Ordered monotone regression

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Agenda

1. Motivating example
2. Problem
3. One monotone curve
4. Two-curve problem
5. Algorithms
6. Smooth estimates
7. Stress-strain example

Motivating example from mechanical engineering

Dynamic material tests, Shim and Mohr (2009).

Determine deformation resistance (strength of material) from uniaxial compression tests at different loading velocities.

Yields stress-strain curves.

x-axis: strain,

- force applied to experimental unit via piston ("Kolben"),
- negative logarithm of ratio of current over initial piston stroke,
- maximum shortening of piston stroke: 63% $\Rightarrow$ x-values lie in $[0, 1]$.
- x-values in fact measured with error $\Rightarrow$ ignored.

y-axis: stress,

- measured compression of the sample,
- computed from cross-sectional area of specimen.

Motivating example from mechanical engineering

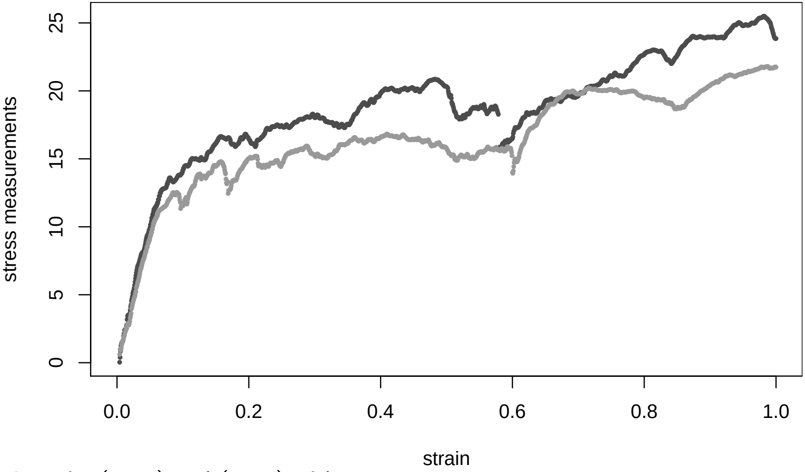
Substantial noise due to

- variability in loading velocity and
- electrical noise in data acquisition.

Regression curves are expected to be

1. monotone increasing $\Rightarrow$ stress $=$ increasing function of strain,
2. ordered $\Rightarrow$ deformation resistance increases as loading velocity increases.

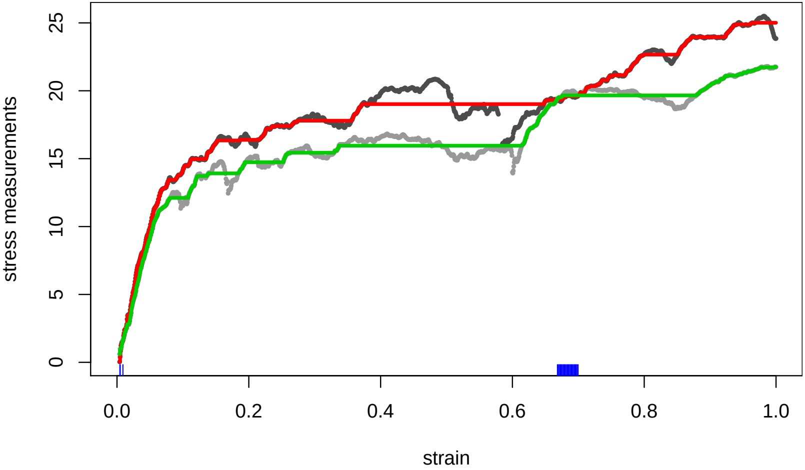
Motivating example from mechanical engineering



1495 pairs (x_i, y_i) and (x_i, z_i) with

- x_i: invoked strain,
- y_i, z_i: stress measurements for two loading velocities.

Naive approach



Two naive approaches to "estimation":

- "Trial and error" with "parametric" functions ⇒ original approach!
- Two independent monotone functions ⇒ ordering not guaranteed.

Problem

For data (x_i, y_i) and (x_i, z_i) find the minimizer of

$$L_2(\mathbf{a}, \mathbf{b}) = \sum_{i=1}^{n} w_{1,i}(y_i - a_i)^2 + \sum_{i=1}^{n} w_{2,i}(z_i - b_i)^2$$

over $(\mathbf{a}, \mathbf{b}) \in \mathbb{R}^n \times \mathbb{R}^n$ such that

- **a** and **b** are increasing and
- $\mathbf{a} \le \mathbf{b}$, with $\mathbf{w}_1, \mathbf{w}_2 \in \mathbb{R}_+^n$ given vectors of weights.

