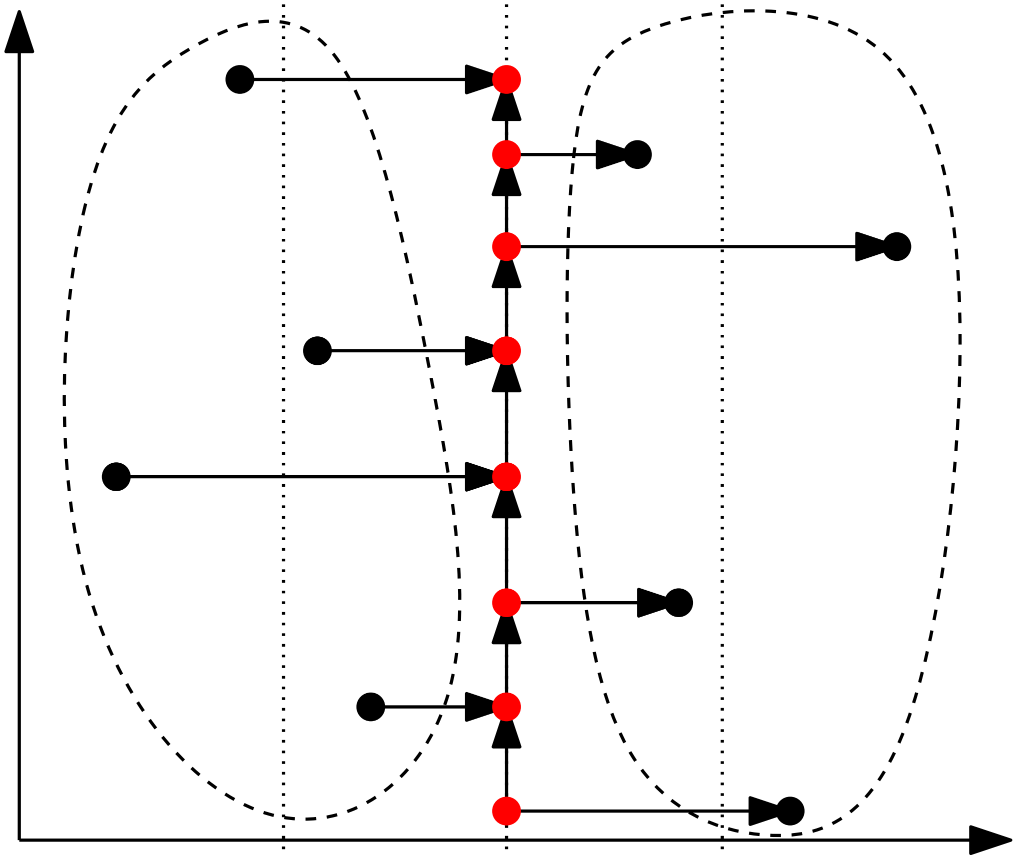

Recurse in each half.
→ $O(n \log n)$ in 2 dimensions.

small Manhattan networks
[Gudmundsson, Klein, Knauer, and Smid 2007]

