# The Fitting of Multifunctions:

# An approach to Nonparametric Multimodal Regression


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GfKl, 10th of March 2005

# 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 $m : \mathbb{R} \longrightarrow \mathbb{R}$ 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

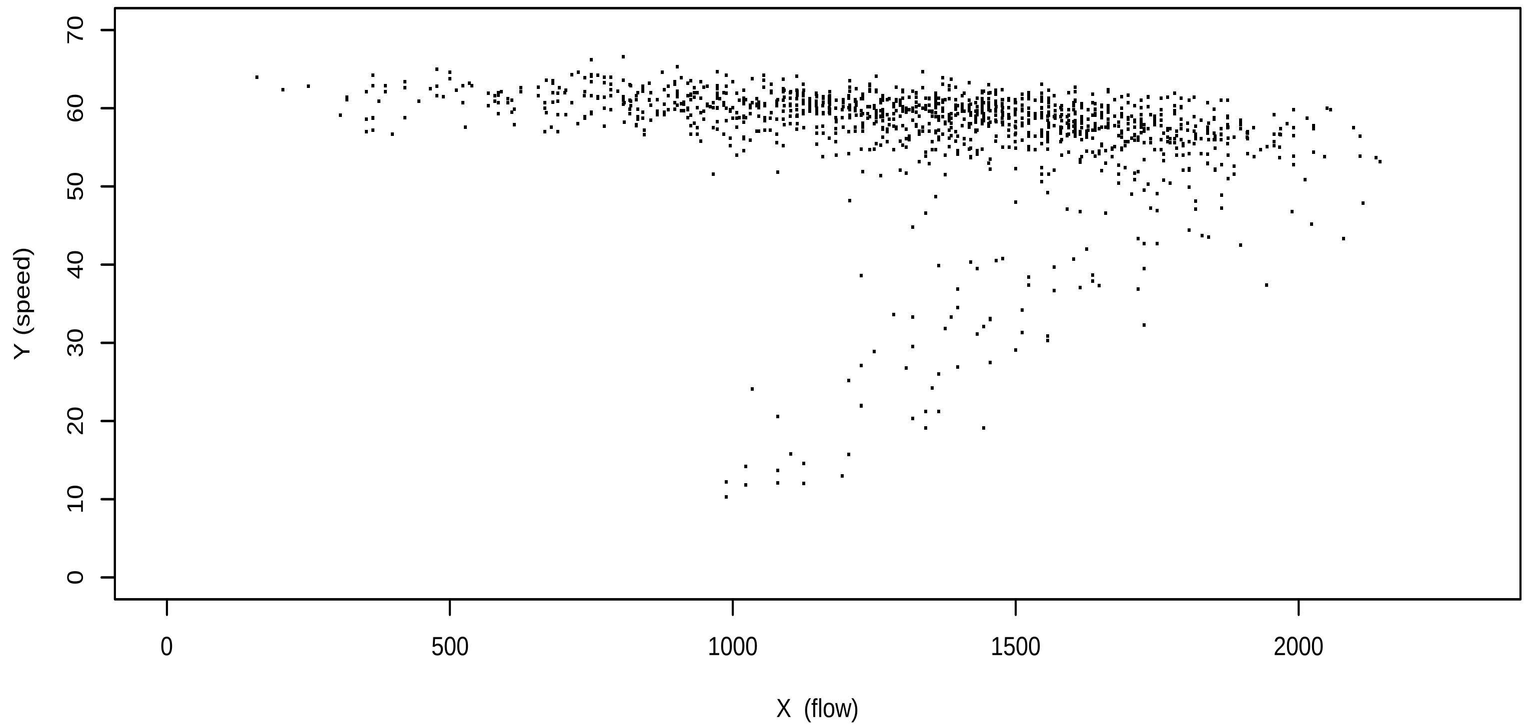
$$m_l(x) = \arg\min_a E(l(Y - a)|X = x),$$

yielding

| | | | |
|---|---|---|---|
| $l(z)$ | $z^2$ | $\|z\|$ | $-\delta(z)$ |
| $\Phi(\cdot)$ | $E(\cdot)$ | $Median(\cdot)$ | $Mode(\cdot)$ |

# Limits of ordinary nonparametric regression

Speed-Flow diagram:



