Statistical Learning

Kernel Density and Regression Estimators

Spring 2024

Outline

- We will introduce a new technique for nonparametric estimations
- An important concept is the kernel function
- We will use this in two different ways
  - Kernel density estimation
  - Kernel regression
- The central idea is to estimate things locally, but the bias-variance trade-off also applies to this problem

Kernel Density Estimation

Kernel Density Estimation

- Given some observations from an unknown distribution, we want to estimate the probability density function (pdf)
- This is an unsupervised problem, however, the technique can be used for regression later
- Suppose we have

$$X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} f(\cdot)$$

- Some popular methods
  - Assume a family of distributions (e.g., Gaussian) $f_\theta(\cdot)$ and estimate the parameters
  - Kernel density estimator

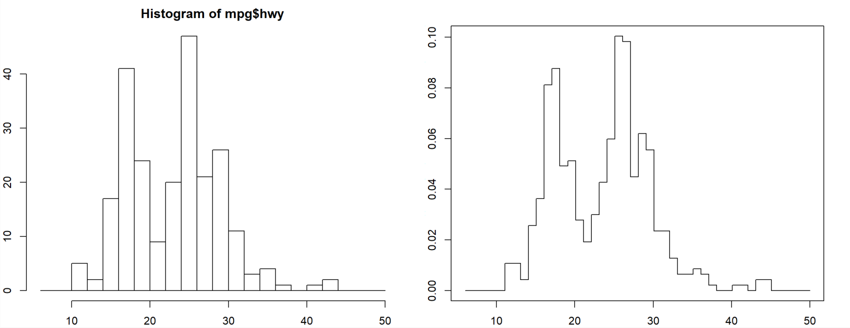
Histogram Estimator of Density Functions

- If a continuous variable $X \sim f(\cdot)$ the following are some facts:
  - $f(u) > 0$ and $\int f(u)du = 1$
  - $\mathsf{P}(x - \frac{\lambda}{2} \leq X \leq x + \frac{\lambda}{2}) = \int_{x-\lambda/2}^{x+\lambda/2} f(u)du$
  - $f(x) = \lim_{\lambda \to 0} \frac{1}{\lambda}\mathsf{P}(x - \lambda/2 \leq X \leq x + \lambda/2)$
- Histogram is a commonly used technique to visualize the data
- A similar and intuitive approach estimator is

$$\widehat{f}(x) = \sum_{i=1}^{n} \frac{\mathbb{1}\left\{x_i \in [x - \lambda/2, x + \lambda/2]\right\}}{\lambda n}$$

- However, this estimation is bumpy and non-smooth

Kernel Density Estimation



Histogram Estimator of Density Functions

- Let's look at the previous estimator in a different way
  - Suppose we put $\frac{1}{n}$ point mass for each observation x_i
  - Further spread that probability onto a region with width λ, e.g., uniformly on $[x_i - \lambda/2, x_i + \lambda/2]$ for all i
  - Add up all such density functions.
- This is exactly the previous estimator (switch x and x_i). For any target point x, the estimator will be affected only by observations within $\lambda/2$

$$\widehat{f}(x) = \sum_{i=1}^{n} \frac{\mathbb{1}\{x \in \overbrace{[x_i - \lambda/2, x_i + \lambda/2]}^{\text{uniform density range}}\}}{\underbrace{\lambda n}_{\text{normalizing constant}}}$$

- What if we use a different distribution, other than uniform?

Kernel Functions

- Denote K a kernel function, centered at 0
- Usually, we use a density function $K(\cdot)$ with
  - $\int K(u)du = 1$
  - $K(-u) = K(u)$
  - $\int K(u)u^2du \leq \infty$
- Furthermore, we introduce a bandwidth λ that controls how "local" this estimator is $K_\lambda(u) = K(u/\lambda)/\lambda$
- In our previous uniform example, $K(u) = \mathbb{1}\{u \in [-\frac{1}{2}, \frac{1}{2}]\}$ and

$$K_\lambda(u) = \frac{1}{\lambda}\mathbb{1}\left\{u \in [-\lambda/2, \lambda/2]\right\}$$

