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Auctions

parametric Regression

Semiparametrics

References

## Nonparametrics and Local Methods

Richard L. Sweeney

based on slides by Chris Conlon

Empirical Methods
Spring 2019

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Nonparametric Density Estimation

Estimation

2 Cross-Validation

Exampl

3 Example: Auctions

parametric Regression

Semiparametric:

parametric

4 Non-parametric Regression

5 Semi-parametrics

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Cross-Validation

Example: Auctions

Nonparametric Regression

Semiparametrics

References

## Section outline

## Why nonparametrics?

- sometimes just interested in the distribution
- sometimes this is the first stage and we want to integrate
- sometimes want to do something semiparametric

In this section, we are interested in estimating the **density** f(x) under minimal assumptions.

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Semi-

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# Let's start with the histogram

One of the more successful and popular uses of nonparametric methods is estimating the density or distribution function f(x) or F(x).

$$\hat{f}_{HIST}(x_0) = \frac{1}{N} \sum_{i=1}^{N} \frac{\mathbf{1}(x_0 - h < x_i < x_0 + h)}{2h}$$

 Divide the dataset into bins, count up fraction of observations in each bins Cross-Validation

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Let's rewrite the histogram estimator

$$\hat{f}_{HIST}(x_0) = \frac{1}{Nh} \sum_{i=1}^{N} K\left(\frac{x_i - x_0}{h}\right)$$

Where 
$$K(z) = \frac{1}{2} \cdot \mathbf{1}(|z| < 1)$$

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# Density estimator interpretation

- for each observation, there is probability mass 1 to spread around
- use the function  $K(\cdot)$  and smoothing parameter h to choose how to allocate this mass
- then, for any given  $x_0$ , sum over these functions that spread out mass, and normalize by dividing by N

## Smooth Kernels

We call  $K(\cdot)$  a Kernel function and h the bandwidth. We usually assume

- (1) K(z) is symmetric about 0 and continuous.
- $\textcircled{\textbf{m}}$  Either (a) K(z)=0 if  $|z|\geq z_0$  for some  $z_0$  or (b)  $|z|K(z)\to 0$  as  $|z|\to \infty$ .
- $\bigvee \int z^K(z)dz = \kappa$  where  $\kappa$  is a constant.

Usually we choose a smooth, symmetric K. But a common nonsmooth choice: K(x)=(|x|<1/2) gives the histogram estimate.

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## Some Common Kernels

**Table 9.1.** Kernel Functions: Commonly Used Examples<sup>a</sup>

Kernel	Kernel Function K(z)	δ
Uniform (or box or rectangular)	$\frac{1}{2} \times 1( z  < 1)$	1.3510
Triangular (or triangle)	$(1- z ) \times 1( z  < 1)$	_
Epanechnikov (or quadratic)	$\frac{3}{4}(1-z^2) \times 1( z  < 1)$	1.7188
Quartic (or biweight)	$\frac{15}{16}(1-z^2)^2 \times 1( z <1)$	2.0362
Triweight	$\frac{35}{32}(1-z^2)^3 \times 1( z <1)$	2.3122
Tricubic	$\frac{70}{81}(1- z ^3)^3 \times 1( z <1)$	_
Gaussian (or normal)	$(2\pi)^{-1/2} \exp(-z^2/2)$	0.7764
Fourth-order Gaussian	$\frac{1}{2}(3-z)^2(2\pi)^{-1/2}\exp(-z^2/2)$	_
Fourth-order quartic	$\frac{15}{32}(3 - 10z^2 + 7z^4) \times 1( z  < 1)$	_

<sup>&</sup>lt;sup>a</sup> The constant  $\delta$  is defined in (9.11) and is used to obtain Silverman's plug-in estimate given in (9.13).

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## Kernel Comparison

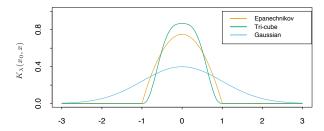


FIGURE 6.2. A comparison of three popular kernels for local smoothing. Each has been calibrated to integrate to 1. The tri-cube kernel is compact and has two continuous derivatives at the boundary of its support, while the Epanechnikov kernel has none. The Gaussian kernel is continuously differentiable, but has infinite support.

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# Mean and Variance of $\hat{f}(x_0)$

Assume that the derivative of f(x) exists and is bounded, and  $\int zK(z)dz=0$ 

Then the estimator has bias

$$b(x_0) = E\left[\hat{f}(x_0)\right] - f(x_0) = \frac{1}{2}h^2f''(x_0)\int z^2K(z)dx$$

The variance of the estimator is

$$V\left[\hat{f}(x_0)\right] = \frac{1}{Nh}f(x_0)\int K(z)^2 dz \left\{+o(\frac{1}{Nh})\right\}$$

So, unsurprisingly, the bias is *increasing* in h, and the variance is *decreasing* in h.

