Second-Order Shape-Constrained Function Fitting

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based on joint work with David Durfee, Yu Gao, and Anup B. Rao

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WADS Algorithms and Data Structures Symposium 2019

Outline

1 Introduction

2 Our Result

3 Geometric Dynamic Programming

4 Conclusion

Regression

here: 2D points

- **Goal:** Given observations (x_i, y_i), find best **function** explaining $y_i \approx f(x_i)$.

"fit" function to points

- "regression analysis" ubiquitous in statistics / machine learning

↝ **stats challenge:** identify reasonable shape restrictions for f (model, prior knowledge)

↝ **cs challenge:** efficiently compute best f for data s. t. shape constraints

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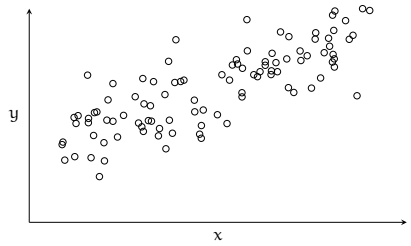

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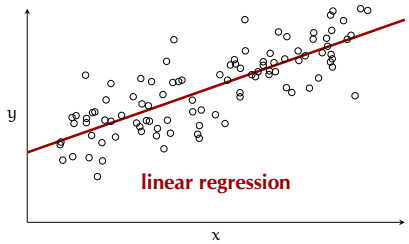

$$f(x) = ax + b$$

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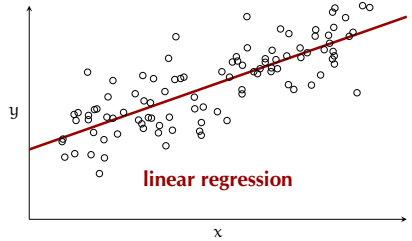

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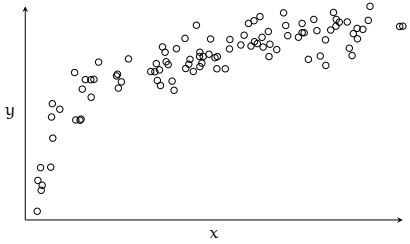

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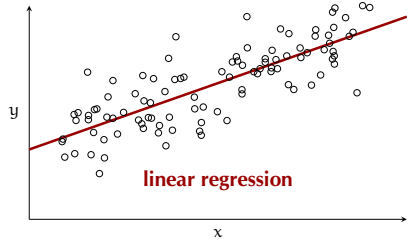

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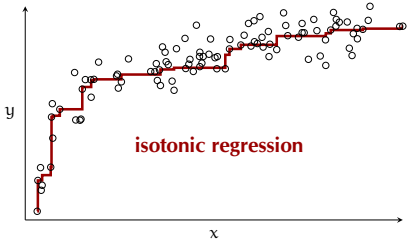

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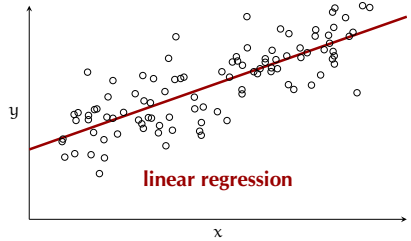

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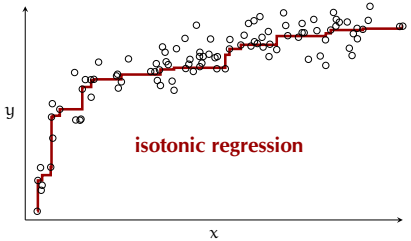

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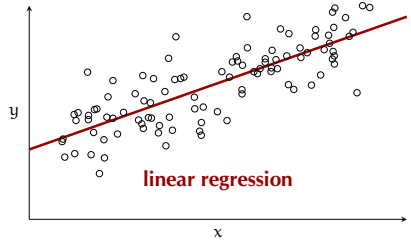

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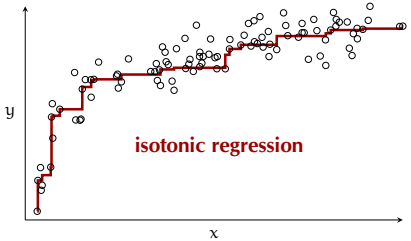

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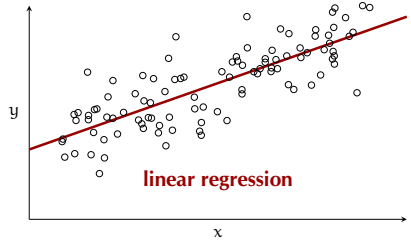

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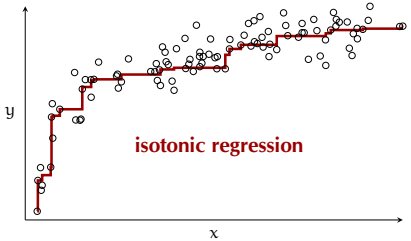

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Shape Constraints

Typical shape constraints for 1D functions

- (bounded)
- monotonic — cumulative density functions, low-dim. metric embedding
- unimodal — dose-response curves
- Lipschitz (bounded derivative) — avoiding overfitting in isotonic regression
- increasing & concave — production functions, utility functions (diminishing returns)
- convex — consumer preferences, value functions in reinforcement learning
- smooth

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all expressible by bounds on first and second derivatives!

