Probability Density Estimation, Smoothed Mean Estimators

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Computational Methods in Statistics and Data Science (Stats 406)

Probability Density Estimation

Setting

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$$X_i \sim F, \quad F(x) = \int_{-\infty}^{x} f(t)\, dt$$

Goal: Estimate f.

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The **empirical density function** is then a discrete probability mass function

$$\widehat{f}_n(x) = \frac{1}{n} \sum_{i=1}^{n} I(X_i = x)$$

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We will start with the **univariate case**. Later we'll consider **bivariate extensions**. After that, we'll see smoothing for **conditional distributions**.

Simulated Data: Mixture of $N(0,1)$ anf $N(3,1)$

```
> x <- rnorm(1000, mean = 3 * rbinom(100, size = 1, 0.25))
```
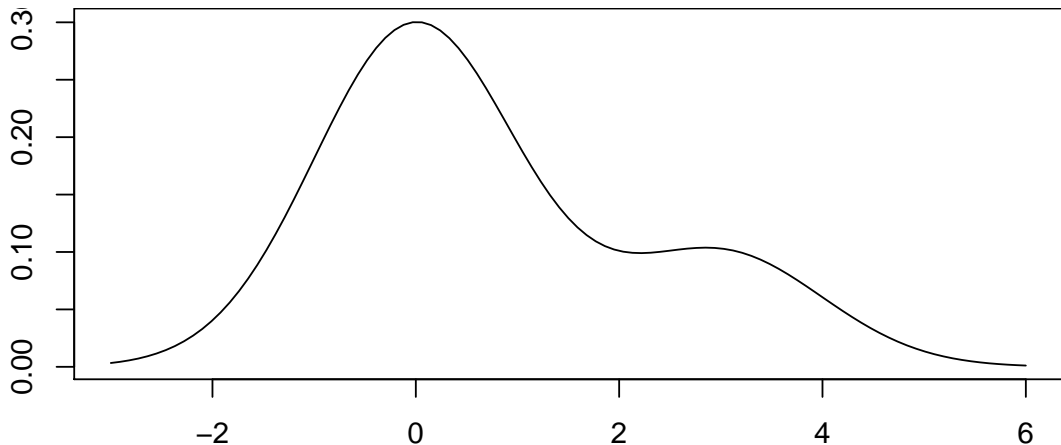
Histograms

A **histogram estimator** creates bins k bins

$$[t_j, t_{j+1}), \quad j = 1, \ldots, k$$

and counts then number of observations X_i that fall in each bin:

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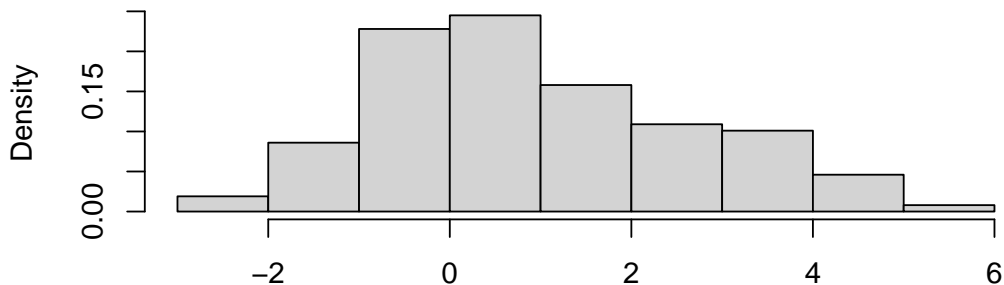
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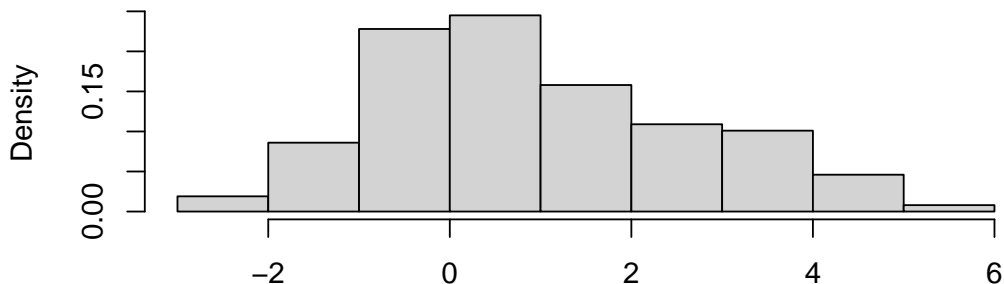Then an estimator of the density at point x is:

$$\widehat{f}(x) = \frac{1}{n} \sum_{j=1}^{k} \frac{V_j}{t_{j+1} - t_j} I(x \in [t_j, t_{j+1}))$$