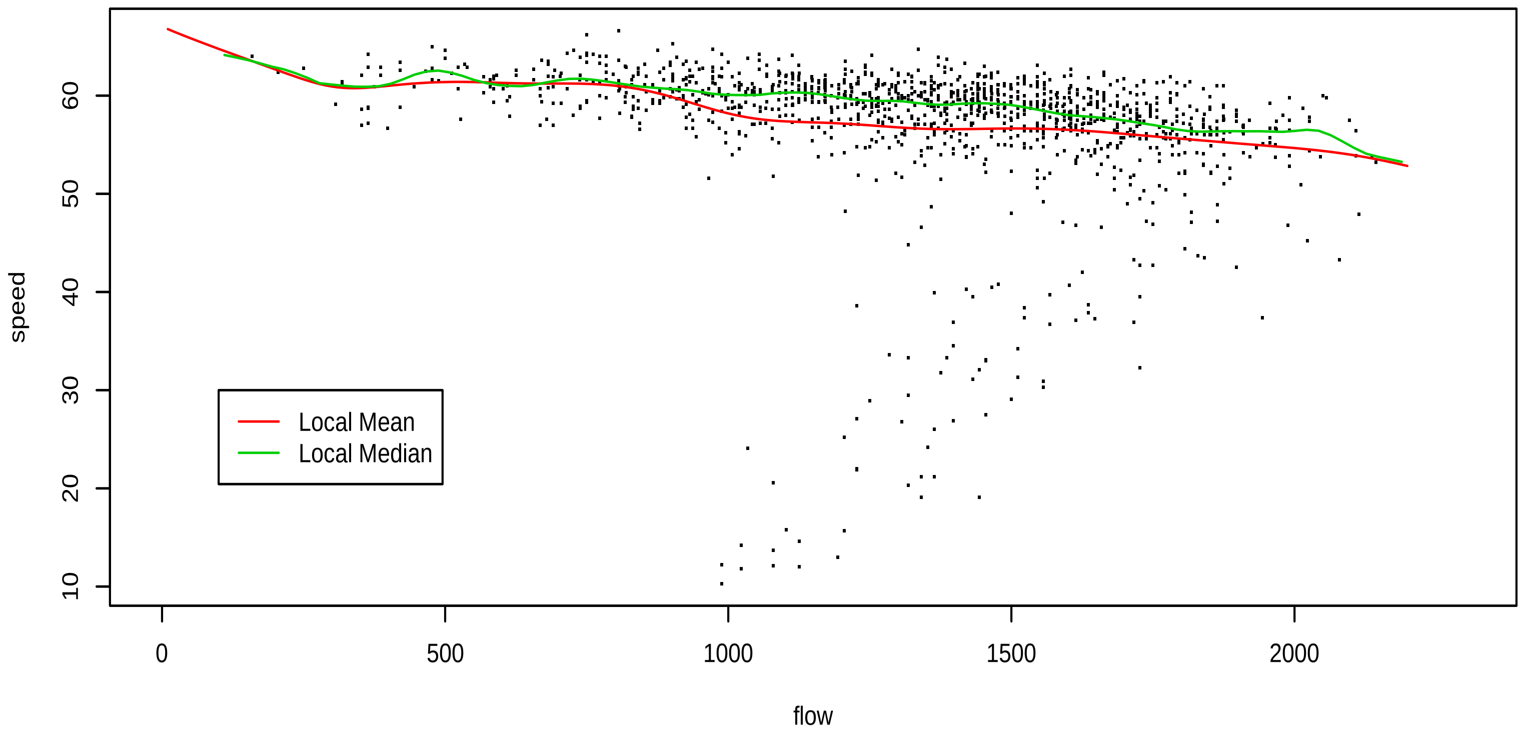

X: traffic flow in cars/hour,     Y: speed in Miles/hour

recorded on a californian “freeway”.