Weighted L_∞ Function Fitting With 2nd-Order Constraints

$$\begin{aligned} \min \quad & \text{error between } \vec{f} \text{ and } \vec{y} \\ \text{s.t.} \quad & \text{bounds on 1st derivative of } \vec{f} \\ & \text{bounds on 2nd derivative of } \vec{f} \end{aligned}$$

given quantities
variables to compute

Weighted L_∞ Function Fitting With 2nd-Order Constraints

$$\min \quad \max_{1 \leqslant i \leqslant n} w_i \cdot |f_i - y_i|$$

s. t. bounds on 1st derivative of $\vec{f}$

bounds on 2nd derivative of $\vec{f}$

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Weighted L_∞ Function Fitting With 2nd-Order Constraints

weights

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$$\text{s.t.} \quad f_i'^{-} \leqslant f'(x_i) \leqslant f_i'^{+} \qquad (i = 2, \ldots, n)$$

given quantities
variables to compute

bounds on 2nd derivative of $\vec{f}$

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discrete derivative

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$$f_i''^- \leqslant \frac{\frac{f_i - f_{i-1}}{x_i - x_{i-1}} - \frac{f_{i-1} - f_{i-2}}{x_{i-1} - x_{i-2}}}{x_i - x_{i-1}} \leqslant f_i''^+ \qquad (i = 3, \ldots, n)$$

discrete 2nd derivative

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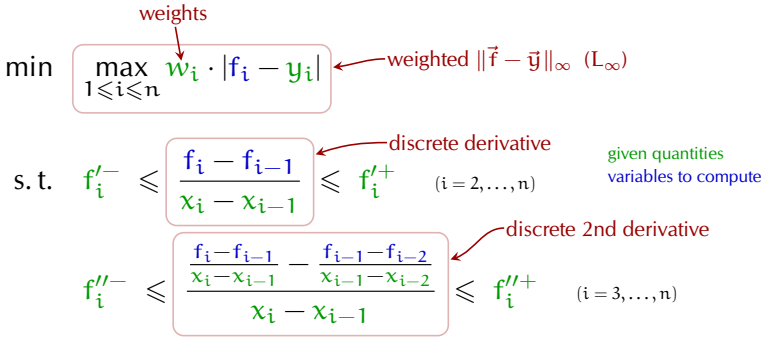

More convenient formulation:

$$f_i'^- \leqslant \frac{f_i - f_{i-1}}{x_i - x_{i-1}} \leqslant f_i'^+$$

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discrete 2nd derivative

More convenient formulation:

For this talk: $x_i = i \rightsquigarrow \alpha_i = 1$ (equidistant points)

general α in paper

$$\underbrace{(x_i - x_{i-1}) f_i'^-}_{y_i^-} \leqslant f_i - f_{i-1} \leqslant \underbrace{f_i'^+ (x_i - x_{i-1})}_{y_i^+}$$

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general α in paper

$$y_i^- \leqslant f_i - f_{i-1} \leqslant y_i^+$$

$$z_i^- \leqslant (f_i - f_{i-1}) - (f_{i-1} - f_{i-2}) \leqslant z_i^+$$

Previous Work

Shape Constraint	Error Norm	Time	Source
linear function	weighted L_2	$O(n)$	[linear least squares]
linear comb. of k fixed functions	weighted L_2	$O(nk^2)$	[linear least squares]
monotonic (isotonic regr. on path)	weighted L_2	$O(n)$	[pool adjacent violators algorithm, Rote 2019]
monotonic	weighted L_1	$O(n \log n)$	[Ahuja&Orlin 2001, Rote 2019]
monotonic	weighted L_∞	$O(n)$	[Stout 2015]
isotonic regr. on general partial orders	*various results surveyed*		[Stout 2019]
unimodal	weighted L_2	$O(n)$	[Stout 2008]
unimodal	weighted L_1	$O(n \log n)$	[Stout 2008]
unimodal	L_∞	$O(n)$	[Stout 2008]
piecewise constant (k-step function)	weighted L_∞	$O(n \log n)$	[Fournier&Vigneron 2013]
piecewise constant (k-step function)	L_∞	$O(n)$ sorted input	[Fournier&Vigneron 2011]
Lipschitz & monotonic	L_2	$O(n \log n)$	[Agarwal&Phillips&Sadri 2010]
Lipschitz & unimodal	L_2	$O(n \operatorname{polylog} n)$	[Agarwal&Phillips&Sadri 2010]
multivar. convex (& Lipschitz)	L_2	quadr. prog. $\Theta(n^2)$ constraints	[Mazumder et al. 2018]

Previous Work

Summary:

- **Near-linear** time exact methods for **first-order** constraints
- Best prior approach for **second-order**: **solve LP**

Shape Constraint			
linear function	weighted L_2	$O(n)$	[linear least squares]
linear comb. of k fixed functions	weighted L_2	$O(nk^2)$	[linear least squares]
monotonic (isotonic regr. on path)	weighted L_2	$O(n)$	[pool adjacent violators algorithm, Rote 2019]
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Lipschitz & monotonic	L_2	$O(n \log n)$	[Agarwal&Phillips&Sadri 2010]
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Previous Work

Summary:

- **Near-linear** time exact methods for **first-order** constraints
- Best prior approach for **second-order**: **solve LP**

Shape Constraint			
linear function	weighted L_2	$O(n)$	[linear least squares]
linear comb. of k fixed functions	weighted L_2	$O(nk^2)$	[linear least squares]
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Outline

1 Introduction

2 Our Result

3 Geometric Dynamic Programming

4 Conclusion

Our result

Main result:
There is a single algorithm computing $\vec{f}$ s. t. **2nd-order constraints** with

$$\max_i w_i \cdot |f_i - y_i| \quad \leqslant \quad \mathrm{OPT} + \varepsilon \qquad (\varepsilon\text{-approximation})$$

in **time** $\mathbf{O}\left(n \log\left(\frac{U}{\varepsilon}\right)\right)$ for $U = (\max w_j)(\max y_j - \min y_j)$.