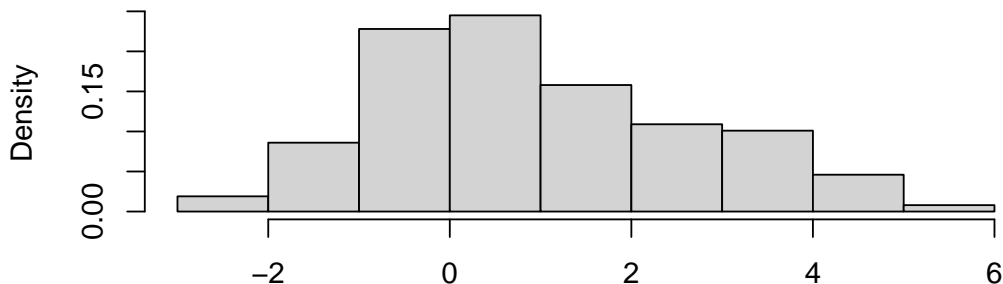**Histogram, further notes**

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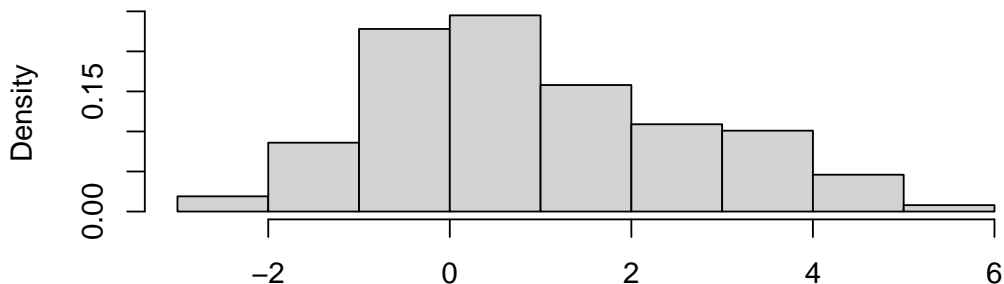
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- We usually make all bins have the same width $h = t_{j+1} - t_j$
- There is a tradeoff between smoothness (large h) and precision (small h).
- There are several options for setting the bin width and locations (see Rizzo, chapter 10).

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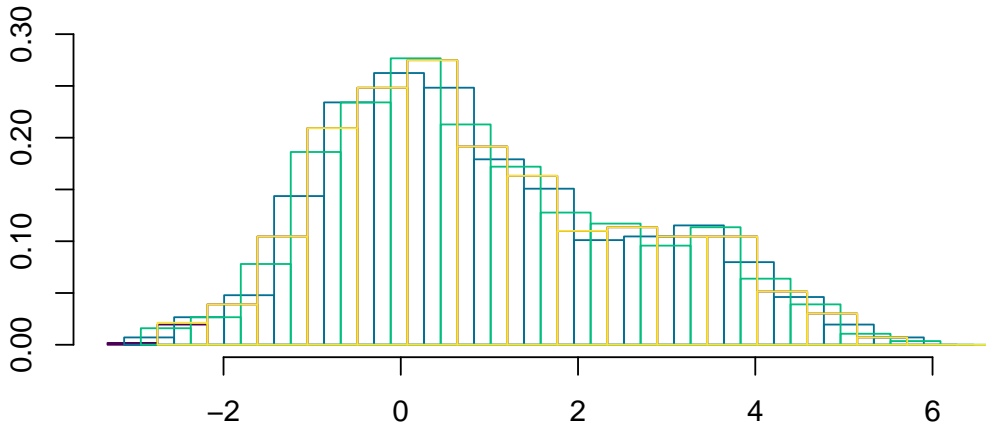
Average Shifted Histogram

Rather than estimate f with a single histogram, we can **average over m histograms**:

$$f_{\text{ASH}}(x) = \frac{1}{m} \sum_{j=1}^{m} \widehat{f}_j(x)$$

where $\widehat{f}_j$ is a histogram with bin size h start at $t^{(j)} = t_0 + h/m$.
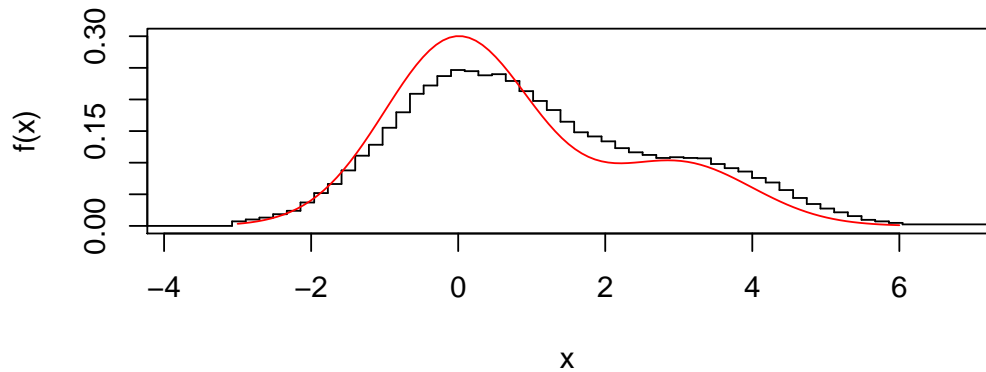
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```
> library(ash)
> ash_x <- ash1(bin1(x), 5, kopt = c(0,0))
```

Taking $m \to \infty$

As we **increase** m (number of histograms in ASH) the approximation will get **more smooth**. What happens when $m \to \infty$?

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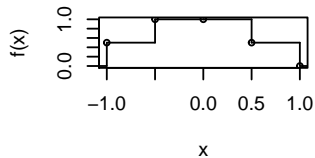Suppose all of the data is within $[-1, 1]$ and we want to estimate $f(0)$.

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Another way of saying this is, if we keep averaging at a single point as $m \to \infty$, what proportion of neighbors within $+1/-1$ are included?
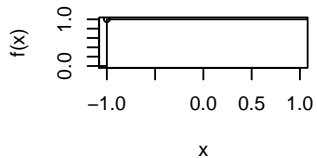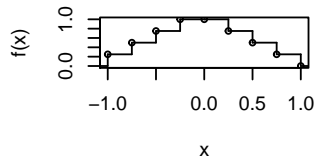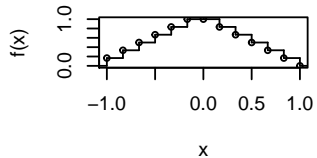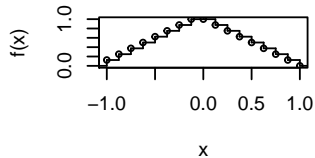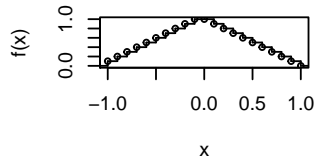
Triangular Distribution

As $m \to \infty$, the ASH becomes

$$\widehat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} I(X_i \in [x - h, x + h]) \left(1 - \frac{|x - X_i|}{h}\right)$$
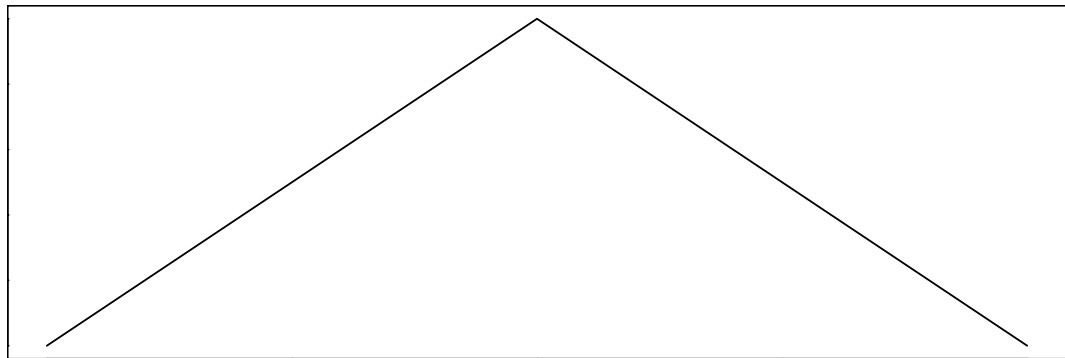
Density objects in R

R has a built in function to perform **density estimation**:

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> fx <- density(x, kernel = "triangular")
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The object is list of two vectors: x values from the sample and $\hat{f}(x)$ estimates

```
> fx$x[1:5]
```

```
[1] -3.905 -3.884 -3.863 -3.842 -3.820
```

```
> fx$y[1:5]
```

```
[1] 9.544e-19 2.537e-18 8.760e-18 1.487e-17 1.626e-17
```

Plotting in Base R