## Attempt: Ordinary nonparametric regression

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

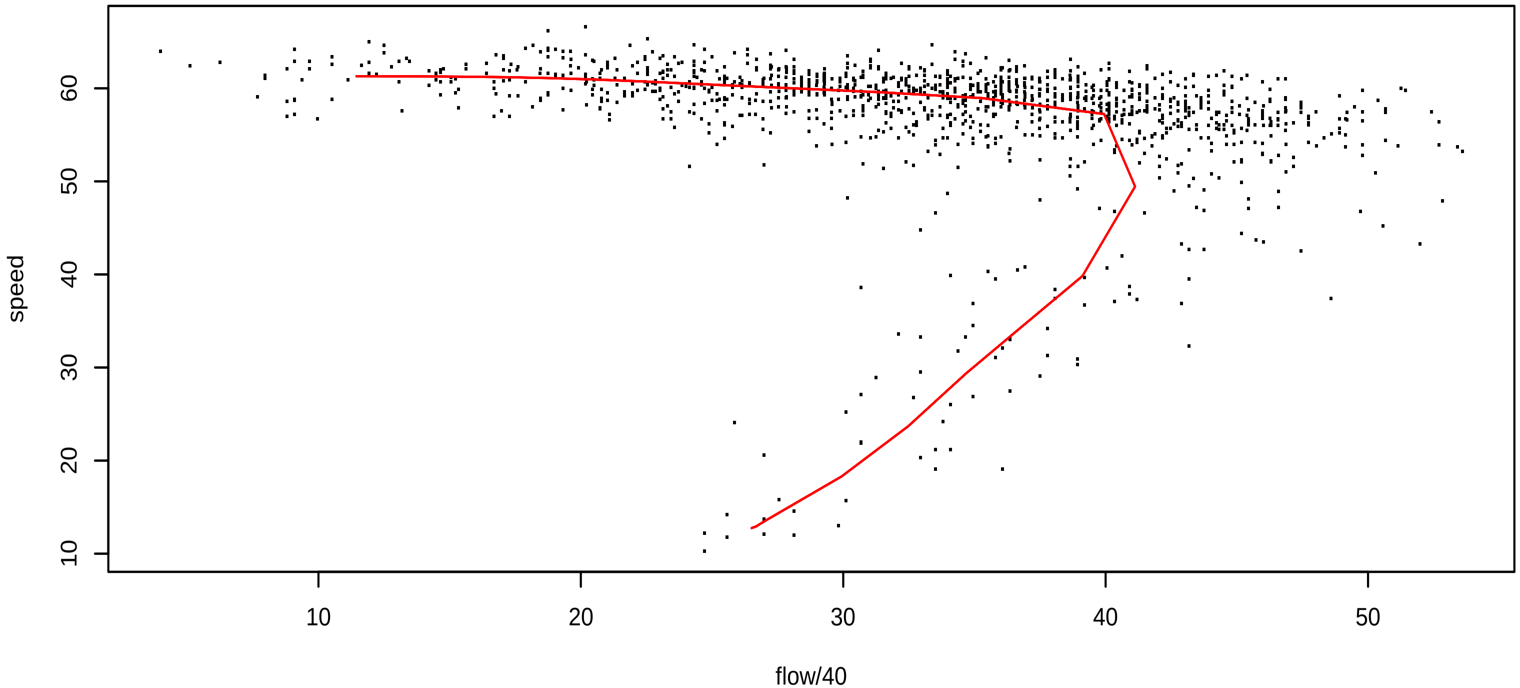
$$Y = m(X) + \epsilon\,; \text{ with a function } m : \mathbb{R} \longrightarrow \mathbb{R}$$




$\longrightarrow$ Obviously some information is discarded!

## Possible solution: Principal curves

$$\begin{pmatrix} X \\ Y \end{pmatrix} = f(t) + \epsilon\,;\; f : \mathbb{R} \longrightarrow \mathbb{R}^2 \qquad \text{(X and Y symmetric!)}$$