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$$\begin{array}{lcccl} & \exists \vec{f} \text{ s. t.} & & & \\ x_i^- & \leqslant & f_i & \leqslant & x_i^+ \quad i = 1..n \\ y_i^- & \leqslant & f_i - f_{i-1} & \leqslant & y_i^+ \quad i = 2..n \\ z_i^- & \leqslant & (f_i - f_{i-1}) - (f_{i-1} - f_{i-2}) & \leqslant & z_i^+ \quad i = 3..n \end{array}$$

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This talk: only Yes/No
But: can find $\vec{f}$ by backtracing ($\rightsquigarrow$ paper)

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Dynamic Programming with Infinite States?

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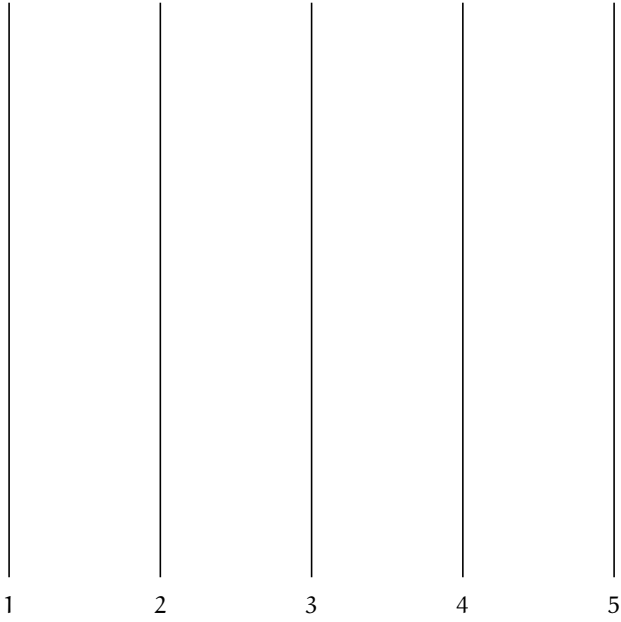

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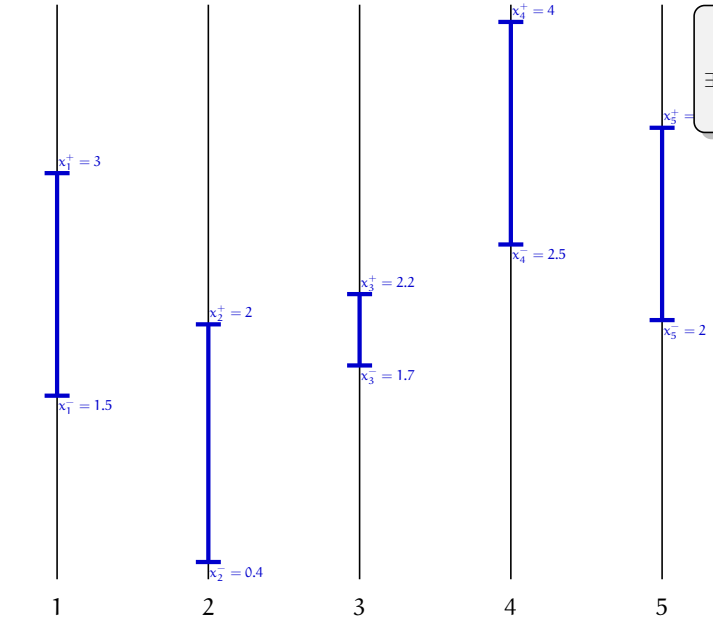

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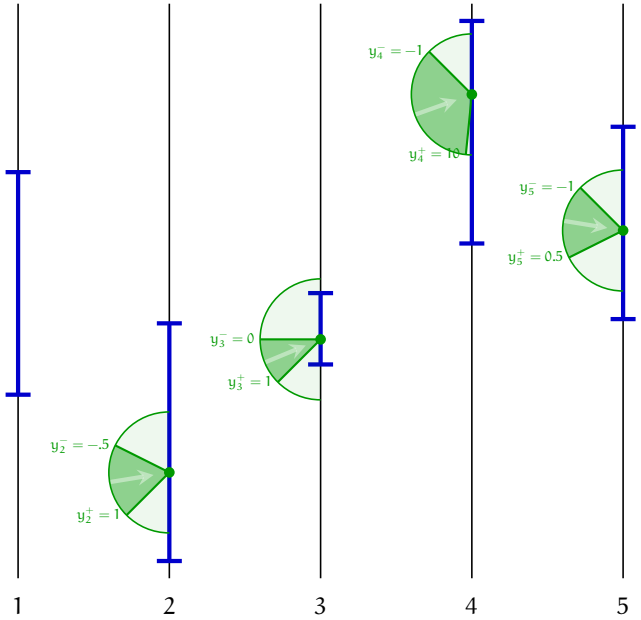