Popular Kernels

- Symmetric Beta family kernel

$$K(u,d) = \frac{(1-u^2)^d}{2^{2d+1}B(d+1,d+1)}\mathbf{1}\{|u| \leq 1\}$$

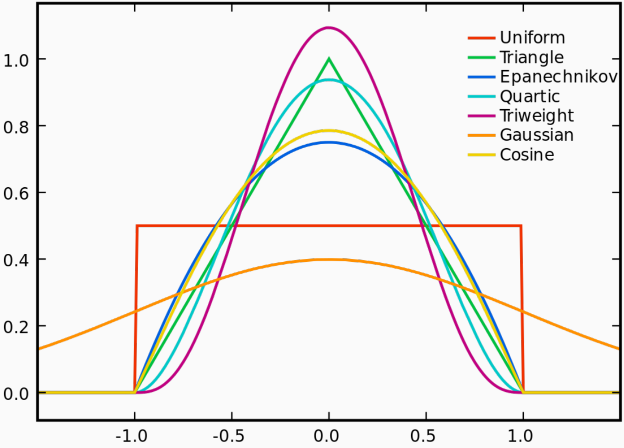
  — Uniform kernel $d = 0$

  — Epanechnikov kernel $d = 1$

  — Bi/Tri weight $d = 2, 3$

- Tri-cube kernel: $K(u) = (1-u^3)^3\mathbf{1}\{|u| \leq 1\}$
- Gaussian kernel: $K(u) = \phi(u) = 1/\sqrt{2\pi}\exp(-u^2/2)$

Kernels


Uniform
Triangle
Epanechnikov
Quartic
Triweight
Gaussian
Cosine
1.0
0.8
0.6
0.4
0.2
0.0
-1.0
-0.5
0.0
0.5
1.0

Kernel Density Estimation

- Parzen estimator

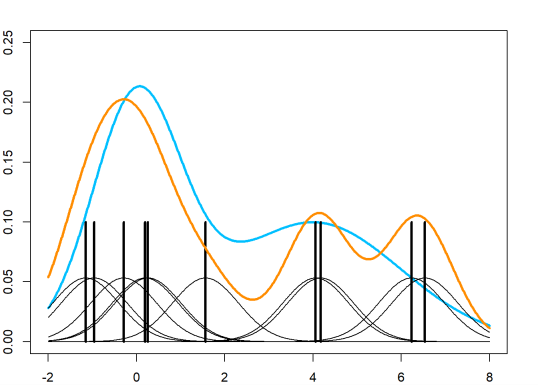
$$\widehat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} K_\lambda(x, x_i)$$

  where $K_\lambda(x, x_i) = K_\lambda(|x - x_i|) = K(\frac{|x-x_i|}{\lambda})/\lambda$

- Popular choice: $K(u)$ is the Gaussian density function with mean zero and standard deviation λ

$$\widehat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\lambda\sqrt{2\pi}} \exp\left\{ \frac{-(x - x_i)^2}{2\lambda^2} \right\}$$

Kernel Density Estimation



Properties of the Kernel Density Estimator

- Under regularity assumptions, the kernel density estimator is asymptotically unbiased for a target point x

$$
\begin{aligned}
E\left[\widehat{f}(x)\right] &= E\left[K\left(\frac{x-x_1}{\lambda}\right)\Big/\lambda\right] \\
&= \int_{-\infty}^{\infty} \frac{1}{\lambda} K\left(\frac{x-x_1}{\lambda}\right) f(x_1)dx_1 \\
&= \int_{\infty}^{-\infty} \frac{1}{\lambda} K(t) f(x-t\lambda) d(x-t\lambda) \\
\text{(Taylor expansion)} \qquad &= f(x) + \frac{\lambda^2}{2} f''(x) \int_{-\infty}^{\infty} K(t)t^2 dt + o(\lambda^2) \\
&\to f(x) \qquad \text{as } \lambda \to 0
\end{aligned}
$$

Properties of the Kernel Density Estimator

- We can further verify that the integrated Bias^2 (integrating the Bias^2 previously over the domain of x) is

$$\begin{aligned}\text{Bias}^2 &= \int \Big(E[\widehat{f}(x)] - f(x)\Big)^2 dx \\ &\approx \frac{\lambda^4 \sigma_K^4}{4} \int \big[f''(x)\big]^2 dx\end{aligned}$$

where $\sigma_K^2 = \int_{-\infty}^{\infty} K(t) t^2 dt$.