Questions:

- Existence?
- Uniqueness?
- Characterization?
- Computation?
- Consistency?
- Test whether regression functions are monotone?
- Or whether they are different from each other?

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A simpler problem

Minimize

$$L_1(\mathbf{a}) \quad = \quad \sum_{i=1}^{n} w_i(y_i - a_i)^2$$

over $\mathbf{a} \in \mathbb{R}^n$ s.t. $a_1 \leq a_2 \leq \cdots \leq a_n$ where $w_i > 0$.

Identify any vector $\mathbf{v} \in \mathbb{R}^n$ with cumsum function $Hy : [0, n] \to \mathbb{R}$:

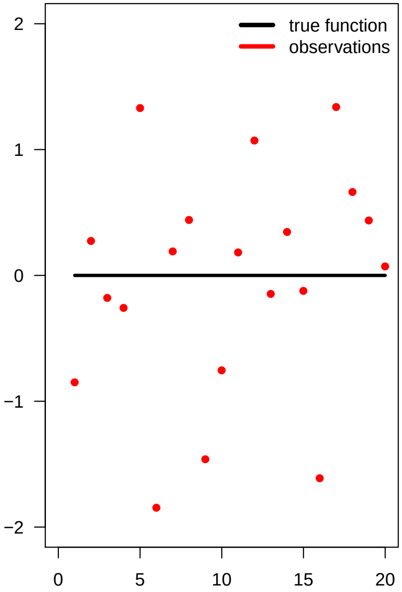
- $Hy(0) = 0$,
- $Hy(k) = \sum_{i=1}^{k} y_i, \;\; k = 1, \ldots, n$,
- and linear on the intervals $[0, 1], \ldots, [n-1, n]$.

Theorem

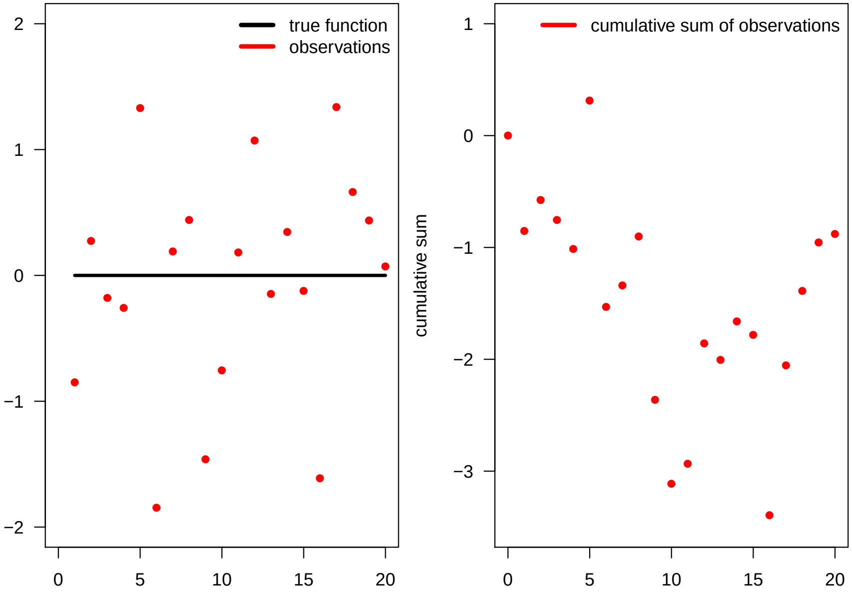
A vector $\widehat{\mathbf{a}}$ *minimizes* L_1 *if and only if*

$$\begin{aligned} H\widehat{\mathbf{a}}(n) &= H\mathbf{y}(n), \\ H\widehat{\mathbf{a}} &\leq H\mathbf{y} \text{ on } [0, n], \\ H\widehat{\mathbf{a}}(t) &= H\mathbf{y}(t) \text{ at knot points } t \in]0, n[\text{ of } H\widehat{\mathbf{a}}. \end{aligned}$$