- 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

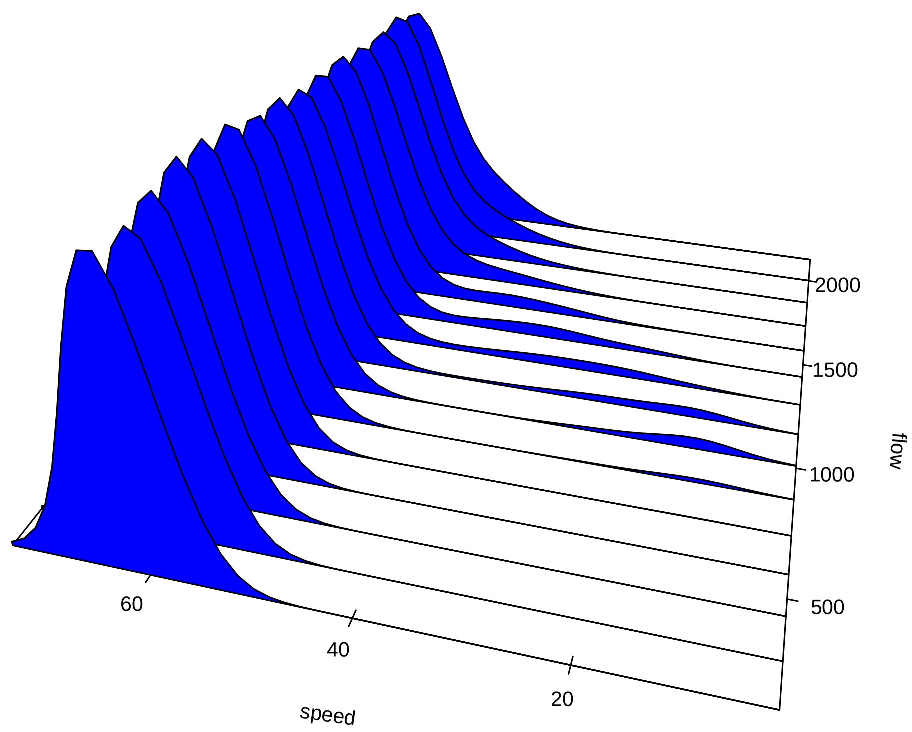
As for ordinary regression, we assume an asymmetric relationship

$$Y = M(X) + \epsilon,$$

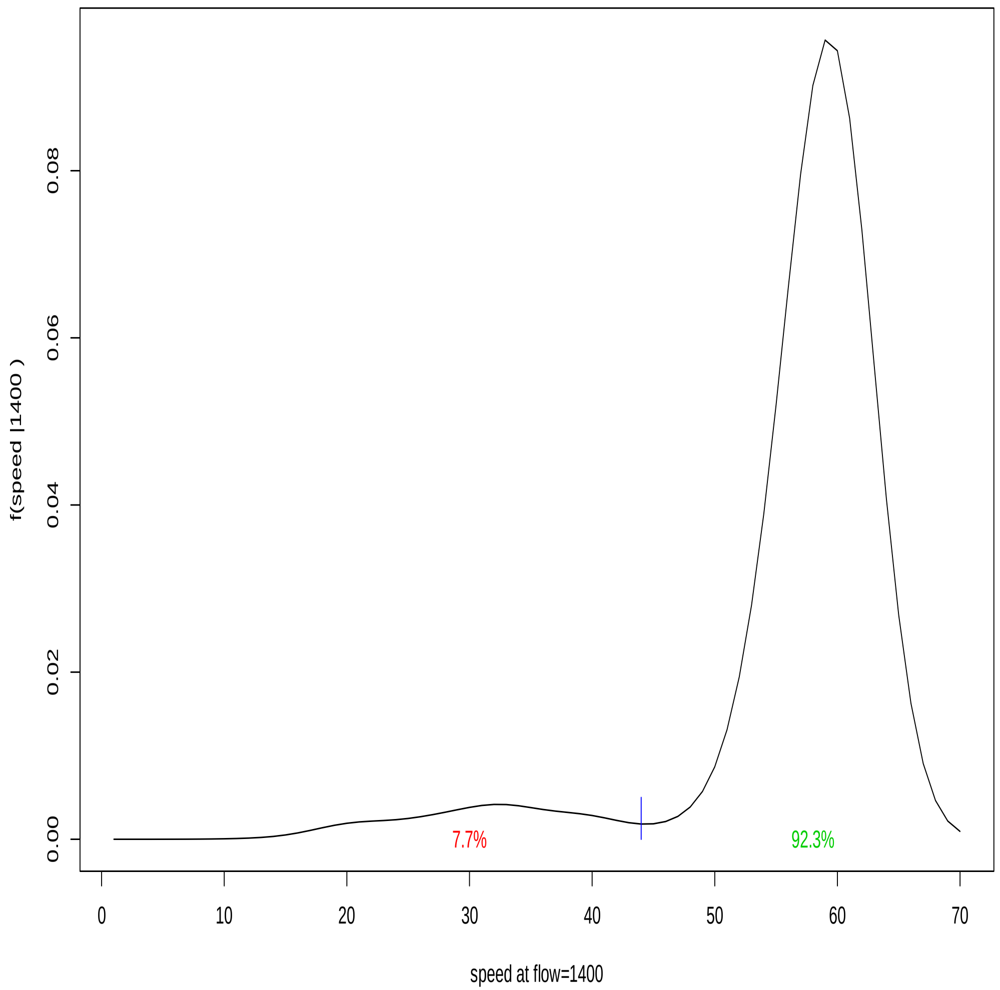
but now employing a multifunction (multi-valued 'function') $M : \mathbb{R} \longrightarrow \mathbb{R}$.