$O(n \log n)$ is optimal in 2 dimensions: Horton sets

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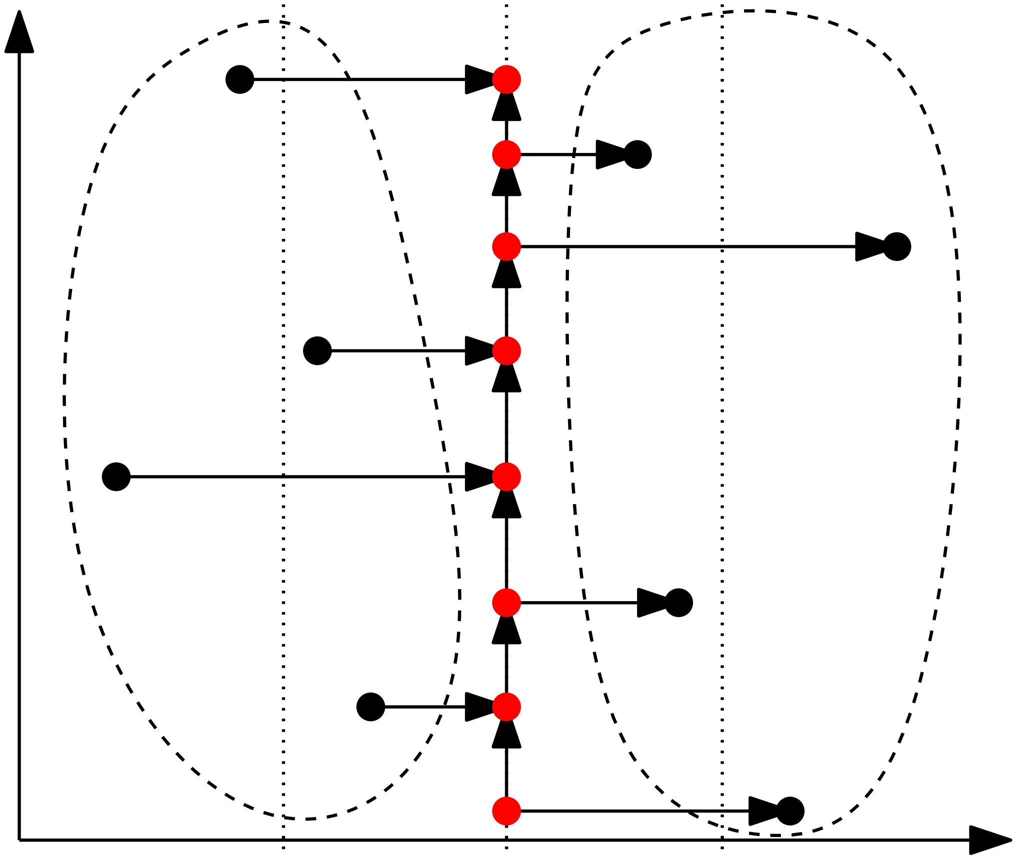

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Rote [2013]: $O(n)$ space and $O(n \log^{d-1} n)$ expected time

L_∞ regression for d-dimensional orders

Rote [2013]: $O(n)$ space and $O(n \log^{d-1} n)$ expected time

- feasibility checking without *explicitly* constructing the DAG
- randomized optimization by Timothy Chan's technique (saves a $\log$-factor.)

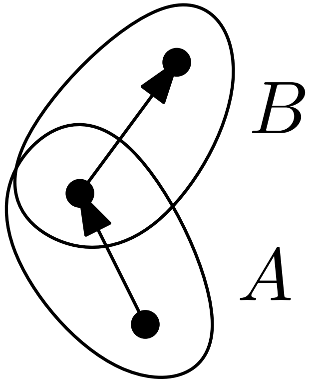
$$x_j^{\text{low}} = \max\{\ell_j, \max\{\, \ell_i \mid p_i \prec p_j \,\}\}$$