Characterization in one-curve problem



Characterization in one-curve problem



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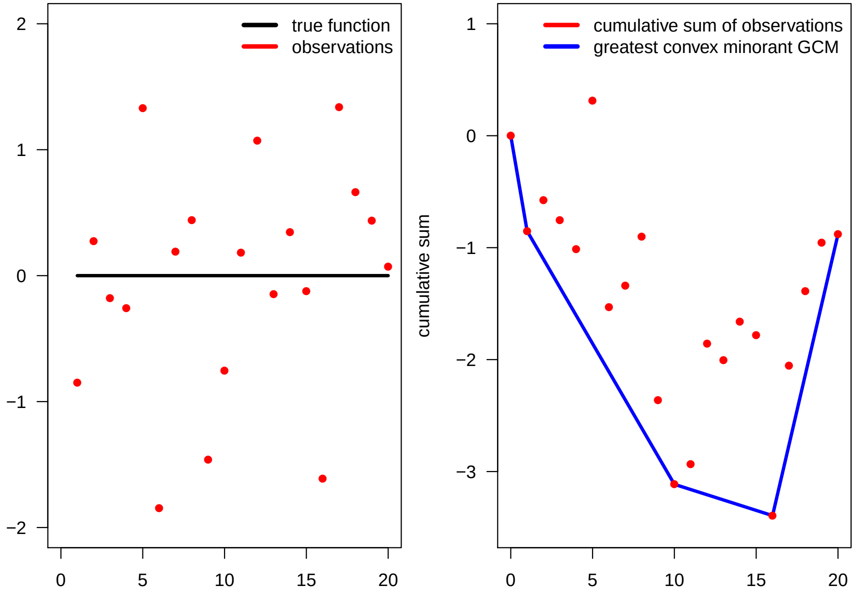

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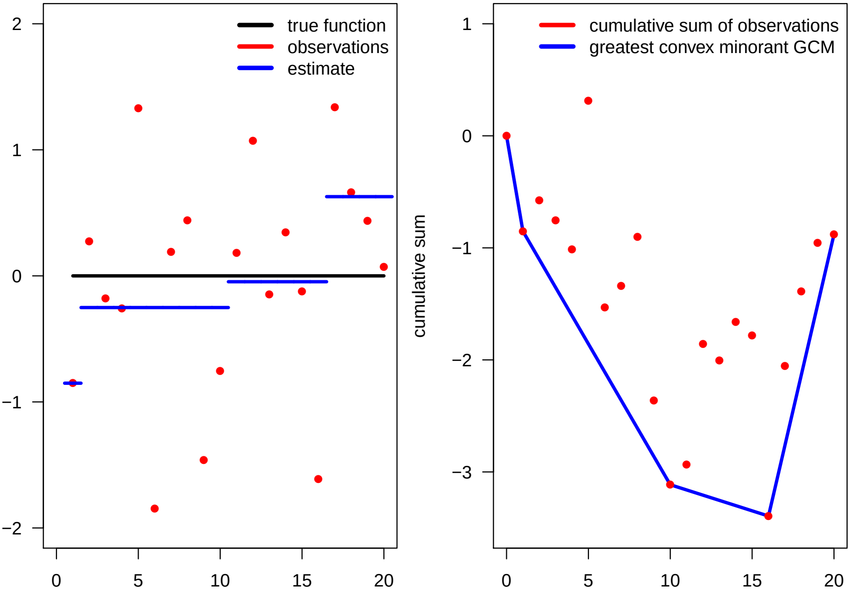

Monotone regression in applications

- Regression curve estimation, especially for small datasets: constrain parameter space ⇒ reduce e.g. MSE.
- Estimation of dose-response curves.
- Regression with ordered covariates:
  - Bayesian GLM: Dunson (2003a, b),
  - Least squares, GLM: R. (2009).
- Econometrics: Engel-curve, demand of a household for a given commodity as a function of income.
- etc.

Numerous density estimation applications, e.g. estimation of p-value density in multiple testing framework (Langaas et al, 2005).

Computation via PAVA

Compute monotone estimate using Pool-adjacent-violaters algorithm (PAVA):

- Initialization: each $x_i = i$ is a subset.
- Find minimal i where $y_i > y_{i+1}$ ($=$ violation), pool corresponding x_i's in one subset, replace y_i, y_{i+1} by $M(y_i, y_{i+1}) = (y_i + y_{i+1})/2$.
- Iterate until no violations are left.

