Introduction to Kernel Smoothing

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Kernel Smoothing

Monographs on Statistics and Applied Probability

Chapman & Hall, 1995.

Introduction

Histogram of some p−values

Introduction

- Estimation of functions such as regression functions or probability density functions.
- Kernel-based methods are most popular non-parametric estimators.
- Can uncover structural features in the data which a parametric approach might not reveal.

Univariate kernel density estimator

Given a random sample X_1, \ldots, X_n with a continuous, univariate density *f*. The kernel density estimator is

$$
\hat{f}(x,h) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)
$$

with kernel *K* and bandwidth *h*. Under mild conditions (*h* must decrease with increasing *n*) the kernel estimate converges in probability to the true density.

The kernel *K*

- Can be a proper pdf. Usually chosen to be unimodal and symmetric about zero.
- \Rightarrow Center of kernel is placed right over each data point.
- \Rightarrow Influence of each data point is spread about its neighborhood.
- \Rightarrow Contribution from each point is summed to overall estimate.

Gaussian kernel density estimate

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The bandwidth *h*

- Scaling factor.
- Controls how wide the probability mass is spread around a point.
- Controls the smoothness or roughness of a density estimate.
- \Rightarrow Bandwidth selection bears danger of under- or oversmoothing

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KDE with b=0.005

Some kernels

Some kernels

$$
K(x, p) = \frac{(1 - x^2)^p}{2^{2p+1}B(p+1, p+1)} 1_{\{|x| < 1\}}
$$
\nwith

\n
$$
B(a, b) = \Gamma(a)\Gamma(b)/\Gamma(a+b).
$$

 $-p = 0$: Uniform kernel.

 $-p = 1$: Epanechnikov kernel.

 $-p = 2$: Biweight kernel.

Kernel efficiency

- Perfomance of kernel is measured by MISE (mean integrated squared error) or AMISE (asymptotic MISE).
- Epanechnikov kernel minimizes AMISE and is therefore optimal.
- Kernel efficiency is measured in comparison to Epanechnikov kernel.

 \Rightarrow Choice of kernel is not as important as choice of bandwidth.

Modified KDEs

- Local KDE: Bandwidth depends on *x*.
- Variable KDE: Smooth out the influence of points in sparse regions.
- Transformation KDE: If *f* is difficult to estimate (highly skewed, high kurtosis), transform data to gain a pdf that is easier to estimate.

Bandwidth selection

- Simple versus high-tech selection rules.
- Objective function: MISE/AMISE.
- R-function density offers several selection rules.
- Normal scale rule.
- Assumes *f* to be normal and calculates the AMISE-optimal bandwidth in this setting.
- First guess but oversmoothes if *f* is multimodal or otherwise not normal.

bw.ucv

- Unbiased (or least squares) cross-validation.
- Estimates part of MISE by leave-one-out KDE and minimizes this estimator with respect to *h*.
- Problems: Several local minima, high variability.

bw.bcv

- Biased cross-validation.
- Estimation is based on optimization of AMISE instead of MISE (as bw.ucv does).
- Lower variance but reasonable bias.

bw.SJ(method=c("ste", "dpi"))

- The AMISE optimization involves the estimation of density functionals like integrated squared density derivatives.
- dpi: Direct plug-in rule. Estimates the needed functionals by KDE. Problem: Choice of pilot bandwidth.
- ste: Solve-the-equation rule. The pilot bandwidth depends on *h*.

Comparison of bandwidth selectors

- Simulation results depend on selected true densities.
- Selectors with pilot bandwidths perform quite well but rely on asymptotics \Rightarrow less accurate for densities with "sharp features" (e.g. multiple modes).
- UCV has high variance but does not depend on asymptotics.
- BCV performs bad in several simulations.
- Authors' recommendation: DPI or STE better than UCV or BCV.

KDE with Epanechnikov kernel and DPI rule