- 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.

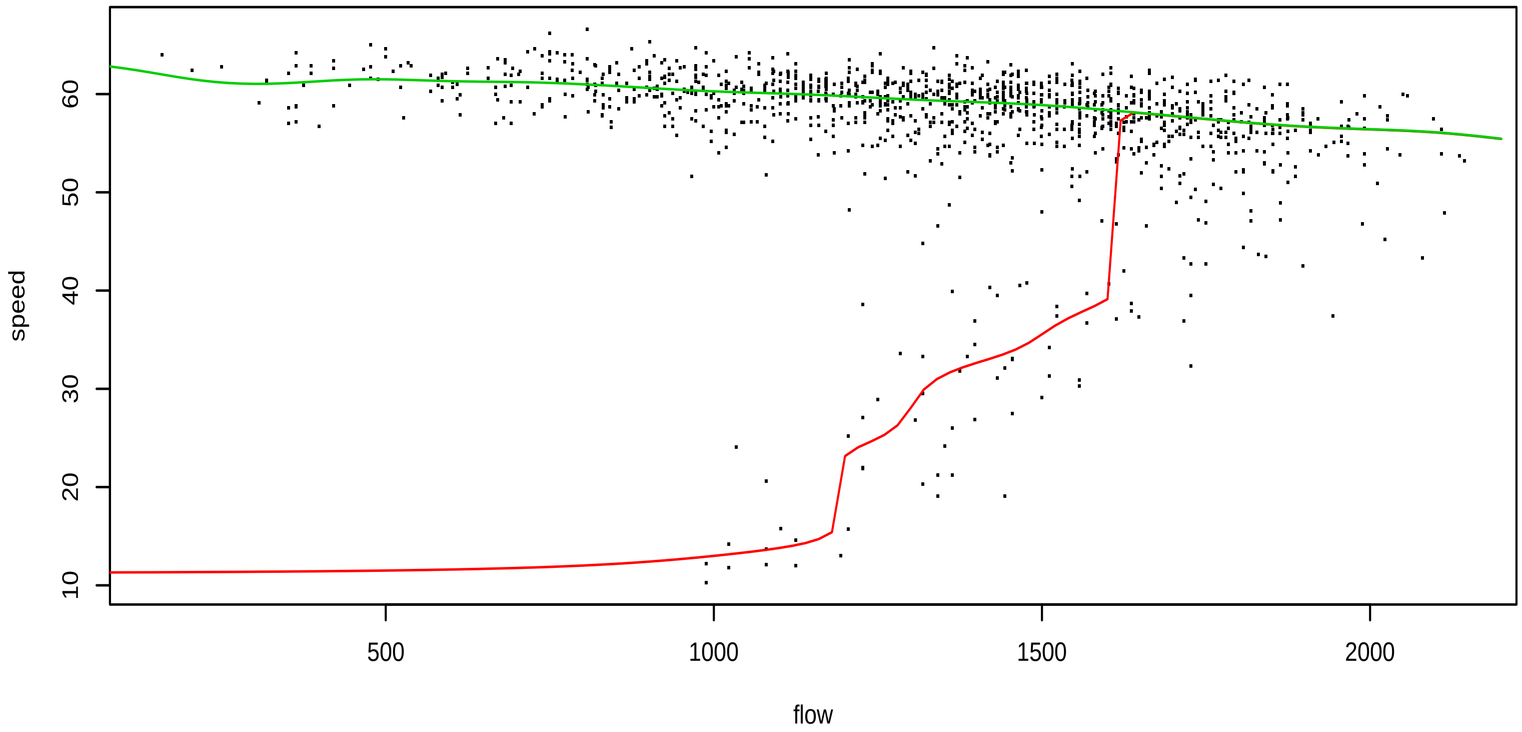


For instance, conditional density at a flow $= 1400$.