```
> plot(fx, ylim = c(0, 0.3))
> truef <- function(x) { 0.75 * dnorm(x) + 0.25 * dnorm(x, mean = 3) }
> curve(truef(x), add = TRUE, col = "red")
```


density.default(x = x, kernel = "triangular")

14
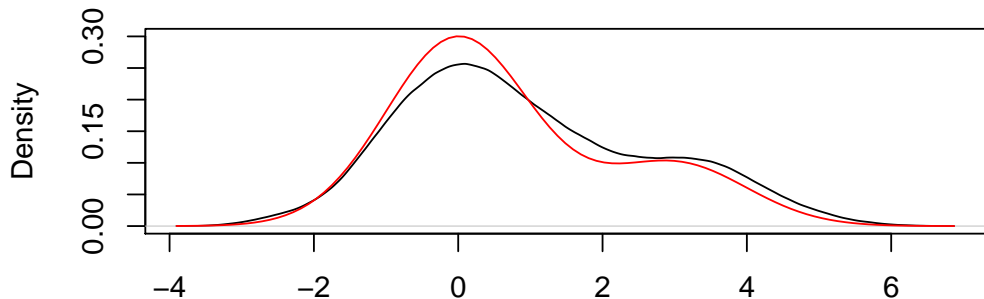
Plotting in ggplot

```
> ggplot(data.frame(x), aes(x = x)) + geom_density(kernel = 'triangular') +
+   stat_function(fun = truef, col = 'red')
```
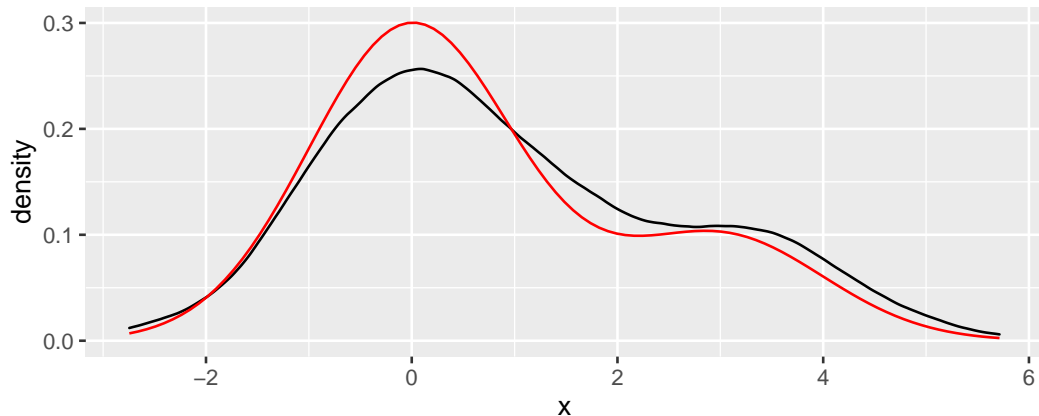
Kernel Density Estimators

In general, we can write:

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Optimal bandwidth depends on the true f. Heuristics discussed in Rizzo.

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Properties of the kernel usually transfer to $\widehat{f}$. E.g., if K is smooth, then $f_{K,h}$ is also smooth.

Multivariate Density Smoothing

Suppose we have $X = (X_1, \ldots, X_d)$ from a **multivariate density**. We can create multivariate kernels two ways:

- Use multivariate kernels (e.g., the multivariate standard Normal distribution):

$$\widehat{f}(x_1, \ldots, x_d) = \frac{1}{n h_1 h_2 \ldots h_d} \sum_{i=1}^{n} K\left(\frac{x_1 - X_{i1}}{h_1}, \frac{x_2 - X_{i2}}{h_2}, \ldots, \frac{x_d - X_{id}}{h_d}\right)$$

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- Create a kernel from the product of unidimensional kernels ("independent joint distribution")

$$\widehat{f}(x_1, \ldots, x_d) = \frac{1}{n h_1 h_2 \ldots h_d} \sum_{i=1}^{n} \prod_{j=1}^{d} K\left(\frac{x_j - X_{ij}}{h_j} \right)$$