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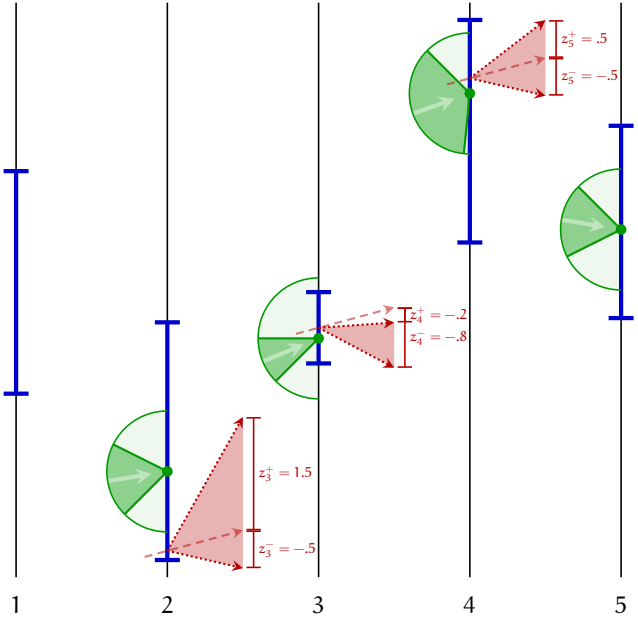

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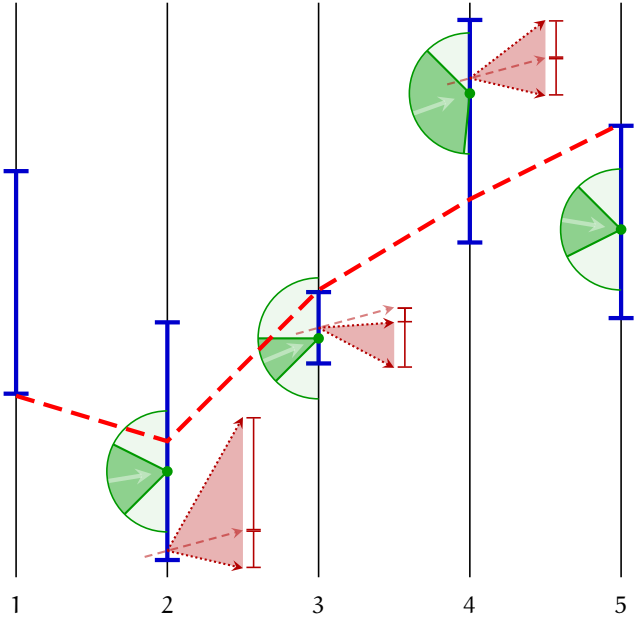

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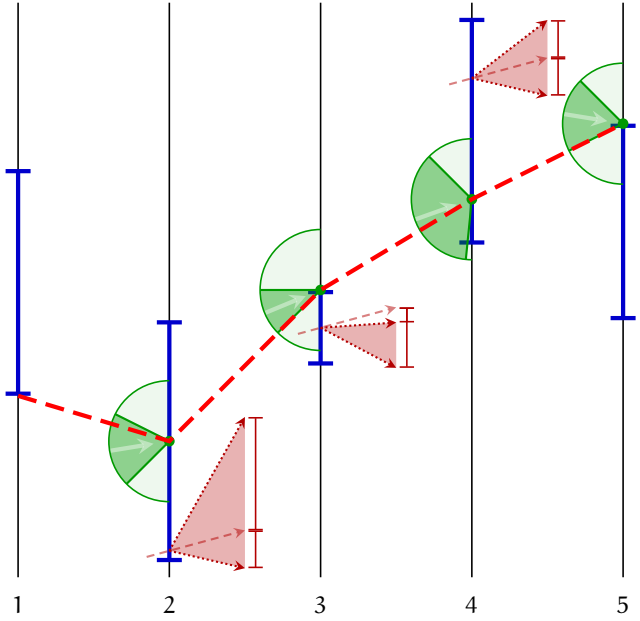

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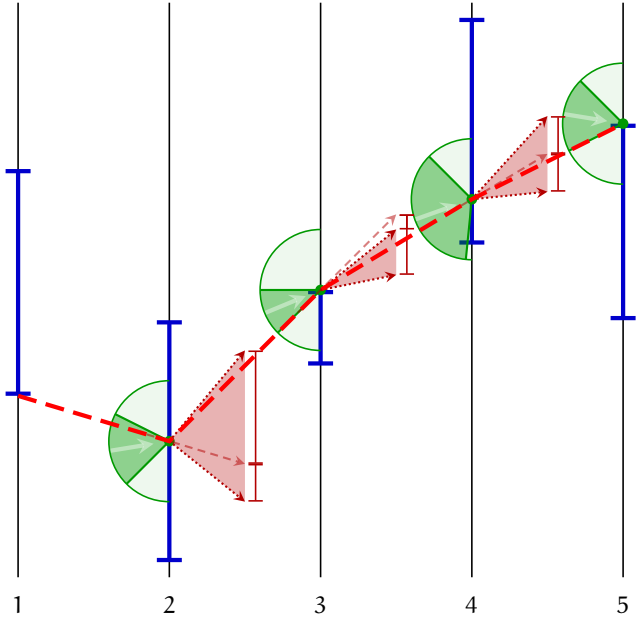