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## How to Choose h

- We want both bias and variance to be as small as possible, as usual.
- In parametric estimation, it is not a problem: they both go to zero as sample size increases.
- In nonparametric estimation reducing h reduces bias, but increases variance; how are we to make his trade off?
- Note that how we set h is going to be much more important than the choice of  $K(\cdot)$

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# Mean Integrated Square Error

• Start with the *local* performance at  $x_0$ 

$$MSE\left[\hat{f}(x_0)\right] = E\left[\left(\hat{f}(x_0) - f(x_0)\right)^2\right]$$

Calculate the *integrated* (as opposed to expected) squared error

$$\int \left( \hat{f}(x) - f(x) \right)^2 dx = - \int \mathsf{bias}^2 \left( \hat{f}(x) \right) + \mathsf{var} \left( \hat{f}(x) \right) dx$$

• Simple approximate expression (symmetric order 2 kernels):

$$(\mathsf{bias})^2 + \mathsf{variance} = Ah^4 + B/nh$$

with 
$$A = \int (f''(x))^2 (\int u^2 K)^2 / 4$$
 and  $B = f(x) \int K^2$ 

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# Optimal bandwidth

• The AMISE is

$$Ah^4 + B/nh$$

• Minimize by taking the FOC

$$h_n^* = \left(\frac{B}{4An}\right)^{1/5}$$

- bias and standard error are both in  $n^{-2/5}$
- and the AMISE is  $n^{-4/5}$ —not 1/n as it is in parametric models.
- But: A and B both depend on K (known) and f(y) (unknown), and especially "wiggliness"  $\int (f'')^2$  (unknown, not easily estimated). Where do we go from here?

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# Optimal bandwidth

Can be shown that the optimal bandwidth is

$$h* = \delta \left( \int f''(x_0)^2 dx_0 \right)^{-0.2} N^{-0.2}$$

where  $\delta$  depends on the kernel used (Silverman 1986) [these  $\delta$ 's are given in the kernel table]

Note the "optimal" kernel is Epanechnikov, although the difference is small.

## Silverman's Rule of Thumb

• If f is normal with variance  $\sigma^2$  (may not be a very appropriate benchmark!), the optimal bandwidth is

$$h_n^* = 1.06\sigma n^{-1/5}$$

• In practice, typically use Silverman's plug-in estimate:

$$h_n^* = 0.9 * \min(s, IQ/1.34) * n^{-1/5}$$

where IQ=interquartile distance

• Investigate changing it by a reasonable multiple.

This tends to work pretty well. But can we do better?

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# Why not search for optimal h in our data?

- Know we want to minimize MISE.
- ullet One option is to find the h that minimizes it in sample
  - Loop through increments of h
  - Calculate MISE
- Example: Old Faithful R data
  - Waiting time between eruptions and the duration of the eruption for the Old Faithful geyser in Yellowstone National Park, Wyoming, USA.
  - See R code in this folder.

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## Cross-validation

• General concept in the whole of nonparametrics: choose h to minimize a criterion CV(h) that approximates

$$AMISE(h) = \int E(\hat{f}_n(x) - f(x))^2 dx.$$

- Usually programmed in metrics software. If you can do it, do it on a subsample, and rescale.
- CV tries to measure what the expected out of sample (OOS or EPE) prediction error of a new never seen before dataset.
- The main consideration is to prevent overfitting.
  - In sample fit is always going to be maximized by the most complicated model.
  - OOS fit might be a different story.
  - ie 1-NN might do really well in-sample, but with a new sample might perform badly.

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# Sample Splitting/Holdout Method and CV

Cross Validation is actually a more complicated version of sample splitting that is one of the organizing principles in machine learning literature.

Training Set This is where you estimate parameter values.

Validation Set This is where you choose a model- a bandwidth h or tuning parameter  $\lambda$  by computing the error.

Test Set You are only allowed to look at this after you have chosen a model. Only Test Once: compute the error again on fresh data.

- Conventional approach is to allocate 50-80% to training and 10-20% to Validation and Test.
- Sometimes we don't have enough data to do this reliably.

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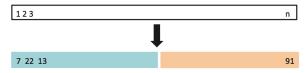
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# Sample Splitting/Holdout Method



**FIGURE 5.1.** A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.

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# Challenge with Sample Splitting

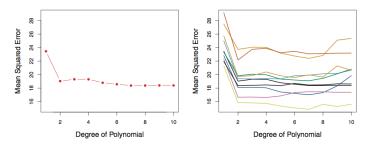


FIGURE 5.2. The validation set approach was used on the Auto data set in order to estimate the test error that results from predicting mpg using polynomial functions of horsepower. Left: Validation error estimates for a single split into training and validation data sets. Right: The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.