More general operation *update*(A, B): $(A, B \subseteq \{1, \ldots, n\})$

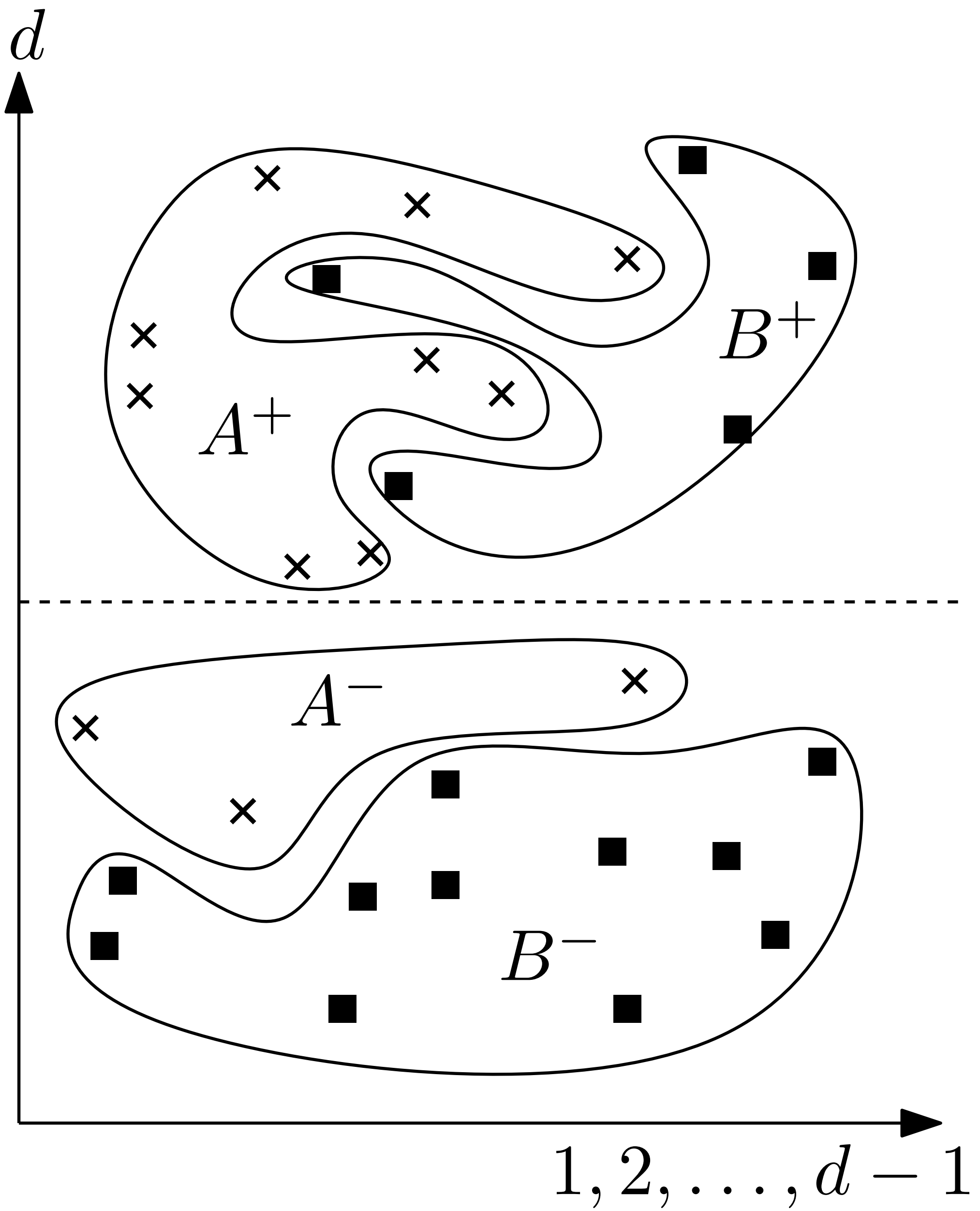
for all $j \in B$: $x_j^{\text{new}} = \max\{x_j^{\text{old}}, \max\{\, x_i^{\text{old}} \mid i \in A,\ p_i \prec p_j \,\}\}$

equivalent formulation:
for all $i \in A$, $j \in B$ (in any order):

if $p_i \prec p_j$ then set $x_j := \max\{x_j, x_i\}$.



Partitioning the *update* operation



```
procedure update$(A, B)$:
    Split $A \cup B$ along
            the last coordinate;
    update$(A^-, B^-)$;
    update$(A^-, B^+)$;
    update$(A^+, B^-)$;
    update$(A^+, B^+)$;
```