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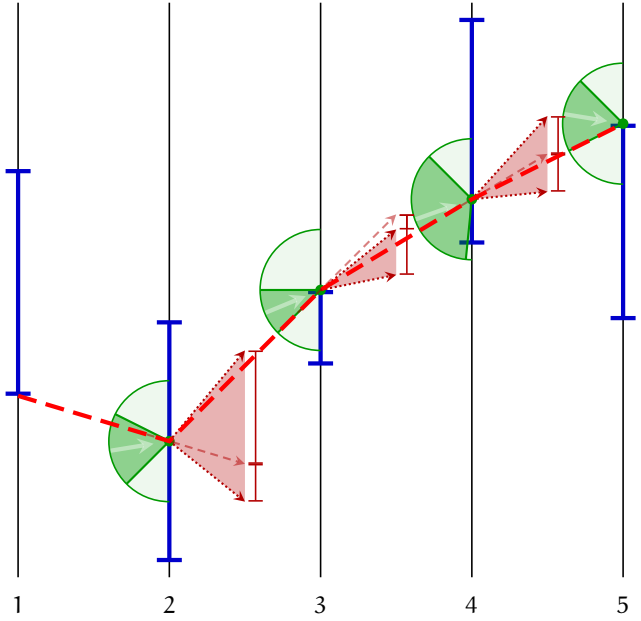

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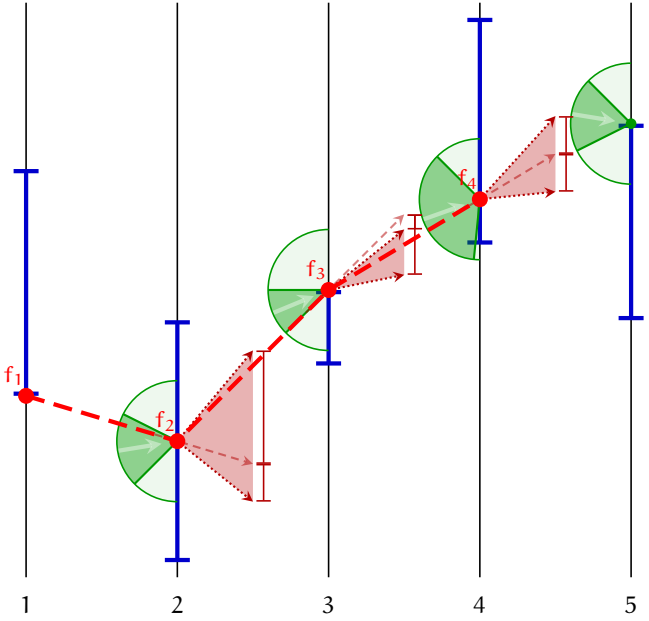

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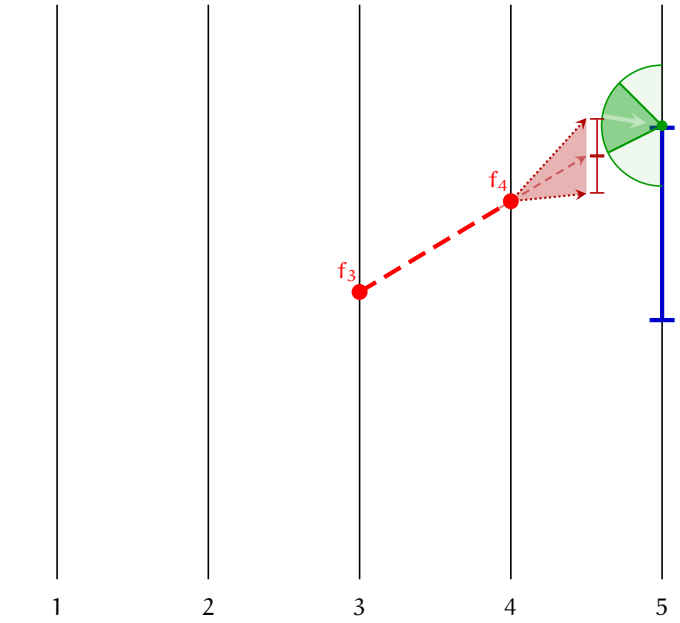

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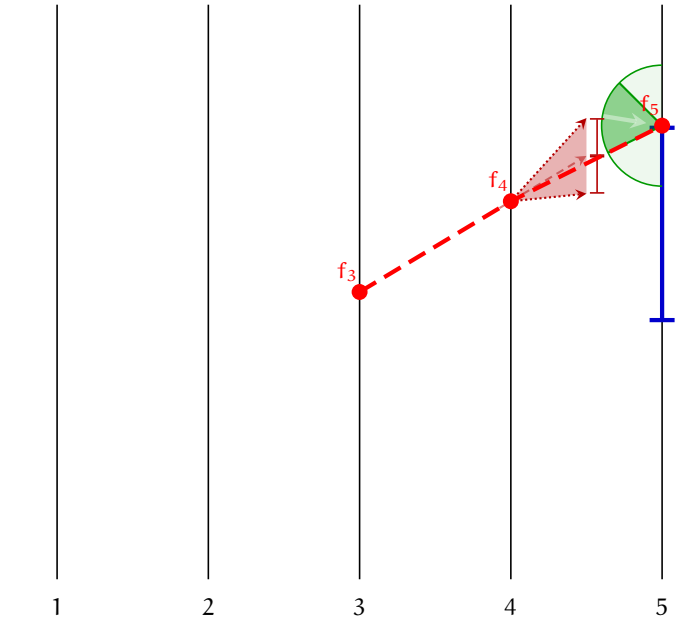