```
> ggplot(nhanes, aes(x = sys_mean, y = dia_mean)) + geom_point()
```
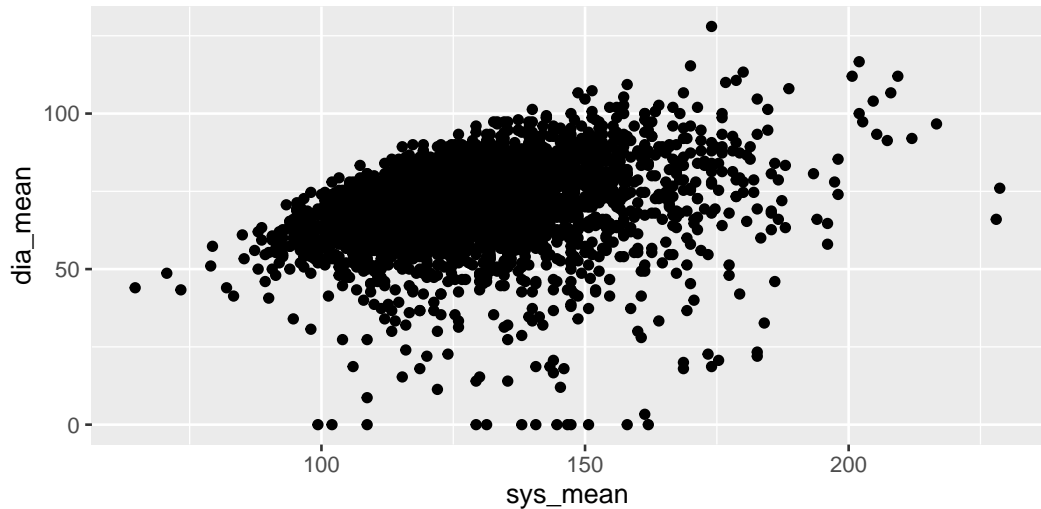
```
> library(MASS)
> contour(kde2d(nhanes$sys_mean, nhanes$dia_mean))
```
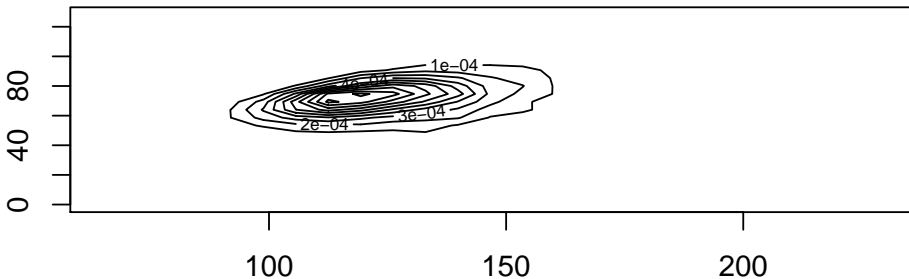
Mixture distributions

Recall our definition of a **mixture distribution**

$$F(x) = \sum_{i=1}^{n} w_i F_i(x)$$

where

- Each F_i is a **valid CDF**.
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If each CDF has a **PDF/PMF** f_j, then

$$f(x) = \frac{d}{dx} \sum_{j=1}^{m} w_i F_i(x) = \sum_{j=1}^{m} w_i f_i(x)$$

Location-scale mixtures

Suppose we have a **mixture** where the F_j come from a single **location-scale family**:

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The mixture density is then

$$f(x) = \sum_{i=1}^{n} w_i \frac{g\left(\frac{x-\mu_j}{\sigma}\right)}{\sigma}$$

Density estimation as a mixture

Now we can see that **kernel density estimator** is fitting a **mixture distribution**:

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

where

- K is the **location-scale density**,
- X_i is the **mean** μ_j
- h is the **scale/sd** σ.
- All **weights are 1/n**.

Gaussian kernel, $h = 1/2$, $X = (0, 1, 3)$
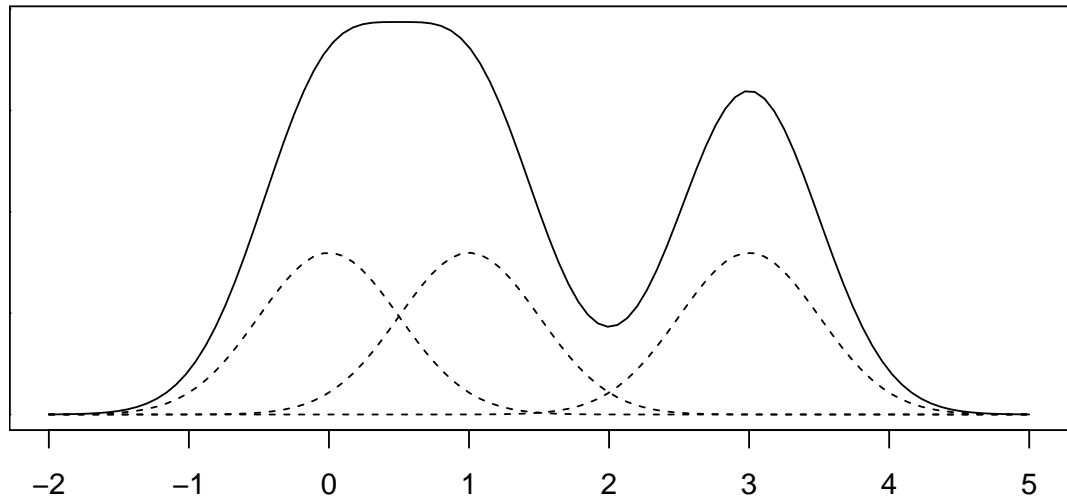
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Smoothed Means

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Goal: Understand the relationship between x_i and Y_i (perhaps for prediction, data reduction, inference).

Mean functions

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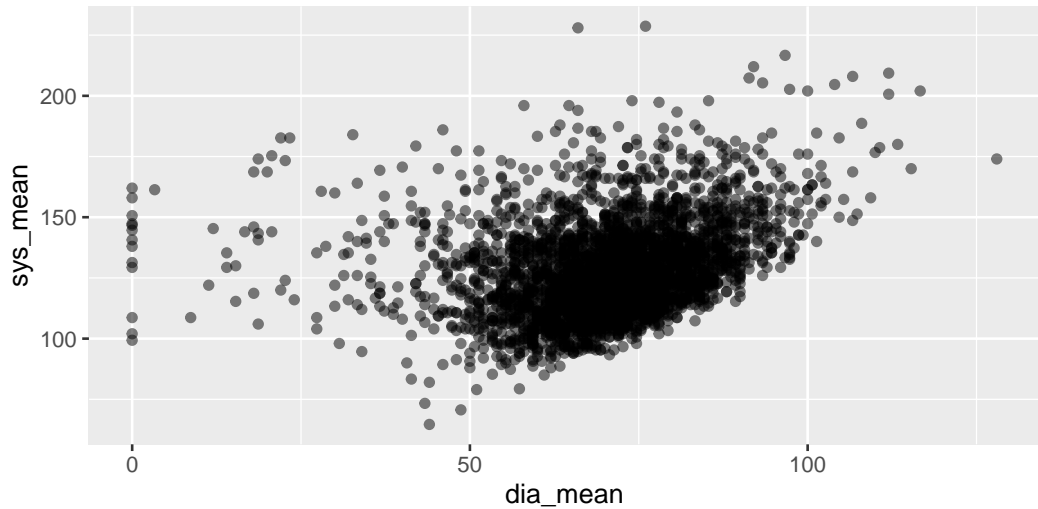where we assume $E(\epsilon) = 0$.

For example,

$$Y = \beta_0 + \beta_1 x + \epsilon$$

Notice because $E(\epsilon) = 0$, we have

$$E(Y|x) = \mu(x)$$