Features of PAVA:

- Only values at x_i's relevant for criterion $\Rightarrow$ define estimate as suitable derivative of GCM on entire interval $[0, n]$.
- At most n iterations.
- Easy to implement and fast.

min-max representation and generalizations

Equivalent representation for least-squares problem:

$$\widehat{a}_i^* \quad = \quad \max_{s \le i} \min_{t \ge i} M(\{s, \ldots, t\})$$

where $M(\{s, \ldots, t\}) = \sum_{i=s}^{t} y_i w_i / \sum_{i=s}^{t} w_i$.

Used to derive theoretical results.

Criterion function: least squares $\Leftrightarrow$ functional in min-max representation: weighted mean.

PAVA is valid in more general framework: A functional M satisfies averaging property if for any sets A and B s.t. $A \cap B = \emptyset$ we have

$$\min\{M(A), M(B)\} \le M(A \cup B) \le \max\{M(A), M(B)\}.$$

Validity of PAVA for general functionals

Subdivision of $\{1, \ldots, n\}$: set of disjoint subsets.

Theorem

PAVA yields subdivision of x_i's s.t.

1. *The functional M is increasing on the sets of the subdivision.*
2. *A finer subdivision would necessarily cause a violation.*
3. *The estimate received by the PAVA is equivalent to that given by the min-max representation.*

Statement for mean functional (least squares): Barlow, Bartholomew, Bremner, and Brunk (1972).

Rigorous proof for general functionals having averaging property: Balabdaoui, R., and Santambrogio (2009).

Functionals satisfying averaging property

- Mean: $M(A) = \sum_{i \in A} w_i a_i / \sum_{i \in A} w_i$,
- Bounded mean: $(M(A) \vee \max_A a_i^1) \wedge \min_A \mathbf{a}^0$ with $\mathbf{a}^0, \mathbf{a}^1 \in \mathbb{R}^n$,
- Median: $\mathrm{med}_A\, \mathbf{a} = \arg\min_{m \in \mathbb{R}} \sum_{i \in A} |a_i - m| w_i$,
- Minimum: $\min_A \mathbf{a} = \min_{i \in A} a_i$,
- Maximum: $\max_A \mathbf{a} = \max_{i \in A} a_i$.

Minimum, maximum, and sum of two functionals M_1 and M_2 satisfying averaging property satisfy it as well.

Back to two-curve problem: obvious questions

- Geometrical characterizations using GCMs?
- PAVA-like algorithm?
- min-max representation?

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- Geometrical characterizations using GCMs? Not found.
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Alternatives:

- Analytical characterizations.
- Projected subgradient algorithm (general), Dykstra's algorithm (least squares).
- First value of lower and last of upper curve.

$$L_2(a, b) = \sum_{i=1}^{n} w_{1,i}(y_i - a_i)^2 + \sum_{i=1}^{n} w_{2,i}(z_i - b_i)^2$$

Theorem (Balabdaoui, R., and Santambrogio, 2009)

- *Estimate* $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}})$ *exists and is unique.*
- *Necessary and sufficient characterization can be given.*
- *We have the following representations:*

$$\widehat{a}_i^* = \max_{s \le i} \min_{t \ge i} \left(M_1(\{s, \ldots, t\}) \wedge \widehat{b}_s^* \right)$$

$$\widehat{b}_i^* = \max_{s \le i} \min_{t \ge i} \left(M_2(\{s, \ldots, t\}) \vee \widehat{a}_t^* \right)$$

for $i = 1, \ldots, n$, *where* M_1 *and* M_2 *are the weighted mean functionals.*

Problem with min-max representation:

- Expression for $\widehat{a}_i^*$ depends on $\widehat{\mathbf{b}}^*$ and vice versa.
- Idea for algorithm: iterate above min-max representations.
  Does not work!

Dykstra's algorithm

Problem of minimizing

$$L_2(a, b) = \sum_{i=1}^{n} w_{1,i}(y_i - a_i)^2 + \sum_{i=1}^{n} w_{2,i}(z_i - b_i)^2$$

over $(a, b) \in \mathbb{R}^n \times \mathbb{R}^n$ s.t. a and b are increasing and $a \leq b$

is equivalent

to least squares projection of $(\mathbf{y}, \mathbf{z})$ on intersection of convex cones

$$\{(a, b) : a \text{ is increasing}\}, \ \{(a, b) : b \text{ is increasing}\}, \text{ and } \{(a, b) : a \leq b\}.$$

What the doctor ordered: algorithm by Dykstra (1983).
Simply iterate projections.