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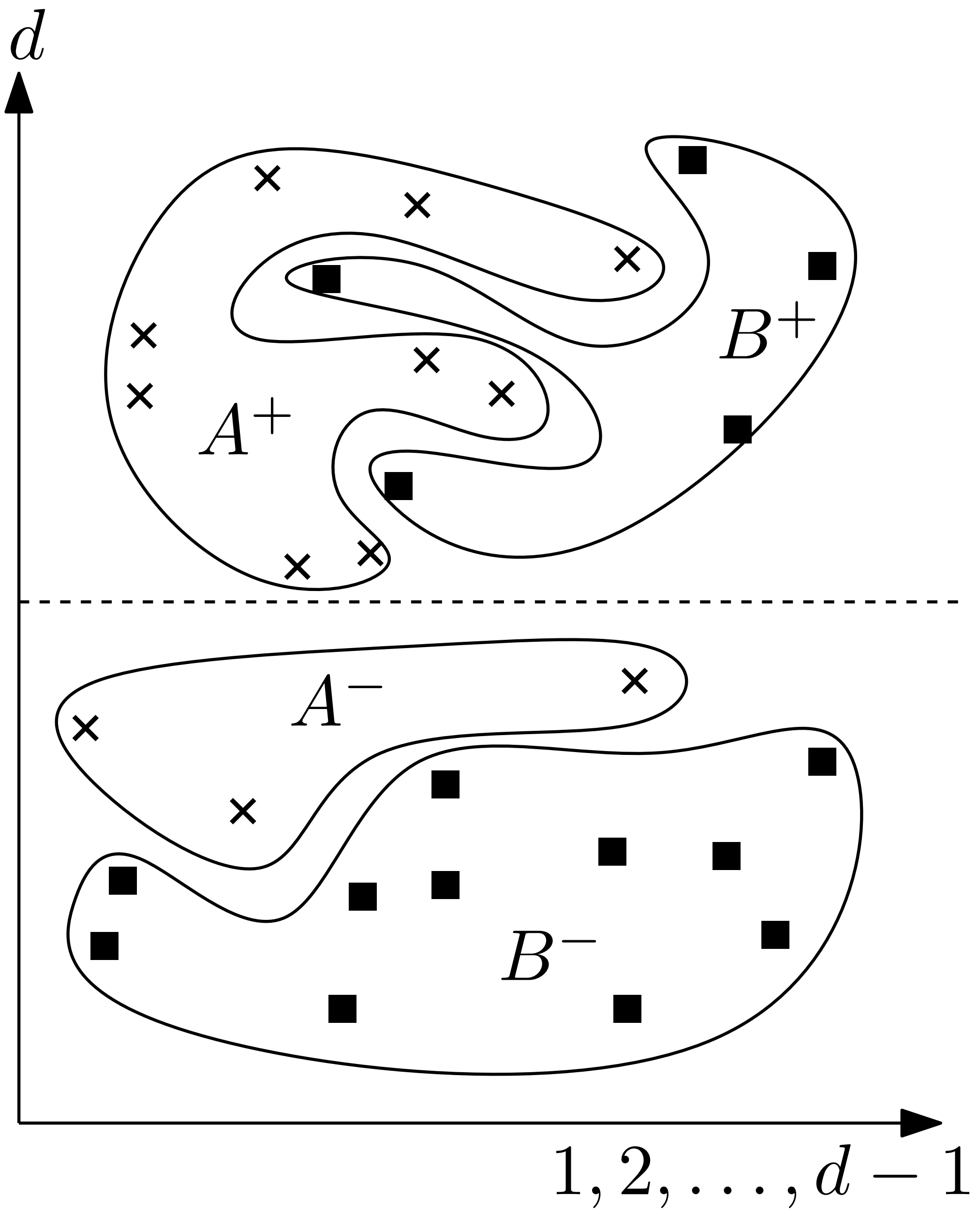

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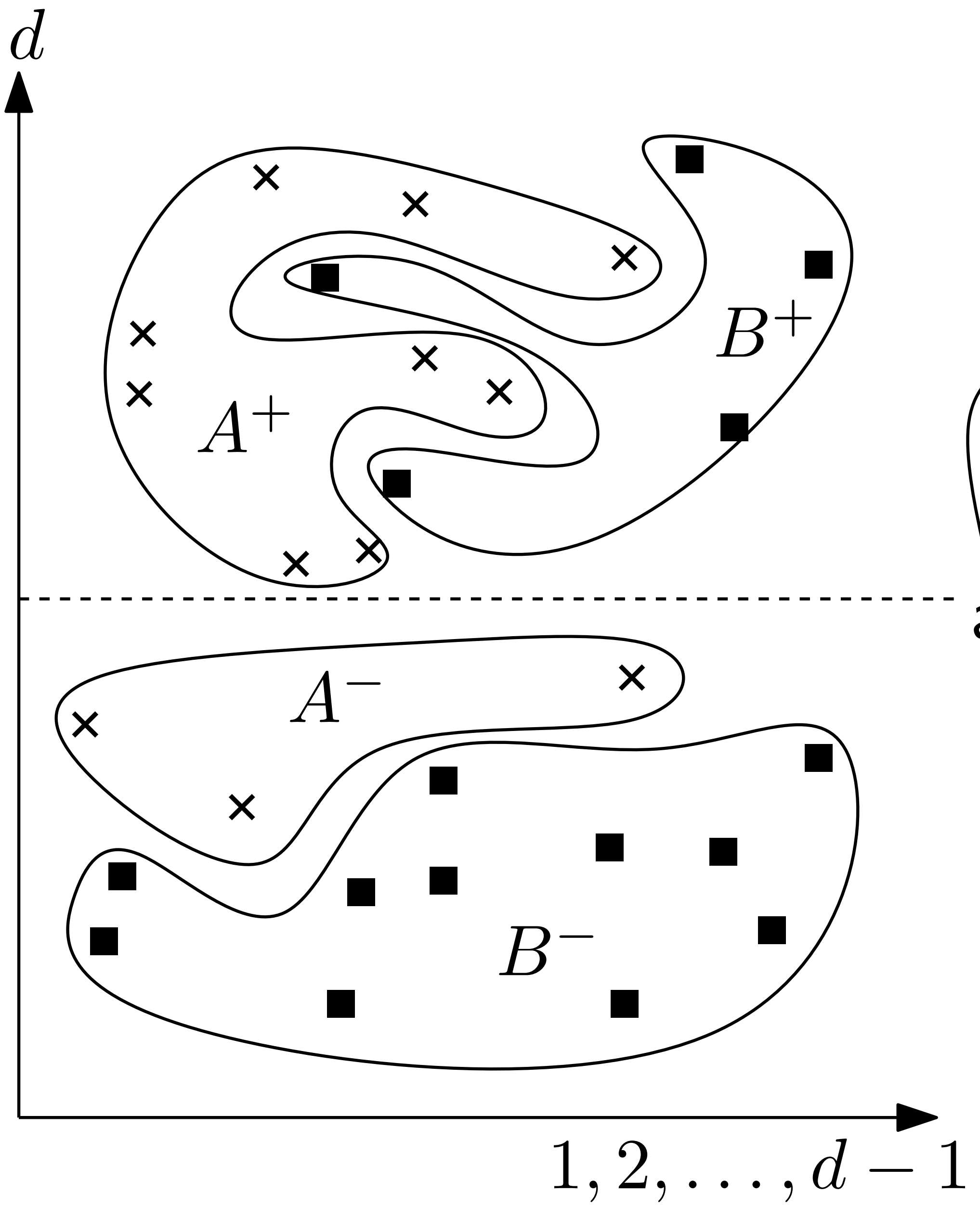