Properties of the Kernel Density Estimator

- ... and the integrated variance is

$$\text{Var} \approx \frac{1}{n\lambda} \int K^2(t)dt$$

- Hence, the optimal bias-variance trade-off happens where the asymptotic mean integrated squared error (AMISE)

$$\text{Bias}^2 + \text{Var}$$

  is minimized

- This leads to $\lambda \approx \left(\frac{\int K^2(t)dt}{n\sigma_K^4 \int [f''(x)]^2 dx} \right)^{\frac{1}{5}}$
- This leads to an optimal convergence rate of $\mathcal{O}(n^{-4/5})$

Popular Kernels

- Epanechnikov kernel minimizes AMISE and is therefore optimal.
- Kernel efficiency is measured in comparison to Epanechnikov kernel:
  - Biweight 0.994; Triangular 0.986; Normal 0.951; Uniform 0.930
- However, choosing kernel is not as important as choosing the bandwidth!

The choice of λ

- The rule of thumb (Silverman 1986) for the bandwidth λ in univariate case is

$$\widehat{\lambda} = 1.06\widehat{\sigma}n^{-1/5}$$

  where $\widehat{\sigma}$ is the standard deviation of the observed data
- This is based on assuming that both f and K are Gaussian
- For multidimensional case (p cannot be too large), the optimal λ is at the rate of $n^{-1/(p+4)}$.

R implementations

- hist makes histograms
- density for kernel density estimator
- bw.nrd and a set of related functions for bandwidth selection
- Library locfit : function locfit can perform both local polynomial regressions and density estimation

Kernel regression

k-Nearest Neighbor Smoother

- k-Nearest Neighbor averaging

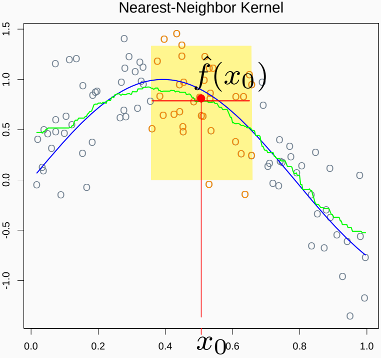
$$\widehat{f}(x) = \sum_{i=1}^{n} w(x, x_i) y_i$$

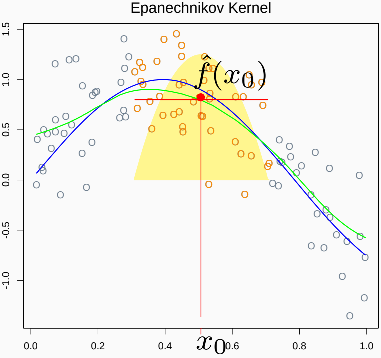
where

$$w(x, x_i) = \begin{cases} \frac{1}{k} & \text{if } x_i \in N_k(x) \\ 0 & \text{o.w.} \end{cases}$$

- The weight $w(x, x_i)$ drops off abruptly to zero outside the neighborhood of x. This accounts for jagged appearance of the fit.

Rectangular vs. Epanechnikov Kernels





Kernel Smoother

- We can still use the local averaging idea:
  - Fit a simple model locally at each point x using only those observations close to it
  - Localization via the weighting function $K(x, x_i)$, the weight of x_i is based on its distance from x
  - Weight decreases as we move further away from x
- For any point $x \in \mathcal{X}$,

$$\widehat{f}(x) = \frac{\sum_i K_\lambda(x, x_i) y_i}{\sum_i K_\lambda(x, x_i)}$$

where $K_\lambda(x, x_i) = K(|x - x_i|/\lambda)/\lambda$ is a kernel function and λ is some tuning parameter for bandwidth.

Kernel Smoother

- The estimator is called Nadaraya-Watson kernel estimator
- It shares the same intuition as the kernel density estimator, but with y_i as the outcome instead of $1/n$ as the point mass
- Requires little or no training time; all the work gets done during prediction (same as kNN).

