The Fitting of Multifunctions:
An approach to Nonparametric Multimodal Regression

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What is “Nonparametric Regression”?

Typical definition:

“Given observations from an explanatory variable $X$ and a response variable $Y$, construct a function, a “smoother”, which at point $x$ estimates the average value of $Y$ given that $X = x$. ”

(Holmström et.al, 2003)
Nonparametric regression

Given \( n \) data points \((X_i, Y_i), i = 1, \ldots, n\), one seeks a smooth function \( m : \mathbb{R} \rightarrow \mathbb{R} \) relating \( X \) and \( Y \) in a proper way, which can be generally expressed in the form

\[
m(x) = \Phi(Y | X = x).
\]

Possible choices of the operator \( \Phi(\cdot) \) are obtained as solutions of the minimization problem

\[
m_l(x) = \arg \min_a E(l(Y - a)|X = x),
\]

yielding

| \( l(z) \) | \( z^2 \) | \( |z| \) | \( -\delta(z) \) |
|---|---|---|---|
| \( \Phi(\cdot) \) | \( E(\cdot) \) | \text{Median}(\cdot) | \text{Mode}(\cdot) |
Limits of ordinary nonparametric regression

Speed-Flow diagram:

X: traffic flow in cars/hour,    Y: speed in Miles/hour
recorded on a Californian “freeway”.

(data from: R package hdrcde)
Attempt: Ordinary nonparametric regression

One assumes an asymmetric relationship between $X$ and $Y$:

$$Y = m(X) + \epsilon; \text{ with a function } m : \mathbb{R} \rightarrow \mathbb{R}$$

\[\begin{array}{c|c|c|c|c|c|c|c|c|}
\hline
\text{flow} & 0 & 500 & 1000 & 1500 & 2000 \\
\text{speed} & 10 & 20 & 30 & 40 & 50 & 60 \\
\hline
\end{array}\]

→ Obviously some information is discarded!
Possible solution: Principal curves

\[
\begin{pmatrix} X \\ Y \end{pmatrix} = f(t) + \epsilon; \quad f : \mathbb{R} \rightarrow \mathbb{R}^2 \quad \text{(X and Y symmetric!)}
\]

- Principal curves are smooth functions passing through the middle of the data cloud.
- They uncover nicely the underlying branched structure.
- However, they are not suitable for prediction of \( Y \) from a given \( X = x \).
New approach: Multi-valued nonparametric regression

As for ordinary regression, we assume an asymmetric relationship

\[ Y = M(X) + \epsilon, \]

but now employing a multifunction (multi-valued ‘function’) \( M : \mathbb{R} \rightarrow \mathbb{R}. \)

- The data cloud is thought of to consist of several smooth branches (regimes).
- For every \( X = x, \) more than one predicted value is possible.
- The estimator for \( M \) at \( x \) is a random set \( \hat{M}(x) = \{\hat{m}_1(x), \ldots, \hat{m}_k(x)\} \), with \( k \)
  being the number branches.
Basic idea: Consider the conditional densities.
For instance, conditional density at a flow = 1400.

- For estimation of $M(x)$, compute the modes of the estimated conditional densities $\hat{f}(y|x)$.
- The area between a mode and the neighboring ‘antimode’ serves as estimated probability, that, given $x$, a value on the corresponding branch is attained.
The estimated branches correspond to the uncongested and congested regimes.

The relevance of the branches varies smoothly with $x$, as long as the branches can be separated.
Estimation of conditional modes

We are interested in all local maxima of the estimated conditional densities

$$
\hat{f}(y|x) = \frac{\hat{f}(x, y)}{\hat{f}(x)} = \frac{\sum_{i=1}^{n} K_1 \left( \frac{x-X_i}{h_1} \right) K_2 \left( \frac{y-Y_i}{h_2} \right)}{h_2 \sum_{i=1}^{n} K_1 \left( \frac{x-X_i}{h_1} \right)}
$$

with kernels $K_1, K_2$ and bandwidths $h_1, h_2$. We assume, that a profile $k(\cdot)$ for kernel $K_2$ exists such that

$$
K_2(\cdot) = c_k k(\cdot)^2,
$$

holds. One calculates

$$
\frac{\partial \hat{f}(y|x)}{\partial y} = \frac{2c_k}{h_2^3} \sum_{i=1}^{n} K_1 \left( \frac{x-X_i}{h_1} \right) k' \left( \left( \frac{y-Y_i}{h_2} \right)^2 \right) (y - Y_i) \overset{!}{=} 0
$$
and obtains

\[ y = \frac{\sum_{i=1}^{n} K_1 \left( \frac{x-X_i}{h_1} \right) G \left( \frac{y-Y_i}{h_2} \right) Y_i}{\sum_{i=1}^{n} K_1 \left( \frac{x-X_i}{h_1} \right) G \left( \frac{y-Y_i}{h_2} \right)}. \] (1)

with \( G(\cdot) = -k'(\cdot)^2 \).

Remarks:

- Applying (1) iteratively, the sequence \((y_j)\) corresponds to a series of ‘local centers of mass’ and converges to a conditional mode of \(Y|X=x\)

  (“mean shift algorithm”, Comaniciu & Meer, 2002).

- The right side of (1) corresponds to the “Sigma-Filter” used in digital image smoothing. Hence, the sigma filter is a one-step approximation to the conditional mode.
Example with 3 branches: Atypical speed-flow curves

Recorded on a line segment for low-speed vehicles in Contra Costa County, California.
(Data from: ‘PemS’)

Highway Layout:
Outlook: Antiregression and Classification

If one plots the antimodes, which are obtained as a by-product of the computation of the relevances, one obtains an antiprediction or antiregression curve.

This curve serves as a separator between the branches, and thus as a tool to classify observations to the uncongested or congested regime.
Summary:

• The conditional mode is more useful for the analysis of multimodal data than the conditional mean or median.

• Maxima of the conditional density can be calculated fast and easily via a conditional mean shift procedure.

• The resulting curves are smooth, but edge-preserving.

• Sometimes problems for very large slopes.

• Function `modalreg` integrated into R package `hdrcde` (maintained by R. Hyndman), available on CRAN.

• To do: Automatic detection of the number of branches.
Literature