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    ~~update($A^+$, $B^-$);~~
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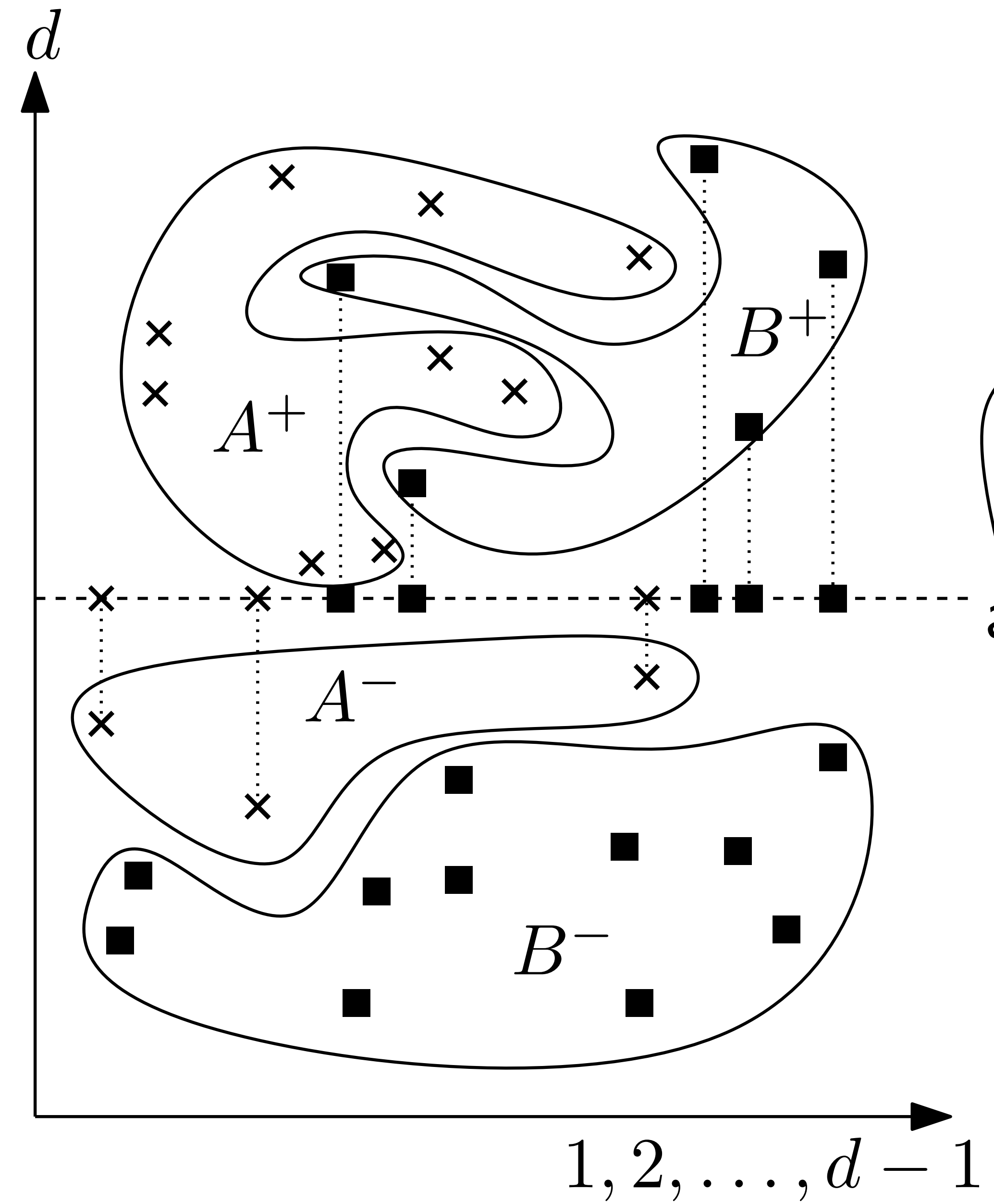
```

a $(d-1)$-dimensional order!