Can we use smoothing to estimate a good mean function?

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The Nardaraya-Watson estimator using a kernel function K:

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

From density estimation to smoothed means

Consider the estimators for the **joint distribution of** (Y, X) and the **marginal distribution of** X:

$$\hat{f}(x, y) = \frac{1}{nh^2} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) K\left(\frac{Y_i - y}{h}\right)$$

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

By the relationship that $f(y \mid x) = f(x, y)/f(x)$, we can plugin in our estimators to get

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

Estimating $E(Y \mid x)$

We want to estimate $E(Y \mid x) = \int y \, f(y \mid x) \, dy$, so let's plug in our estimate $\hat{f}(y \mid x)$:

$$\int y \, \hat{f}(y \mid x) \, dy = \int y \, \frac{\frac{1}{h} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) K\left(\frac{Y_i - y}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right)} \, dy$$

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$$

$$
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$$

We're done if we can show

$$
\frac{1}{h} \int y\, K\left(\frac{Y_i - y}{h}\right)\, dy = Y_i
$$

Final step

Recall that K **is a density function** for some random variable V, **symmetric about 0**. Let's do a little **change of variables**.

$$v = \frac{y - Y_i}{h} \Rightarrow y = Y_i + hv, dy = hdv$$

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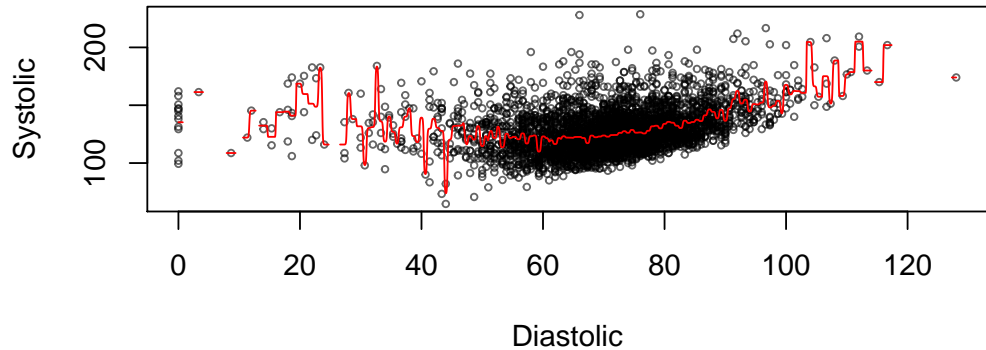$$v = \frac{y - Y_i}{h} \Rightarrow y = Y_i + hv, dy = hdv$$

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Narrow bandwidth