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## k-fold Cross Validation

- Break the dataset into k equally sized "folds" (at random).
- Withhold i=1 fold
  - Estimate the model parameters  $\hat{\theta}^{(-i)}$  on the remaining k-1 folds
  - Predict  $\hat{y}^{(-i)}$  using  $\hat{\theta}^{(-i)}$  estimates for the ith fold (withheld data).
  - Compute  $MSE_i = \frac{1}{k \cdot N} \sum_j (y_j^{(-i)} \hat{y}_j^{(-i)})^2$ .
  - Repeat for  $i = 1, \ldots, k$ .
- Construct  $\widehat{MSE}_{k,CV} = \frac{1}{k} \sum_{i} MSE_{i}$

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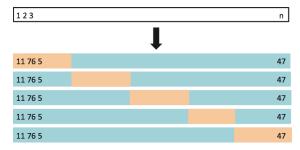
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## k-fold Cross Validation



**FIGURE 5.5.** A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.

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# Leave One Out Cross Validation (LOOCV)

Same as k-fold but with k = N.

- ullet Withhold a single observation i
- Estimate  $\hat{\theta}_{(-i)}$ .
- Predict  $\hat{y}_i$  using  $\hat{ heta}^{(-i)}$  estimates
- Compute  $MSE_i = \frac{1}{N} \sum_j (y_i \hat{y}_i(\hat{\theta}^{(-i)}))^2$ .

Note: this requires estimating the model N times which can be costly.

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## LOOCV vs k-fold CV

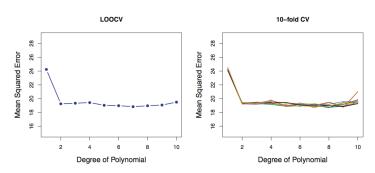


FIGURE 5.4. Cross-validation was used on the Auto data set in order to estimate the test error that results from predicting mpg using polynomial functions of horsepower. Left: The LOOCV error curve. Right: 10-fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.

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## Cross Validation

- Main advantage of cross validation is that we use all of the data in both estimation and in validation.
  - For our purposes validation is mostly about choosing the right bandwidth or tuning parameter.
- We have much lower variance in our estimate of the OOS mean squared error.
  - Hopefully our bandwidth choice doesn't depend on randomness of splitting sample.

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- In Statistics/Machine learning there is a tradition to withhold 10% of the data as Test Data.
- This is completely new data that was not used in the CV procedure.
- The idea is to report the results using this test data because it most accurately simulates true OOS performance.
- We don't do much of this in economics. (Should we do more?)

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## Local Bandwidths

If you only care about f(y) at some given point, then

$$A=f''(y)^2\left(\int u^2K\right)^2/4$$
 and  $B=f(y)\int K^2.$ 

So in a low-density region, worry about variance and take h larger. In a curvy region, worry about bias and take h small.

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# Higher-Order Kernels

- K of order r iff  $\int x^j K(x) dx = 0$  for j < r and  $\int x^r K(x) dx \neq 0$ . Try r > 2?
- The beauty of it: bias in  $h^r$  if f is at least  $C^r$ ...so AMISE can be reduced to  $n^{-r/(2r+1)}$ , almost  $\sqrt{n}$ -consistent if r is large.
- But gives wiggly (and sometimes negative) estimates  $\rightarrow$  leave them to theorists.

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## Back to the CDF

Since now we have estimated the density with

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

a natural idea is to integrate; let  $\mathcal{K}(x) = \int_{-\infty}^{x} K(t) dt$ , try

$$\hat{F}_n(y) = \frac{1}{n} \sum_{i=1}^n \mathcal{K}\left(\frac{y - y_i}{h}\right)$$

as a reasonable estimator of the cdf in y.

Very reasonable indeed:

- when  $n\longrightarrow\infty$  and h goes to zero (at rate  $n^{-1/3}\dots$ ) it is consistent at rate  $\sqrt{n}$
- it is nicely smooth
- by construction it accords well with the density estimator
- ... it is a much better choice than the empirical cdf.

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# Example application: Auctions

- Why auctions?
- Great introduction to structural approach. Arguably the most successful application.
- Auctions are an example of a game with assymetric information: participants know the primitives of the game, but do not know their rivals exact valuations.
- By imposing rationality/ profit maximization, we can recover the distribution of values.
- Can then run counterfatuals

For more detail, check out Chris Conlon's slides in this folder, or John Asker's PhD lecture notes.