Partitioning the *update* operation



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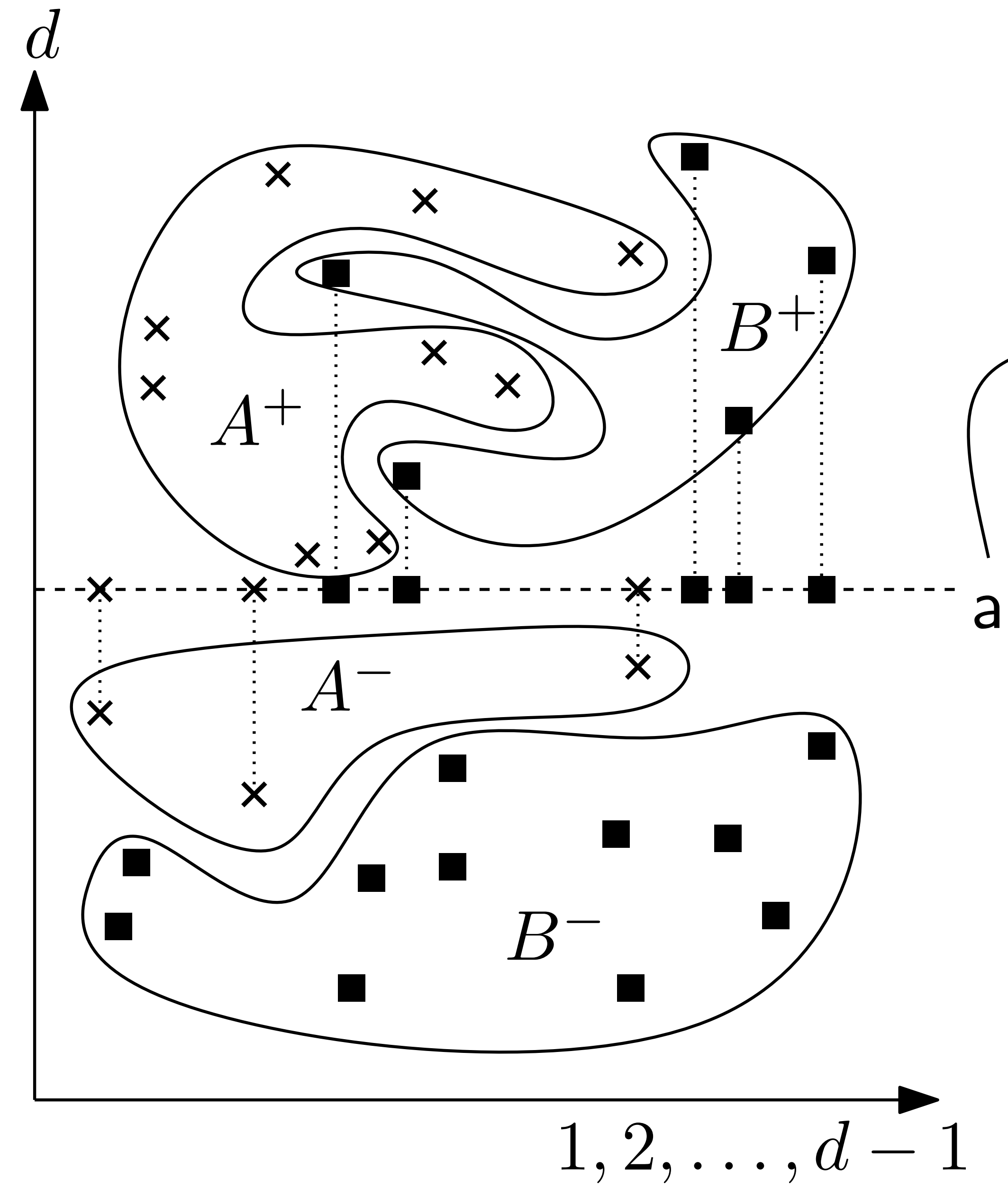
a $(d{-}1)$-dimensional order!

Partitioning the *update* operation



a $(d-1)$-dimensional order!