Dykstra's algorithm

$$\begin{aligned} C_1 &:= \{(a,b) : a \text{ is increasing}\}, \\ C_2 &:= \{(a,b) : b \text{ is increasing}\}, \\ C_3 &:= \{(a,b) : a \le b\}. \end{aligned}$$

Computation of projections:

- C_1, C_2: PAVA,
- C_3: replace each pair (a_i, b_i) violating constraint (i.e. $a_i > b_i$) by weighted average $(w_{1,i}a_i + w_{2,i}b_i)/(w_{1,i} + w_{2,i})$.

Algorithm often converges slow ⇒ but here very fast ⇒ only three projections involved.

Implemented in `R` package `OrdMonReg`.

Projected subgradient algorithm

Dykstra's algorithm: only applicable to functionals of type

$$L_2(a, b) = \sum_{i=1}^{n} w_{1,i}(y_i - a_i)^2 + \sum_{i=1}^{n} w_{2,i}(z_i - b_i)^2$$

Projected subgradient algorithm: can handle

$$L_3(a, b) = F(\mathbf{a}, \mathbf{y}, \mathbf{w}_1) + \sum_{i=1}^{n} w_{2,i}(z_i - b_i)^2$$

where F is convex and differentiable.

Second term can likely be generalized as well.

Derivation and implementation more involved.
Computes solution in least squares case slower.

A smoothed version of the estimates

In fact: estimates only determined at x_i's.

One-curve problem: estimate step function $\Rightarrow$ derivative of GCM of cumsum. We define estimates in two-curve as step functions as well $\Rightarrow$ non-smooth.

Define smooth estimates for some kernel K_h:

$$\tilde{a}_h^*(x) \;=\; \frac{\sum_{i=1}^n K_h(x-x_i)\widehat{a}_i^*}{\sum_{i=1}^n K_h(x-x_i)} \qquad \tilde{b}_h^*(x) \;=\; \frac{\sum_{i=1}^n K_h(x-x_i)\widehat{b}_i^*}{\sum_{i=1}^n K_h(x-x_i)}.$$

Theorem (Mukerjee, 1988)

A monotone function remains monotone after smoothing if the kernel is log-concave.

Proof: Log-concave densities have monotone likelihood ratio.

Ordering: maintained if we use same kernel and bandwidth for both functions $\Rightarrow$ smoothing is simply taking weighted means.

Back to our motivating example

1495 pairs (x_i, y_i), (x_i, z_i).

y_i, z_i: stress results for two different loading velocities.

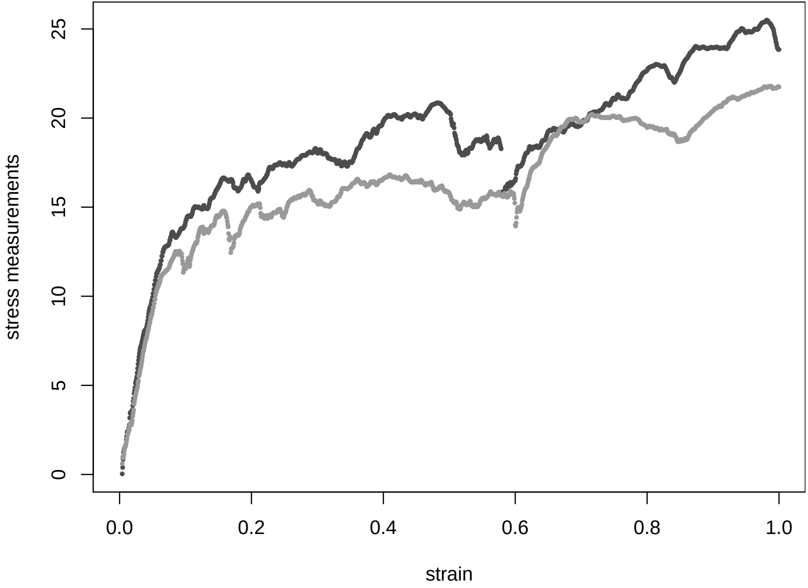
Estimated curves have to be isotonic, ordered, and ideally smooth.