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Let's consider the first price sealed bid (FPSB) auction Denote the equilibrium bid as  $B_i$ , with realizations  $b_i$ 

Perfect Bayes Nash equilibrium:

$$\max_{\tilde{b}} \left( E\left[ U_i | X_i = x_i \right] - b, \max_{j \in N_{-i}} B_j \le \tilde{b} \right)$$
$$Pr\left( \max_{j \in N_{-i}} B_j \le \tilde{b} | X_i = x_i \right)$$

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# Can find bid as a function of primitives

$$v(x_i, \mathbf{x_i}; N) = b_i + \frac{G_{M_i|B_i}(b_i|b_i; N)}{g_{M_i|B_i}(b_i|b_i; N)}$$

where  $G_{M_i \mid B_i}$  and  $g_{M_i \mid B_i}$  are the CDF and PDF of the max bids given  $b_i$  and N

- we are typically interested in the LHS
- RHS is stuff we can observe or compute
- nice linear structure makes this easy to work with
- Guerre, Perrigne and Vuong (2000): can leverage assumption of equilibrium best response and invertibility of b to recover v

# Estimation strategy |

[Assumption: FPSB with symmetric IPV]

1 Leverage independence assumption:

$$G_{M_i|B_i}(m_i|b_i;N) = G_{M_I|n}$$
  
=  $Pr(\max_{j \neq i} B_j \leq m_i|n)$ 

2 Value equation becomes

$$u = b + \frac{G_B(b|n)}{(n-1)g_B(b|n)}$$

where G and g are the marginal distribution of bids and the densities in n bidder auctions

 $oldsymbol{3}$  can estimate G and g using kernels

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# Estimation strategy II

4 now have

$$\hat{u} = b + \frac{\hat{G}_B(b|n)}{(n-1)\hat{g}_B(b|n)}$$

**5** finally, can recover the distribution of values with another kernel

$$\hat{f}(u) = \frac{1}{T_n h_f} \sum_{T=1}^{n} \frac{1}{n_t} \sum_{i=1}^{n} K\left(\frac{u_i - \hat{u}_{it}}{h_f}\right)$$

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# Algoritm

- for each  $b_o$ , estimate  $\hat{G}_B(b_0|n)$  and  $\hat{g}_B(b_0|n)$  using all the data
- infer  $\hat{u}(b_0)$
- ullet estimate  $\hat{f}$
- plot bids, adjust bandwidth etc
- run counterfactuals

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# Something Familiar

Let's start with something we all know, how to calculate:

$$E[Y_i|X_i] = \beta_0 + \beta_1 X_1 + \ldots + \varepsilon_i$$

 The Gauss-Markov theorem (remember that?) tells us that OLS is best among linear unbiased estimators.

#### Identification

What does it mean for a model to be identified?

$$\hat{\beta}_{OLS} = \arg \max_{\beta} (\mathbf{y} - \mathbf{x}\beta)' (\mathbf{y} - \mathbf{x}\beta)$$

- We need there to be a unique value of  $\beta$  that solves the above equation.
- For OLS this reduces to solving a linear system of  $\dim(X) = k$  equations and unknowns.
- The OLS estimator produces  $\hat{\beta}_{OLS} = \beta + (X'X)^{-1}X'\varepsilon$ .
  - Identification: means that we require (X'X) is invertible (no perfect multicollinearity).
  - When  $E[X'\varepsilon] = 0$  then this converges in probability to true  $\beta$ .

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## A Little More Complicated

- For many cases that we care about,  $E[X'\varepsilon] \neq 0$ . (Endogeneity)
- We know this is not the end of the world if we have an instrument Z:
- Now we need that Z'X is invertible.

$$E[\mathbf{x}'(\mathbf{y} - \mathbf{x}\beta)] \neq 0$$

$$E[\mathbf{z}'(\mathbf{y} - \mathbf{x}\beta)] = 0$$

$$\rightarrow \hat{\beta}_{TSLS} = E(Z'X)^{-1}E[Z'Y]$$

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#### Some more information

This leads to the common terminology:

- Under-identified: if  $\dim(X) > \dim(Z)$ .
- Just-identified: if  $\dim(X) = \dim(Z)$ .
- Over-identified: if  $\dim(X) < \dim(Z)$ .

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Auctions
Non-

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Semiparametrics

References

# What does this mean exactly

To understand this we usually construct the GMM form of the moment conditions:

$$E[\mathbf{z}'(\mathbf{y} - \mathbf{x}\beta)] = 0$$
  
$$f(\beta) = (\mathbf{y} - \mathbf{x}\beta)'\mathbf{z} \cdot W \cdot \mathbf{z}'(\mathbf{y} - \mathbf{x}\beta)$$

- Because  $f(\beta)$  is a quadratic form, and when W is PSD then  $f(\beta) \geq 0$ .
- Just-identified: There is exactly one solution to  $f(\beta)=0$  which does not depend on W.
- Under-identified:  $f(\beta)=0$  has many solutions because we have fewer instruments (or moment restrictions) than parameters.
- Over-identified: There are no solutions and  $f(\beta) > 0$ . Instead we choose  $\beta$  to minimize the distance from zero with distance metric W.

