MATH 829: Introduction to Data Mining and Analysis
Kernel smoothing

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

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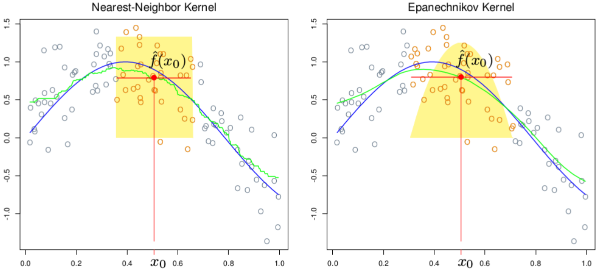
- As we will see, this can be naturally done, without significantly increasing the number of parameters to estimate.
- We will use local information to fit each local linear model.
- Localization is achieved via a weighting function (*kernel*) $K(x, x_i)$, or a parametric family of kernels $K_\lambda(x, x_i)$ for $\lambda \in \Lambda$.

Recall the k-nearest-neighbor average

$$\hat{f}(x) = \text{Ave}(y_i : x_i \in N_k(x))$$

approximates the regression function $E(Y|X = x)$.



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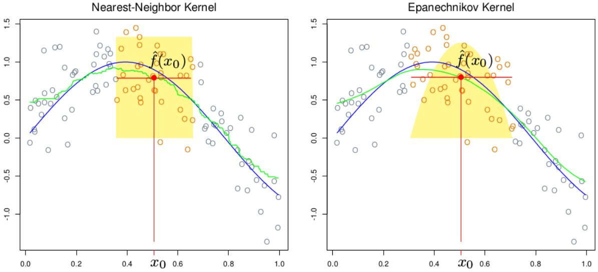

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As x moves from left to right, $N_k(x)$ changes. This results in discontinuities in $\hat{f}(x)$. A *weighed average* naturally solves this problem.

Kernel smoothers

Given a function $K : \mathbb{R}^p \times \mathbb{R}^p \to [0, \infty)$, we can construct the estimator:

$$\hat{f}(x) = \frac{\sum_{i=1}^n K(x, x_i) y_i}{\sum_{i=1}^n K(x, x_i)}.$$

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We usually:

- Use a kernel that decays at some rate (to give more weight to local observations).
- Work with a parametrized family of kernels $K_\lambda(x, y)$, where λ controls the *window size*.
- Known as the Nadaraya–Watson estimator.

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For example, the *Epanechnikov* quadratic kernel is given by

$$K_\lambda(x, x') = D\left(\frac{|x - x'|}{\lambda}\right),$$

where

$$D(t) := \begin{cases} \frac{3}{4}(1 - t^2) & \text{if } |t| \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

Resulting prediction function is continuous.

A few remarks:

1. More generally, one can use an adaptive neighborhood: let $h(x_i)$ determine the width of the neighborhood at x_i. Then one can use
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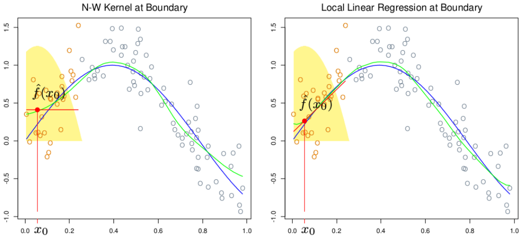
5. Non-parametric approach.

Local linear regression

Kernel smoothers can have poor performance near the boundary of the domain or in regions with very little observations.



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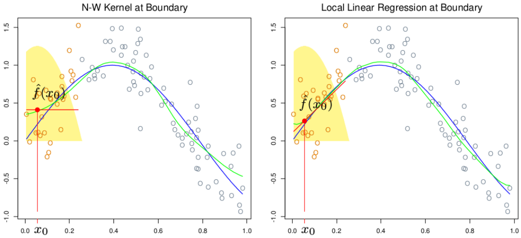

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Locally weighted regression solves a separate weighted least squares problem at each target point x_0:

$$\min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{n} K(x_0, x_i)[y - \alpha(x_0) - \beta(x_0)x_i]^2.$$

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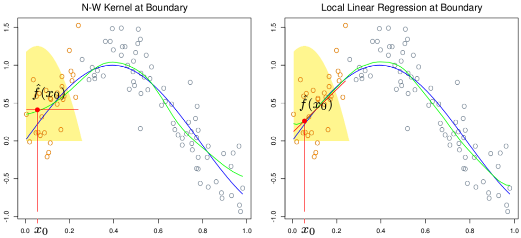

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The estimate is then

$$\hat{f}(x_0) = \alpha(x_0) + \beta(x_0)x_0.$$

Local linear regression (cont.)

- Obtaining the solution is not harder than usual.
- More generally, note that for $y \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, and

$w = (w_i) \in (0, \infty)^n$,

$$\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^{n} w_i (y_i - x_i^T \beta)^2 \quad \Leftrightarrow \quad \min_{\beta \in \mathbb{R}^p} \sum_{i=1}^{n} (\tilde{y}_i - \tilde{x}_i^T \beta)^2,$$

where $\tilde{y}_i := \sqrt{w_i} y_i$ and $\tilde{x}_i = \sqrt{w_i} x_i$.

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So the solution is:

$$\hat{\beta} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X} \tilde{y} = (X^T W X)^{-1} X^T W y.$$

Local linear regression (cont.)

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The prediction at x_0 becomes:

$$\begin{aligned}\hat{f}(x_0) &= x_0^T (X^T W(x_0) X)^{-1} X^T W(x_0) y \\ &= \sum_{i=1}^{n} l_i(x_0) y_i.\end{aligned}$$

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Remark:

1. Estimate is still linear in y.
2. The weights $l_i(x_0)$ combine the weighting kernels $K_\lambda(x_0, x_i)$, and the least squares operations.
3. Same ideas can be applied to local regression with other function bases (e.g. local polynomial regression, see ESL 6.1.2).

Local linear regression - higher dimension

The same ideas apply to higher dimension. Given $K_\lambda : \mathbb{R}^p \times \mathbb{R}^p \to [0, \infty)$, one can solve:

$$\min_{\beta(x_0) \in \mathbb{R}^p} \sum_{i=1}^n K(x_0, x_i)[y_i - x_i^T \beta]^2.$$

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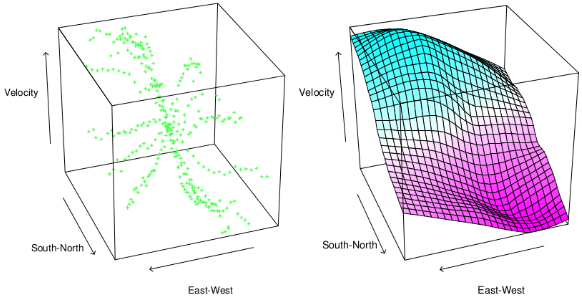

ESL, Figure 6.8. Local linear regression smoothing for velocity of a galaxy data.

Structured local linear regression models

- When the sample size is small compared to the dimension, local linear regression may not perform well.
- As we did before, we can impose more constraints on the model (i.e., add more structure).
- For example, we can weight dimensions differently.

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Structured kernels: use a positive semidefinite matrix A to weight the coordinates:

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Structured Regression Functions, Local Likelihood methods, etc. (see ESL).