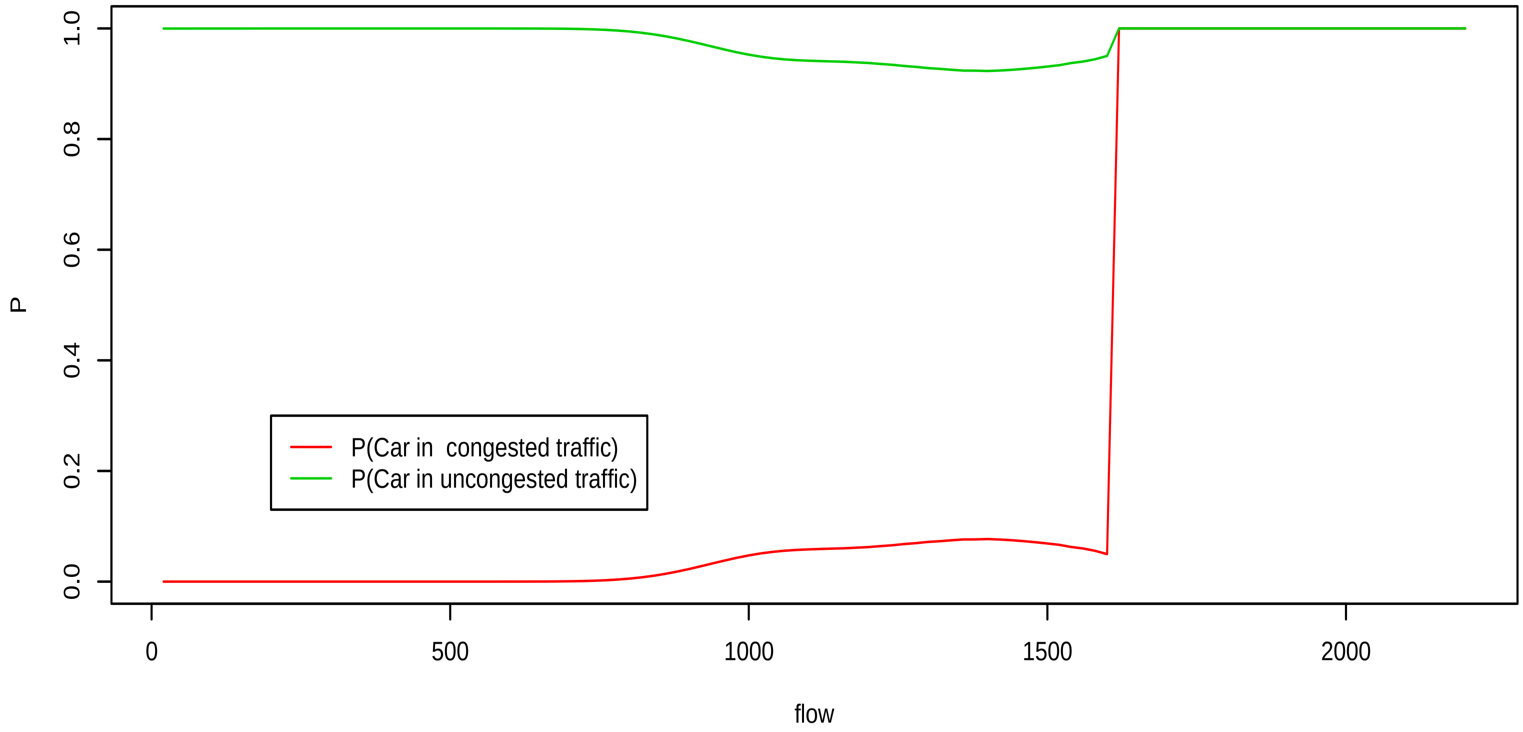

- For estimation of $M(x)$, compute the modes of the estimated conditional densities $\hat{f}(y|x)$.
- The area between a mode and the neighboring 'antimode' serves as estimated probability, that, given $x$, a value on the corresponding branch is attained.

# Estimated multifunction




The estimated branches correspond to the uncongested and congested regimes.