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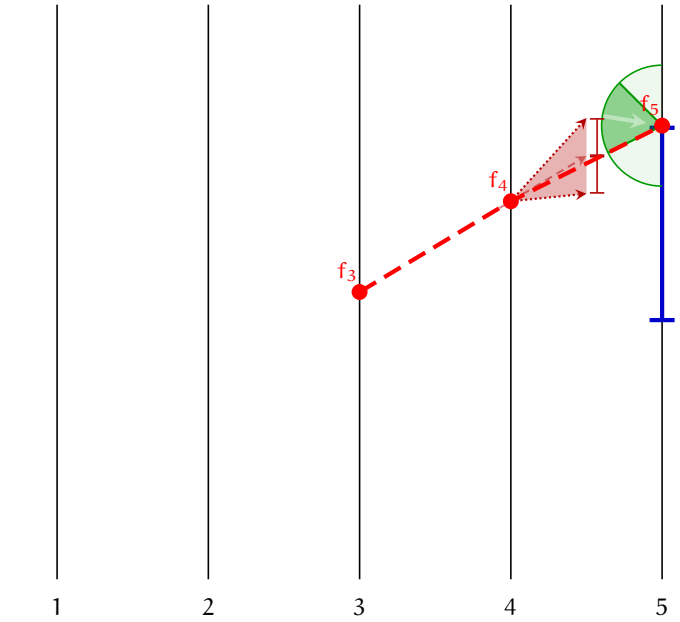

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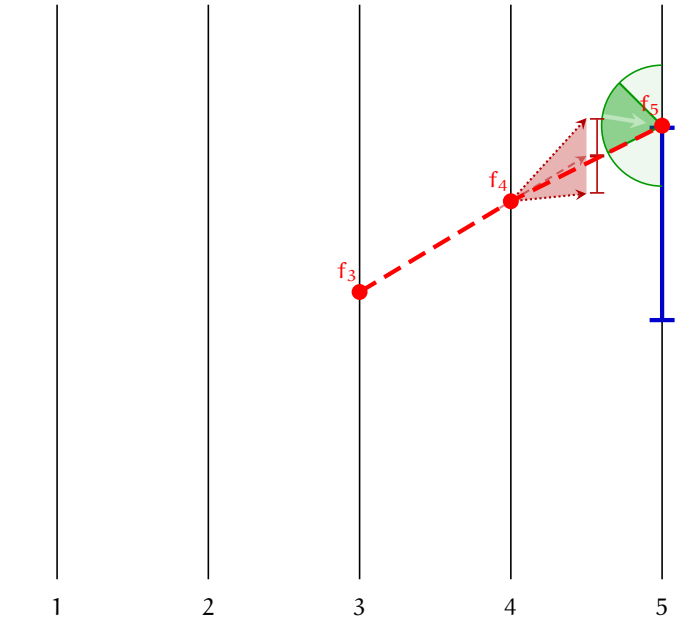

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Continuous problem! Infinitely many candidates $\vec{f}$!

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There is a **finite** representation
for **all** prefix **candidates**

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possible last components of prefix solutions

Dynamic Programming with Infinite States!



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From P_{i-1} to P_i – Step 1

$$P_i = \left\{ (f_i, f_i - f_{i-1}) \,:\, \exists (f_1, \ldots, f_{i-2}) \;\; \forall j \leqslant i \;\; (x_j), (y_j), (z_j) \right\}$$

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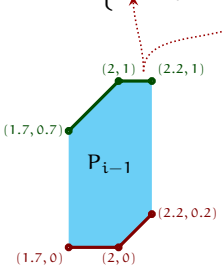

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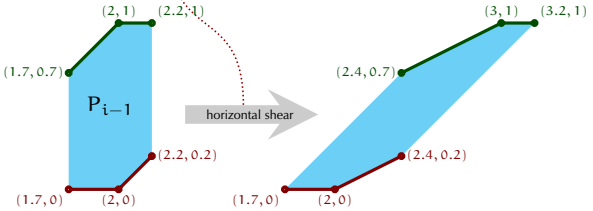

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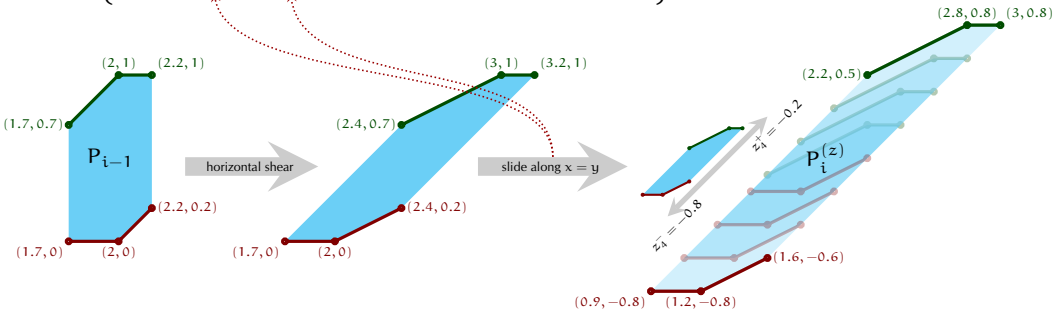

From P_{i-1} to P_i – Step 2

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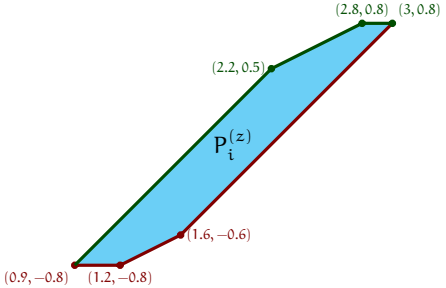