# The Binary Case

Now let's think about a case where  $Y \in \{0, 1\}$ :

$$y_i = \mathbf{1}[F(X_i) - \varepsilon_i > 0]$$

- There are different choices of  $F(X_i)$  and  $f(\varepsilon)$
- Probit:  $F(X_i) = \beta X_i$  where  $\varepsilon_i \sim N(0,1)$ .
- Logit: same  $F(\cdot)$  but different  $f(\varepsilon)$  (Type I Extreme Value).  $P(Y_i=1|X_i)=1/(1+exp[-\beta X_i]).$
- These choices of F are strong and somewhat arbitrary, we choose them out of convenience because both transformations are monotonic in  $\beta X_i$ , and continuously map  $[-\infty,\infty] \to [0,1]$

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Semi-

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# The Binary Case

What is the least I can assume in the binary case and still learn something?

$$y_i = \mathbf{1}[F(X_i) - \varepsilon_i > 0]$$

- Suppose instead we observe  $P(x) = Pr(y_i = 1|x_i)$  at many values of  $x_i$ . (Often refer to this as the CCP).
- Sometimes CCPs are all we care about. (if we are lucky).

Instead we can try and solve:

$$P(x) = \int \mathbf{1}(F(x) - \varepsilon > 0) dH(\varepsilon | x) = H(F(x) | x)$$

- Identification asks, what is the least we need to assume in order to recover F, H?
- Even with  $\varepsilon \perp X$  we still have too many degrees of freedom.

#### Are we stuck?

- We know that Logit and Probit are identified.
- Start with  $\varepsilon \perp X$ .
- $F(X_i) = G(X_i\beta)$  is a very powerful assumption often called (single) index model
- Can use Marginal Rate of Substitution (MRS) of P(x) to identify  $\beta_k/\beta_l$ .
  - How do conditional probabilities respond to changes in  $X^{(k)}$  versus  $X^{(l)}$ ?
  - Suggests the average derivative estimator which doesn't require normality assumptions of probit
  - More robust, but potentially less efficient if true distribution of  $\varepsilon \sim N(0,1)$ .
- Can we extend the general intuition to more cases?

# Single-Index Models

Consider

$$E[y|\mathbf{x}] = g(\mathbf{x}'\beta)$$

such as logit and probit.

ullet With conditional mean of change in  $x_j$ 

$$\frac{\partial [y|\mathbf{x}]}{\partial x_j} = g'(\mathbf{x}'\beta)\beta_j$$

• Can use Marginal Rate of Substitution (MRS) to identify  $\beta_k/\beta_l$ .

$$\frac{\partial \left[y|\mathbf{x}\right]/\partial x_{j}}{\partial \left[y|\mathbf{x}\right]/\partial x_{k}} = \frac{\beta_{j}}{\beta_{k}}$$

- Suggests the average derivative estimator which doesn't require normality assumptions of probit
- More robust, but potentially less efficient if true distribution of  $\varepsilon \sim N(0,1)$ .
- Can we extend the general intuition to more cases?

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Reference

# A Fake Data Example

Following the THF textbook example, we can generate some fake data and let:

$$Y = ORANGE \text{ if } Y* > 0.5$$
  
 $Y = BLUE \text{ if } Y* \leq 0.5$ 

- Easiest way to recover Y\* is by running OLS on the linear probability model.
- Draws from bivariate normal distribution with uncorrelated components but different means (2 overlapping types)
- Mixture of 10 low variance (nearly point mass) normal distributions where the individual means were drawn from another normal distribution. (10 nearly distinct types).

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Example Auctions

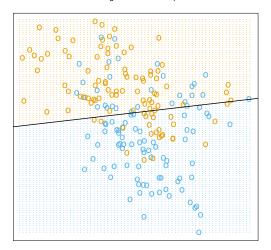
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### Linear Probability Model

Linear Regression of 0/1 Response



**FIGURE 2.1.** A classification example in two dimensions. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by linear regression. The line is the decision boundary defined by  $x^T \hat{\beta} = 0.5$ . The orange shaded region denotes that part of input space classified as ORANGE, while the blue region is classified as BLUE.

#### Alternative

- Lots of potential alternatives to our decision rule.
- A simple idea is to hold a majority vote of neighboring points

$$Y^* = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$$

- To avoid including "yourself" in your neighborhood, we often estimate on one sample and validate on another
- How many parameters does this model have: None? One?
   k?
- Technically it has something like N/k.
- As N → ∞ this means we have an infinite number of parameters! (This is a defining characteristic of non-parametrics).

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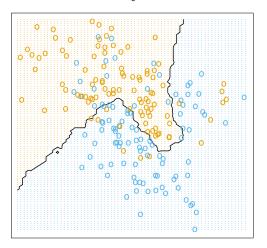
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### 15 Nearest Neighbor

15-Nearest Neighbor Classifier



**FIGURE 2.2.** The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1) and then fit by 15-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the 15-nearest neighbors.

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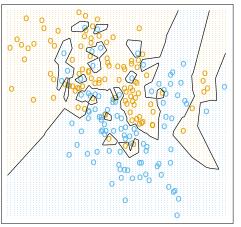
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## Extreme: 1 Nearest Neighbor

#### 1-Nearest Neighbor Classifier



**FIGURE 2.3.** The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (BLUE = 0, QRANGE = 1), and then predicted by 1-nearest-neighbor classification.