Choice of λ

- The bandwidth λ again controls how "local" the estimator is
- In many kernels (except Gaussian), only points within $[x - \lambda, x + \lambda]$ receive positive weights
- Small λ: rougher estimate, bias $\downarrow$, variance $\uparrow$
- Large λ: smoother estimate, bias $\uparrow$, variance $\downarrow$
- Although there are some theoretical values (e.g., Fan and Gijbels (1992, 1995)) for the optimal λ, most may fail in practice (violation of assumptions)
- We can choose λ using CV in practice

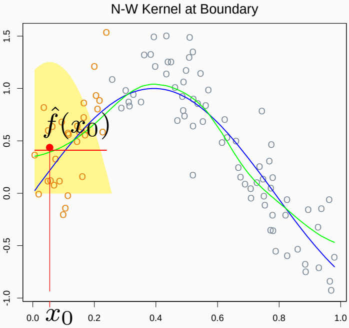
Drawbacks of Local Averaging

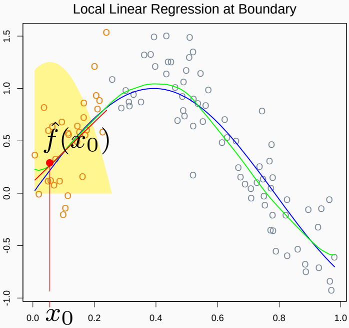
- The kernel averaging formulation can be badly biased on the boundaries of the domain due to the asymmetry of the kernel in that region (we have already seen this)
- Locally weighted linear regression can make a first order correction (straight lines vs. constants)
- Minimizing the objective function

$$\underset{\beta_0(x_0),\beta_1(x_0)}{\text{minimize}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)\big[y_i - \beta_0(x_0) - \beta_1(x_0)x_i\big]^2$$

- The estimation is extremely simple
- The solution $\widehat{f}(x_0) = \widehat{\beta}_0(x_0) + \widehat{\beta}_1(x_0)x_0$ is evaluated only at x_0
- Correct the boundary bias of the kernel estimator

Kernel Boundary Bias





Local Linear Regression

- The objective function can still be solved similarly as a linear regression
- If we let $\mathbf{W}(x_0) = \text{diag}(K_\lambda(x_0, x_1), K_\lambda(x_0, x_2), \ldots, K_\lambda(x_0, x_n))$
- Then the objective function (for target point x_0) is

$$\ell(\boldsymbol{\beta}) = \big(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\big)^{\mathsf{T}}\mathbf{W}(x_0)\big(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\big)$$

- The solution is

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathsf{T}}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{W}\mathbf{y}$$

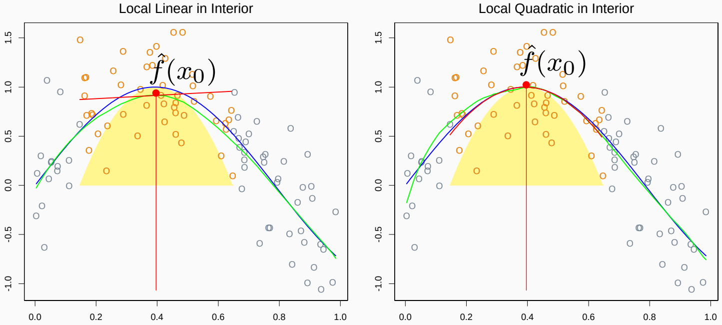
Local Polynomial Regression

- Locally weighted d polynomial regression
- Minimizing the objective function

$$\underset{\beta_0(x_0),\beta_r(x_0)}{\text{minimize}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)\left[y_i - \beta_0(x_0) - \sum_{r=1}^{d} \beta_j(x_0)x_i^r\right]^2$$

- Still a weighted linear regression problem at each target point x_0
- $\widehat{f}(x_0) = \widehat{\beta}_0(x_0) + \sum_{r=1}^{d} \widehat{\beta}_r(x_0)x_0^r$
- Correct the boundary bias of the kernel estimator
- Reduce bias in regions of curvature, however, at a price of higher variance

Kernel Boundary Bias



R implementation

- R function loess provides fitting of the local polynomial regressions
- The most important parameter span = α controls the degree of smoothing: only αn number of closest points are used based on the distance $|x - x_i|$, forming the neighborhood "$N(x)$"
- A weighted least-square linear regression is fit within the neighborhood
- The weights uses tri-cube kernel: $w_{x,i} = (1 - u^3)^3$ with

$$u_i = \frac{|x_i - x|}{\max_{N(x)} |x_j - x|}$$

- degree specifies the degree of the polynomial
- Other implementations such as locfit and locpoly (use Gaussian kernel)