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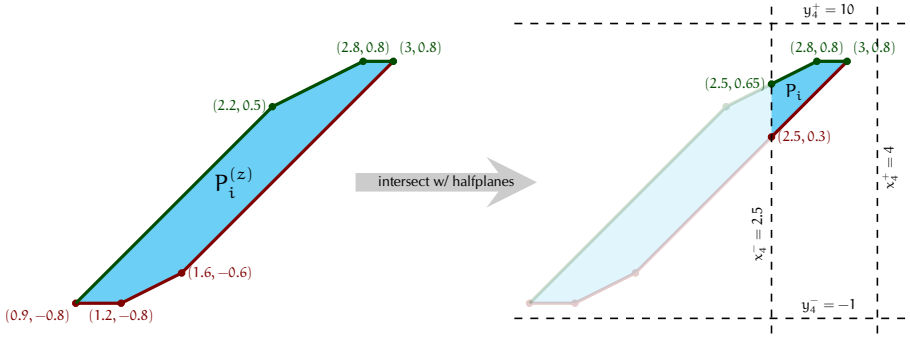

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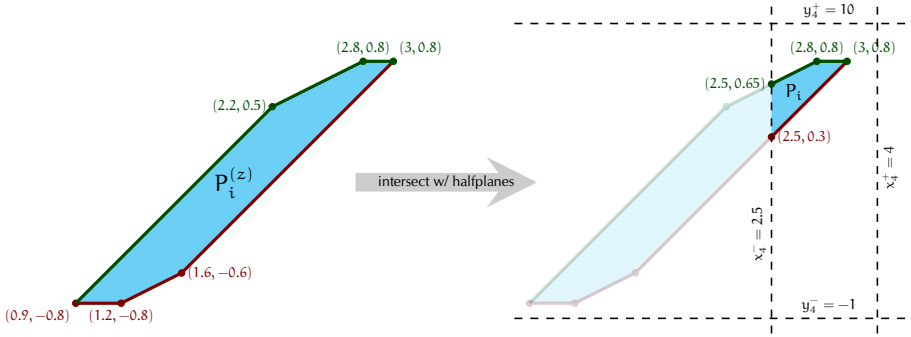
$$P_i = \Big\{(x,y) \ : \ x \in [x_i^-, x_i^+],\ y \in [y_i^-, y_i^+],\ \exists u\ (x-y,u) \in P_{i-1},\ y-u \in [z_i^-, z_i^+]\Big\}$$



$\rightsquigarrow$ Can compute $P_2, \dots, P_n$ iteratively, check if P_n nonempty.

Data Structures & Implicit Updates

But: *Not yet done!*

- P_i has $O(i)$ vertices

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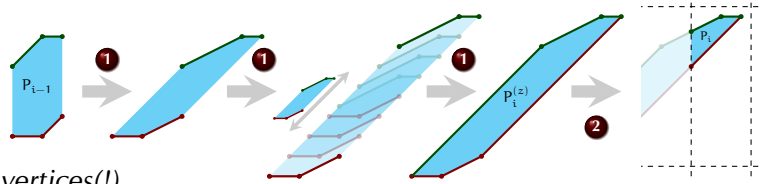

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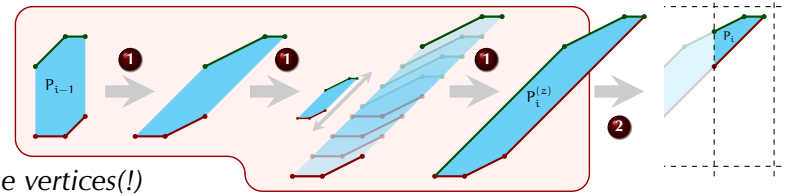



+append 1 vertex each

Step 1 (mostly) applies **same linear** transformations to vertices in **upper** resp. **lower hull**.

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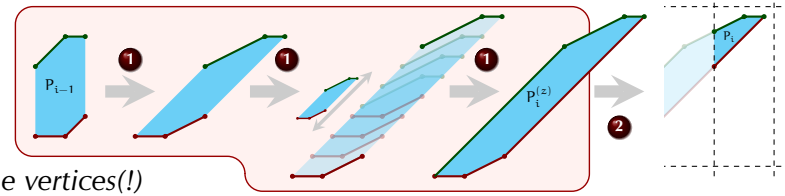



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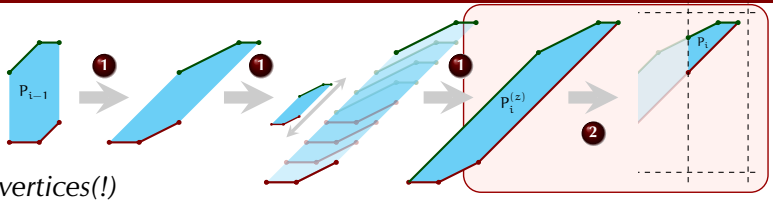



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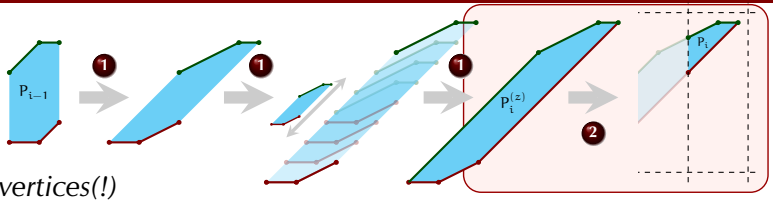