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## Comparisons

- What would happen if  $K \to N$ ?
- The k-NN model is locally constant.
- The k-NN approach tends to be really bumpy which can be undesirable.
- The OLS model is globally linear (is this always true?)

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#### What about?

- If we fixed the fact that there are discrete jumps in who is in the neighborhood by smoothly weighting observations and varying those weights instead (Kernels).
- Another drawback of k-NN is that we consider distance in each X dimension on the same scale, perhaps we could rescale the data to improve our "closeness" measure.
- Instead of fitting a constant locally, we fit a linear function locally (Lowess).
- Instead of using a global linear approximation in OLS use a more flexible nonlinear one.
- There is a bias/variance tradeoff. explain.

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## Bias Variance Decomposition

We can decompose any estimator into two components

$$\underbrace{E[(y-\hat{f}(x))^2]}_{MSE} = \underbrace{\left(E[\hat{f}(x)-f(x)]\right)^2}_{Bias^2} + \underbrace{E\left[\left(\hat{f}(x)-E[\hat{f}(x)]\right)^2\right]}_{Variance}$$

- In general we face a tradeoff between bias and variance.
- In k-NN as k gets large we reduce the variance (each point has less influence) but we increase the bias since we start incorporating far away and potentially irrelevant information.
- In OLS we minimize the variance among unbiased estimators assuming that the true f is linear.

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## Bias Variance Decomposition

What minimizes MSE?

$$f(x_i) = E[Y_i|X_i]$$

- Seems simple enough (but we are back where we started).
- How do we compute the expectation ?
- k-NN tries to use local information to estimate conditional mean
- OLS uses entire dataset and adds structure  $y=x\beta$  to the problem.

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## Big Data

- It used to be that if you had N=50 observations then you had a lot of data.
- Those were the days of finite-sample adjusted t-statistics.
- Now we frequently have 1 million observations or more, why can't we use k-NN type methods everywhere?

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# Curse of Dimensionality

Take a unit hypercube in dimension p and we put another hypercube within it that captures a fraction of the observations r within the cube

- Since it corresponds to a fraction of the unit volume, r each edge will be  $e_p(r)=r^{1/p}$ .
- $e_{10}(0.01) = 0.63$  and  $e_{10}(0.1) = 0.80$ , so we need almost 80% of the data to cover 10% of the sample!
- If we choose a smaller r (include less in our average) we increase variance quite a bit without really reducing the required interval length substantially.

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## Curse of Dimensionality

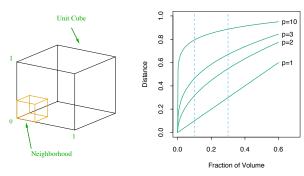


FIGURE 2.6. The curse of dimensionality is well illustrated by a subcubical neighborhood for uniform data in a unit cube. The figure on the right shows the side-length of the subcube needed to capture a fraction r of the volume of the data, for different dimensions p. In ten dimensions we need to cover 80% of the range of each coordinate to capture 10% of the data.

# Curse of Dimensionality

Don't worry, it only gets worse:

$$d(p, N) = \left(1 - \left(\frac{1}{2}\right)^{1/N}\right)^{1/p}$$

- d(p,N) is the distance from the origin to the closest point.
- N=500 and p=10 means d=0.52 or that the closest point is closer to the boundary than the origin!
- Why is this a problem?
- In some dimension nearly every point is the closest point to the boundary – when we average over nearest neighbors we are extrapolating not interpolating.

# Density/Distribution Estimation

One of the more successful and popular uses of nonparametric methods is estimating the density or distribution function f(x) or F(x).

- Estimating the CDF is easy and something you have already done
- Q-Q plots, etc.

$$\hat{F}_{ECDF}(x_0) = \frac{1}{N} \sum_{i=1}^{N} (x_i \le x_0)$$

• Differentiating to get density is unhelpful :  $F_{ECDF}^{\prime}(x)=0$  in most places.

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## What if y is of dimension $p_y > 1$ ?

"Easy": use  $p_y$ -dimensional K (often a  $p_y$ -product of 1-dim kernels) and bandwidth h, and do

$$\hat{f}_n(y) = \frac{1}{nh_y^p} \sum_{i=1}^n K\left(\frac{y-y_i}{h}\right).$$

- 1st minor pitfall: the various dimensions may have very different variances, so use  $(h_1, \ldots, h_{p_n})$ .
- 2nd minor pitfall: they may be strongly correlated; then sphericize first.
- Major problem: next slide...

# The Curse of Dimensionality

- Computational cost increases exponentially.
- Much worse: to achieve precision  $\epsilon$  in dimension  $p_y$ , the number of observations you need increases as

$$n \simeq \epsilon^{-(2+p_y/2)}$$
.

• The *empty space* phenomenon: if  $(y_1,\ldots,y_{p_y})$  all are iid uniform on [-1,1], then only  $n/(10^{p_y})$  observations on average have all components in [-0.1,0.1]. Bias still in  $h^2$ , but variance in  $1/nh^{p_y}$  now.