```
> ## default bandwidth is 0.5
> bp_smooth <- ksmooth(nhanes$dia_mean,
+                      nhanes$sys_mean,
+                      kernel = "normal")
> str(bp_smooth)

List of 2
 $ x: num [1:3567] 0 0.0359 0.0718 0.1077 0.1436 ...
 $ y: num [1:3567] 135 135 135 135 135 ...
```
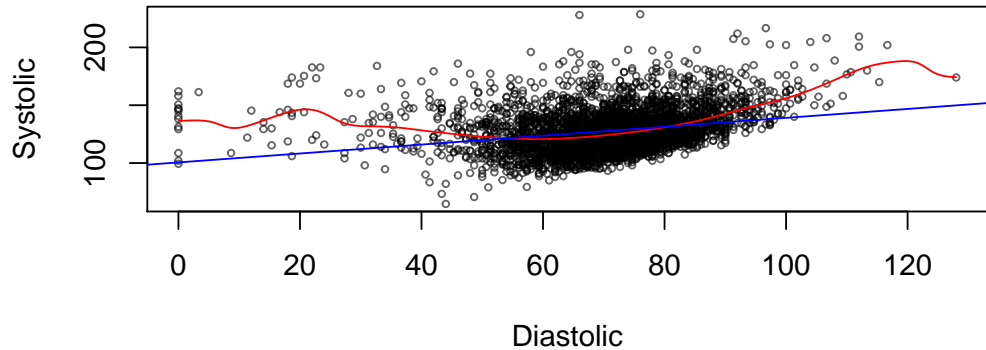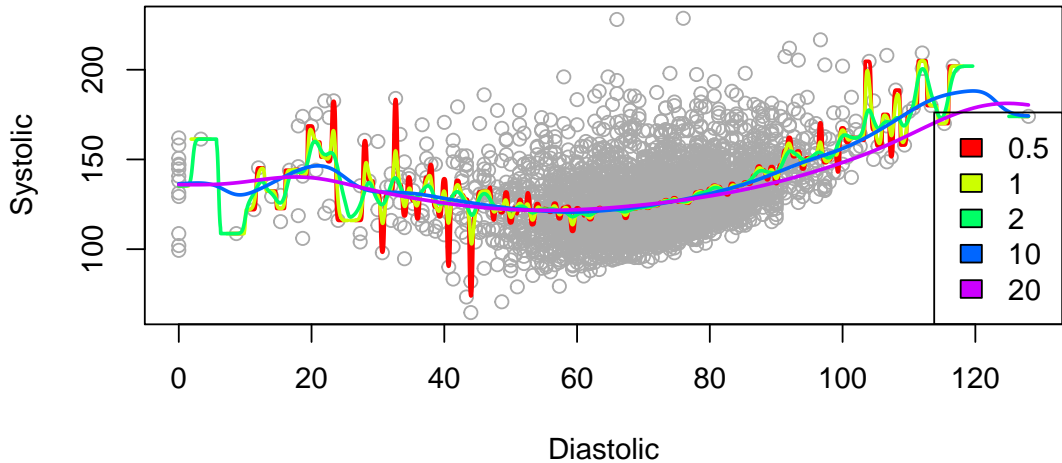
Better bandwidth

```
> bp_smooth_2 <- ksmooth(nhanes$dia_mean,
+                        nhanes$sys_mean,
+                        kernel = "normal", bandwidth = 10)
> bp_linea <- lm(sys_mean ~ dia_mean, data = nhanes)
```

Picking a bandwidth using CV

Recall that **cross validation** splits the data into (many) training and test sets and estimates **prediction loss** (costs paid for estimating new values).

Let's pick bandwidth using **leave one out cross validation** with **squared error loss**.