# Relevance assessment




The relevance of the branches varies smoothly for varying $x$, as long as 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

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

and obtains

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

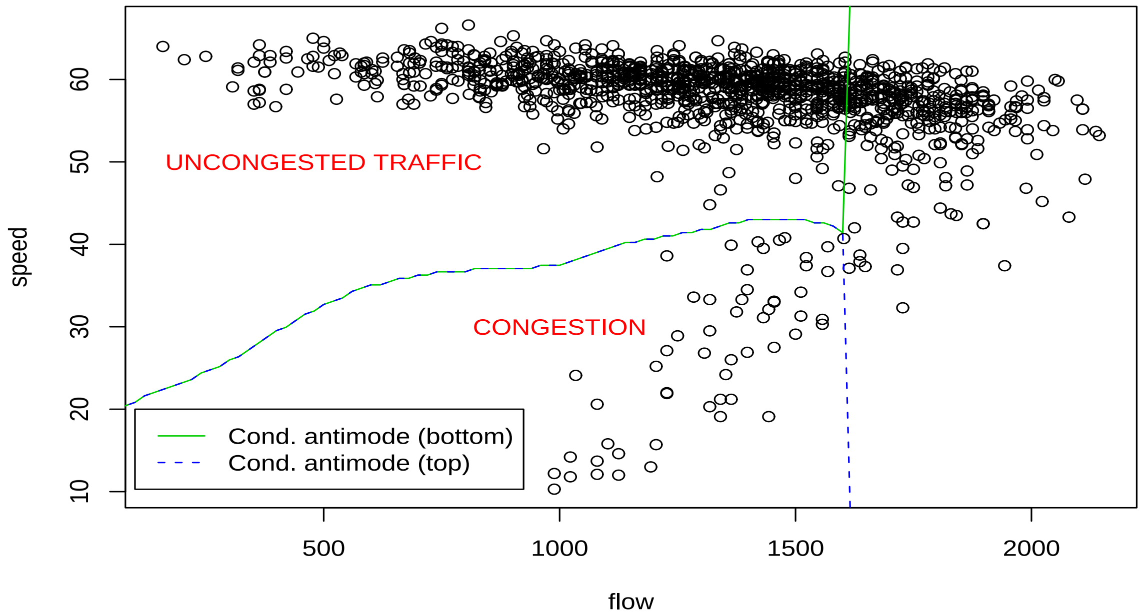
with $G(\cdot) = -k'((\cdot)^2)$.

Remarks:

- The right side of (1) can be seen as a conditional mean shift! Thus, applying (1) iteratively, the sequence $(y_j)$ converges to a conditional mode of $Y|X = x$ (Comaniciu & Meer, 2002).
- The right side of (1) corresponds also to the "Sigma-Filter" used in digital image smoothing. Thus, the sigma filter is a one-step approximation to the conditional mode.

# 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 as the conditional mean or median.
- The mode is robust to outliers $and$ is edge-preserving.
- Maxima of the conditional density can be calculated fast and easily via a conditional mean shift procedure.

To do:

- Bandwidth selection (for conditional densities already available: Fan et al., 1996)
- Bias, Variance? Asymptotics? (for cond. modes: Berlinet et al., 1998)
- Automatic detection of the number of branches.

# Literature


- Principal Curves

  Hastie & Stuetzle, (1989): Principal Curves. *JASA, 84, 502–516*.

  Einbeck, Tutz, & Evers, (2004): Exploring Multivariate Data Structures with Local Principal Curves, *to appear in Proceedings GFKL 2004*

  Chen, Zhang, Tang, & Wang, (2004): Freeway Traffic Stream Modeling Based on Principal Curves and Its Analysis, *IEEE Trans. Intell. Transp. Systems*, 5, 246-258.

- Multi-valued nonparametric regression

  Einbeck, J, & Tutz, G.(2004): Modelling beyond regression functions: An application of multimodal regression to speed-flow data , *SFB 386 Discussion Paper No. 395, University of Munich*

  ⋮ ?

- “Related Literature”:


Comaniciu & Meer (2002): Mean shift: A robust approach towards feature space analysis. *IEEE Trans. Pattern Anal. Machine Intell. 24, 603-619*.

Berlinet, Gannoun & Matzner-Løber (1998): Normalité aymptotique d'estimateurs convergents du mode conditionnel. *Canadian Journal of Statistics, 26, 365–380*.

Fan, Yao & Tong (1996): Estimation of conditional densities and sensitivity measures in nonlinear dynamical systems. *Biometrika, 83, 189–206*

Davies & Kovac (2004): Densities, Spectral Densities and Modality, *Annals of Statistics, 32, 1093–1136*.