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### Silverman's Table

Silverman (1986 book) provides a table illustrating the difficulty of kernel estimation in high dimensions. To estimate the density at 0 of a N(0,1) with a given accuracy, he reports:

Dimensionality Required	Sample Size
1	4
2	19
5	786
7	10,700
10	842,000

Not to be taken lightly... in any case convergence with the optimal bandwidth is in  $n^{-2/(4+p_y)}$  now—and Silverman's rule of thumb for choosing  $h_n^*$  must be adapted too.

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# Usually we care about conditional densities

That is: we have covariates x, we want the density f(y|x). Again, "easy":

- $oldsymbol{0}$  get a kernel estimator of the joint density f(y,x);
- 2 and one of the marginal density f(x);
- 3 then define

$$\hat{f}_n(y|x) = \frac{\hat{f}_n(y,x)}{\hat{f}_n(x)} = \frac{\frac{1}{nh_y^{p_y}h_x^{p_x}} \sum_{i=1}^n K\left(\frac{y-y_i}{h_y}\right) K\left(\frac{x-x_i}{h_x}\right)}{\frac{1}{h_y^{p_y}} \sum_{i=1}^n K\left(\frac{x-x_i}{h_x}\right)}.$$

But the joint density is  $(p_x + p_y)$  dimensional... and the curse strikes big time.

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# What if my distribution is discrete-continuous?

Very often in microeconometrics some covariates only take discrete values (e.g. gender, race, income bracket...). Say the only discrete variable is gender, we care about the density of income of men.

- The kernel approach adapts directly: we separately estimate a density for men (on the corresponding subsample).
- Better: mix the two subsamples! Add women, but with a small weight w.
- Intuition: by doing so we increase the bias (the density for women is probably different than for men)  $\rightarrow$  bad, in  $w^2$  but we reduce the variance, by O(w); and this dominates for small w. (cf Li-Racine).

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## The Seminonparametric Approach

- If we are "pretty sure" that f is almost  $f_{m,\sigma}$  for some family of densities indexed by  $(m,\sigma)$ , then we can choose a family of positive functions of increasing complexity  $P^1_{\theta}, P^2_{\theta}, \ldots$
- Choose some M that goes to infinity as n does (more slowly), and maximize over  $(m,\sigma,\theta)$  the loglikelihood

$$\sum_{i=1}^{n} \log f_{m,\sigma}(y_i) P_{\theta}^{M}(y_i).$$

It works...but it is hard to constrain it to be a density for large  ${\cal M}.$ 

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#### Mixtures of Normals

A special case of seminonparametrics, and usually a very good approach: Let y|x be drawn from

$$N(m_1(x,\theta),\sigma_1^2(x,\theta))$$
 with probability  $q_1(x,\theta)$ ;

$$N(m_K(x,\theta),\sigma_K^2(x,\theta))$$
 with probability  $q_K(x,\theta)$ .

where you choose some parameterizations, and the  $q_k$ 's are positive and sum to 1.

Can be estimated by maximum-likelihood:

$$\max_{\theta} \sum_{i=1}^{n} \log \left( \sum_{k=1}^{K} \frac{q_k(x_i, \theta)}{\sigma_k(x, \theta)} \phi \left( \frac{y_i - m_k(x_i, \theta)}{\sigma_k(x_i, \theta)} \right) \right).$$

Usually works very well with  $K \leq 3$  (perhaps after transforming y to  $\log y$ , e.g).

## Nonparametric Regression

Data  $(y_i,x_i)_{i=1}^n$  now, we are after E(g(y,x)|x)=m(x) for some function g.

- Best-fit approach, quite unbiased:
  - if  $x = x_i$  then  $\hat{m}_n(x) = g(y_i, x_i)$ ; otherwise ... whatever.

But: very jagged estimate; variance independent of n, so not consistent.

 Better and most usual: Nadaraya-Watson, inspired from kernel idea:

$$\hat{m}_n(x) = \frac{\sum_{i=1}^n g(y_i, x_i) K\left(\frac{x - x_i}{h}\right)}{\sum_{i=1}^n K\left(\frac{x - x_i}{h}\right)}.$$

again, bias in  $h^2$  and variance in 1/nh if  $p_x=1$ . Pitfall 1: very unreliable where f(x) is small. Pitfall 2: the formal for the optimal bandwidth h is very ugly.

Nonparametric Regression

# Choosing h

- Plug-in estimates work badly.
- Fortunately, cross-validation amounts to

$$\min_{h} \sum_{i=1}^{n} \frac{(g(y_i, x_i) - \hat{m}_n(x_i; h))^2}{1 - k_i(h)}$$

where 
$$k_i(h) = K_h(0) / \sum_{j=1}^n K_h(x_i - x_j)$$
.

 So not that hard, and can be done on a subsample and rescaled.