Practitioners: fit "parametric" models using trial-and-error until above properties are met $\Rightarrow$ ad-hoc, time-consuming.

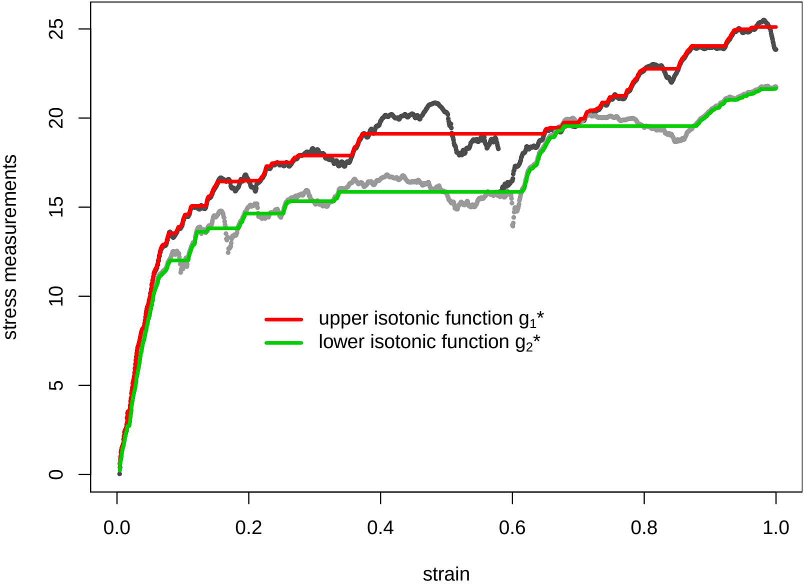
We use normal kernel $K_h(x) = \phi(x/h) \Rightarrow$ log-concave.

Bandwidth: $h = 0.1n^{-1/5} = 0.023$.

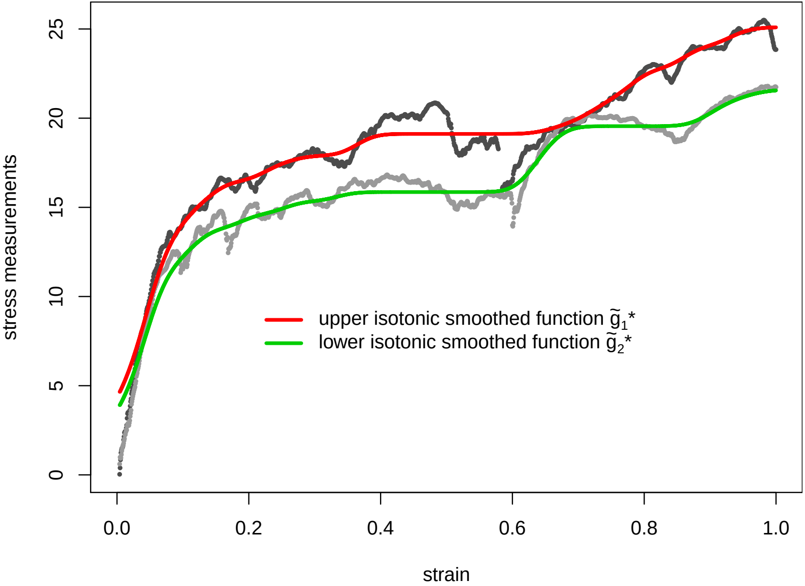
Example: data



Example: ordered monotone estimates



Example: ordered monotone smoothed estimates



Summary

- Monotone regression can be computed using PAVA.
- PAVA valid not only for weighted mean functional, but for any functional satisfying averaging property.
- Rigorous proof of this fact and that PAVA solution is equal to min-max solution.
- Existence, uniqueness, and characterization of two-curve solution.
- Dykstra's and projected subgradient algorithm.
- Smoothed estimates that maintain ordering and monotonicity.

Algorithms for one- and two-curve problem implemented in `R` package `OrdMonReg`.

Outlook

Initial problem of practitioners was solved.

But:

- Now: estimation, then smoothing. Penalize (non-)smoothness as well?
- Asymptotics: presumably even more difficult than in one-curve problem.
- Further applications?
- More than two curves algorithm by Beran & Dümbgen (2010)?

Thank you for your attention.