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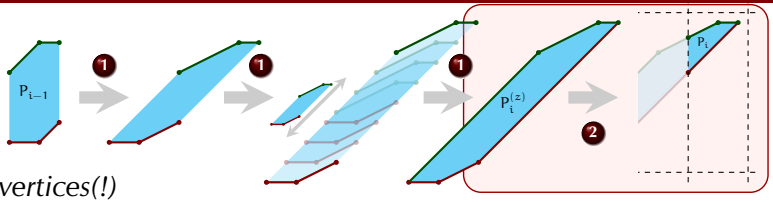

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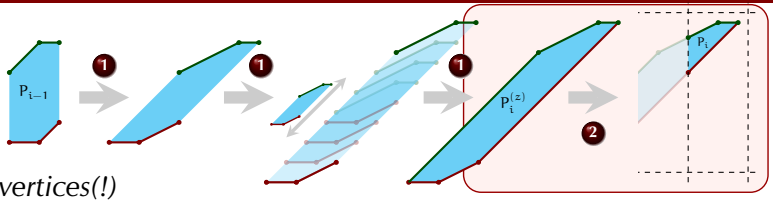



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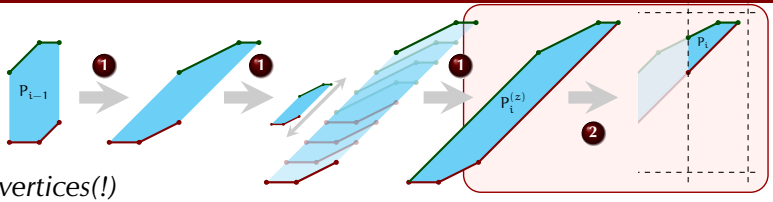

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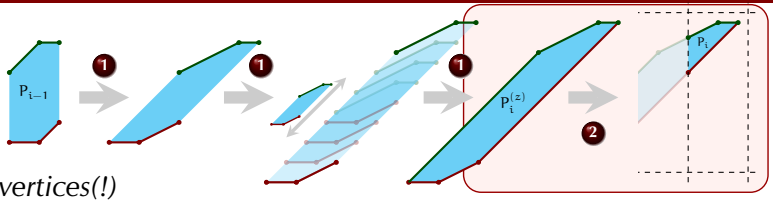

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⇝ Linear search for intersections costs $O(n)$ in total (search cost = # deleted vertices)

Our result

Main result:
There is a single algorithm computing $\vec{f}$ s. t. **2nd-order constraints** with

$$\max_i w_i \cdot |f_i - y_i| \quad \leqslant \quad \mathrm{OPT} + \varepsilon \qquad (\varepsilon\text{-approximation})$$

in **time** $O\big(n \log(\frac{U}{\varepsilon})\big)$ for $U = (\max w_j)(\max y_j - \min y_j)$.

Overview:

- $O(n)$ alg. for **decision** version:
  Given L, $\exists \vec{f}$ with error $\leqslant L$?
- **Binary search** for smallest L
  $\rightsquigarrow O\big(\log(\frac{U}{\varepsilon})\big)$ iterations

This talk: only Yes/No
But: can find $\vec{f}$ by backtracing ($\rightsquigarrow$ paper)

2nd-order-diff constrained decision problem:

$$\exists \vec{f} \text{ s. t.}$$

$$\begin{array}{rcccll}
x_i^- & \leqslant & f_i & \leqslant & x_i^+ & i = 1..n \\
y_i^- & \leqslant & f_i - f_{i-1} & \leqslant & y_i^+ & i = 2..n \\
z_i^- & \leqslant & (f_i - f_{i-1}) - (f_{i-1} - f_{i-2}) & \leqslant & z_i^+ & i = 3..n
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2 Our Result

3 Geometric Dynamic Programming

4 Conclusion

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You've seen

- First **near-linear** algorithm for a regression problem with **2nd-order** shape constraints
- Geometric dynamic programming

You have not seen → paper

- Handling **general** α (non-equidistant x_i's)
- Simple $O(n)$ algorithm for special case of **unweighted** L_∞ **convex** regression.
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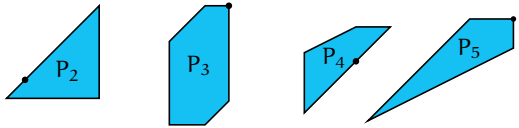

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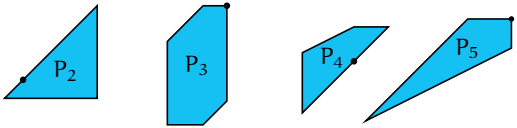

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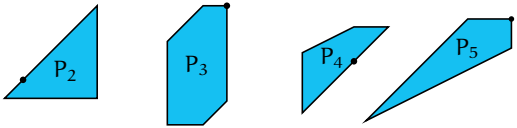

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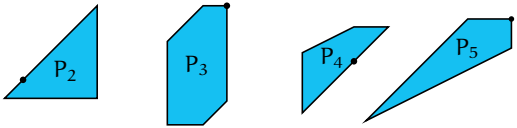

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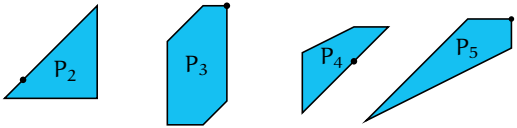

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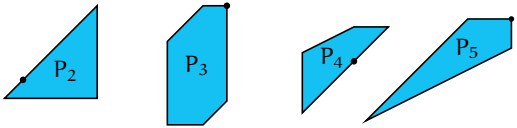

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