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### Local Linear Regression

- The Nadaraya-Watson estimator in x can be obtained very simply by regressing  $g(y_i,x_i)$  on 1, weighting each observation by  $K((x-x_i)/h)$ .
- We could also regress on 1 and  $(x-x_i)$  (going to higher terms has problems) instead; Advantages:
  - the bias becomes 0 if the true m(x) is linear.
  - the coefficient of  $(x-x_i)$  estimates m'(x).
  - behaves better in "almost empty" regions.

Disadvantages: hardly any, just do it!

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#### Local Linear

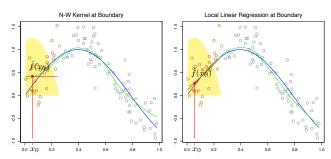


FIGURE 6.3. The locally weighted average has bias problems at or near the boundaries of the domain. The true function is approximately linear here, but most of the observations in the neighborhood have a higher mean than the target point, so despite weighting, their mean will be biased upwards. By fitting a locally weighted linear regression (right panel), this bias is removed to first order.

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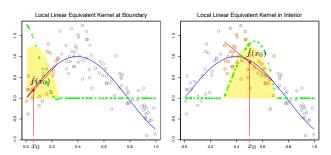
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#### Local Linear



**FIGURE 6.4.** The green points show the equivalent kernel  $l_i(x_0)$  for local regression. These are the weights in  $\hat{f}(x_0) = \sum_{i=1}^N l_i(x_0)y_i$ , plotted against their corresponding  $x_i$ . For display purposes, these have been rescaled, since in fact they sum to 1. Since the yellow shaded region is the (rescaled) equivalent kernel for the Nadaraya-Watson local average, we see how local regression automatically modifies the weighting kernel to correct for biases due to asymmetry in the smoothing window.

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# Local Quadratic

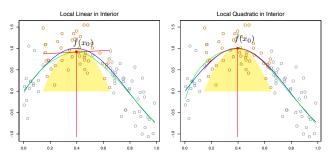


FIGURE 6.5. Local linear fits exhibit bias in regions of curvature of the true function. Local quadratic fits tend to eliminate this bias.

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# Nonparametric Regression, summary, 1

Nadaraya-Watson for E(y|x)=m(x)

$$\hat{m}(x) = \frac{\sum_{i} y_i K_h(x - x_i)}{\sum_{i} K_h(x - x_i)}$$

- bias in  $O(h^2)$ , variance in  $1/(nh^{p_x})$
- optimal h in  $n^{-1/(p+4)}$ : then bias, standard error and RMSE all converge at rate  $n^{-2/(p+4)}$
- to select h, no rule of thumb: cross-validate on a subsample and scale up.

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# Nonparametric Regression, summary, 2

Nadaraya-Watson=local constant regression: to get  $\hat{m}(x)$ ,

- 1 regress  $y_i$  on 1 with weight  $K_h(x-x_i)$
- 2 take the estimated coeff as your  $\hat{m}(x)$ .

Better: local linear regression

- **1** regress  $y_i$  on 1 and  $(x_i x)$  with weight  $K_h(x x_i)$
- 2 take the estimated coeffs as your  $\hat{m}(x)$  and  $\hat{m}'(x)$ .

To estimate the standard errors: bootstrap on an undersmoothed estimate (so that bias is negligible.)

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# $\begin{array}{c} {\sf Seminonparametric}\;(=&{\sf Flexible})\\ & {\sf Regression} \end{array}$

Idea: we add regressors when we have more data

- $\rightarrow$  series or sieve estimators: choose a basis of functions  $P_k(x_i)$  ( $x_i^k$ , or orthogonal polynomials, or sines...)
- ightarrow run linear regression  $y_i = \sum_{k=1}^M P_k(x_i) heta_k + \epsilon_i$
- a reasonable compromise (again, M must go to infinity, more slowly than n).

Still curse of dimensionality, and nonparametric asymptotics.

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# Splines: trading off fit and smoothness

Choose some  $0 < \lambda < \infty$  and

$$\min_{m(.)} \sum_{i} (y_i - m(x_i))^2 + \lambda J(m),$$

Then we "obtain" the natural cubic spline with  $knots=(x_1,\ldots,x_n)$ :

- m is a cubic polynomial between consecutive  $x_i$ 's
- it is linear out-of-sample
- ullet it is  $C^2$  everywhere.

"Consecutive" implies one-dimensional... harder to generalize to  $p_x>1$ .

Orthogonal polynomials: check out Chebyshev,  $1, x, 2x^2 - 1, 4x^3 - 3x \dots$  (on [-1, 1] here.)

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Semiparametric

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## Review: What was the point?

- OLS is lowest variance among linear unbiased estimators.
- But there are nonlinear estimators and potentially biased estimators.
  - Everything faces a bias-variance tradeoff.
  - Nearly anything can be written as Kernel.

Acknowledgements/ References