Kernel smoothing

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March 21, 2016
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- We now explore how one can fit a different but simple model separately at each query point.
- 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 $E(Y|X = x)$.

ESL, Figure 6.1.
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approximates the regression function $E(Y|X = x)$.

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.
Given a function \( K : \mathbb{R}^p \times \mathbb{R}^p \rightarrow [0, \infty) \), 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 $\lambda$ 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.
Kernel smoothers can have poor performance near the boundary of the domain or in regions with very little observations.

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

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

The estimate is then

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

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

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

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

Letting $W = \text{diag}(w_1, \ldots, w_n)$, we have $\tilde{y} = \sqrt{W} y$, $\tilde{X} = \sqrt{W} X$. So the solution is:

$$\hat{\beta} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} = (X^T WX)^{-1} X^T W y.$$
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Local linear regression (cont.)

In the case of local linear regression, the weights are:

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$$\hat{f}(x_0) = x_0^T (X^T W(x_0) X)^{-1} X^T W(x_0)y$$

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**Note:** We need to solve a linear regression problem at every \( x_0 \) where the estimator has to be evaluated.
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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).
The same ideas apply to higher dimension. Given $K_\lambda : \mathbb{R}^p \times \mathbb{R}^p \to [0, \infty)$, one can solve:

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For example, one can use a radial Epanechnikov kernel:

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(Note: better to scale predictors)
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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.

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

$$K_{\lambda,A}(x,x') = D((x-x')^T A (x-x'))^{\lambda}.$$

For example, $A$ could be a diagonal matrix that assigns different weights to different dimensions.
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Structured Regression Functions, Local Likelihood methods, etc. (see ESL).