```
**procedure** update$(A, B)$:
    Split $A \cup B$ along
            the last coordinate;
    update$(A^-, B^-)$;
    update$(A^-, B^+)$;
    ~~update$(A^+, B^-)$;~~
    update$(A^+, B^+)$;
```

```
**procedure** update$_k(A, B)$:
    Split $A \cup B$ along
            the $k$-th coordinate;
    update$_k(A^-, B^-)$;
    update$_{k-1}(A^-, B^+)$;
    update$_k(A^+, B^+)$;
```

Partitioning the *update* operation (2)

```
procedure update_k(A, B):
    Split $A \cup B$ into two equal parts along the $k$-th coordinate;
    update_k$(A^-, B^-)$;
    update_{k-1}$(A^-, B^+)$;
    update_k$(A^+, B^+)$;
```

Initially sort along all coordinates in $O(n \log n)$ time.
→ Splitting takes linear time.

Initial call: *update*$_d(P, P)$ with $P = \{1, \ldots, n\}$

Base case: *update*$_1(A, B)$ is a linear scan. Takes $O(n)$ time.

Induction: *update*$_k(A, B)$ in $O(n \log^{k-1} n)$ time. ($n = |A \cup B|$)

Remark: *update*$_d(A, B)$ is always called with $A = B$.
update$_k(A, B)$ for $k < d$ is always called with $A \cap B = \emptyset$.

Randomized optimization technique

- The problem is decomposable: $z^* = \max\{\, z_{ij} \mid i \prec j \,\}$

  Define $z(P) := \max\{\, z_{ij} \mid i, j \in P,\ i \prec j \,\}$

  If $P = P_1 \cup P_2 \cup P_3$, then

  $$z(P) = \max\{z(P_1 \cup P_2), z(P_1 \cup P_3), z(P_2 \cup P_3)\}$$

  (Similar problems: Diameter, closest pair)

- We can check feasibility: Is $z(P) \le \varepsilon$?

Lemma. (Chan 1998)
$\Longrightarrow$ The solution can be computed in the same expected time as checking feasibility.

Randomized maximization

```
Permute subproblems $S_1, S_2, \ldots, S_r$ into random order.
$z^* := -\infty$;
for $k = 1, \ldots, r$ do
    if $z(S_k) > z^*$ then                 $(*)$
        $z^* := z(S_k)$;                   $(**)$
```

Proposition.
The test $(*)$ is executed r times, and the computation $(**)$ is executed in expectation at most

$$1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{r} = H_r \leq 1 + \ln r$$

times.

L_∞ regression in d dimensions

Partition P into 10 equal subsets $P_1 \cup \cdots \cup P_{10}$ (for example along the d-axis).

Form 45 subproblems (P_i, P_j) for $1 \le i \le j \le 10$ and permute them into random order.

```
$z^* := -\infty$;
**for** $k = 1, \ldots, 45$ **do**
    Let $(P_i, P_j)$ the $k$-th subproblem.
    Feasibility check: Is $z(P_i \cup P_j) \le z^*$?                (*)
    **if** not **then** compute $z(P_i \cup P_j)$ recursively        (**)
                 and set $z^* := z(P_i \cup P_j)$;
```

$$T(n) = O(\mathsf{FEAS}(n)) + H_{45} \cdot T(2n/10)$$

$$\le O(n \log^{d-1} n) + 4.395 \cdot T(n/5) = O(n \log^{d-1} n)$$