```
> loss_one <- function(i, h) {
+     yhat_i <- ksmooth(bandwidth = h, kernel = "normal",
+                       x = nhanes$dia_mean[-i],
+                       y = nhanes$sys_mean[-i],
+                       x.points = nhanes$dia_mean[i])
+     (yhat_i$y - nhanes$sys_mean[i])^2 ## loss
+ }
> loss_LOOCV <- function(h) { mean(sapply(1:nrow(nhanes), loss_one, h = h)
```

```
> hs <- seq(0.4, 20, length.out = 50)
> h_loss <- sapply(hs, loss_LOOCV)
> (best <- hs[which.min(h_loss)])
```

[1] 7.6
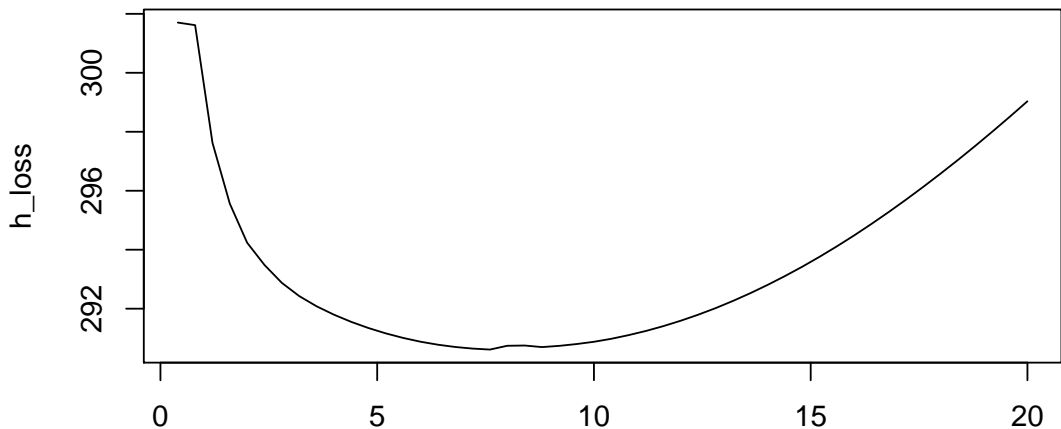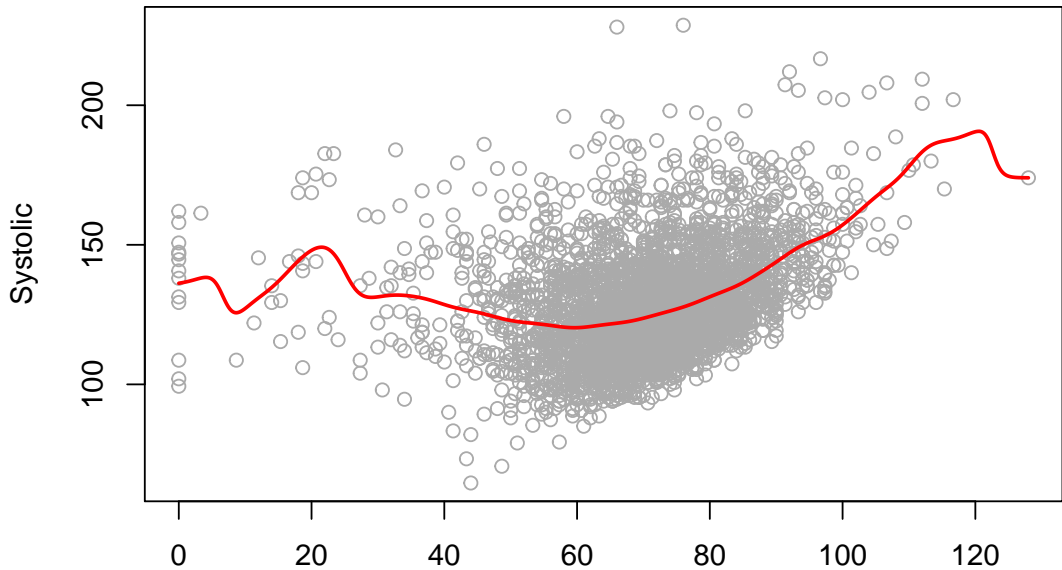
Comparing smoothed mean functions

Question: Is the mean function for aspirin takers the same as the mean function for non-apsirin takers?

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A little setup to make sure we compute the smooothers at the same point:

```
> range_d1 <- range(nhanes$dia_mean[nhanes$taking_aspirin])
> range_d2 <- range(nhanes$dia_mean[!nhanes$taking_aspirin])
> bounds <- c(max(range_d1[1], range_d2[1]),
+             min(range_d1[2], range_d2[2]))
```

Implementing the smoothers

```
> compute_smoother <- function(y, x, z) {
+     # we'll use the optimal bandwidth from before,
+     # but this could be computed within groups
+     ksmooth(x[z], y[z], bandwidth = 7.6,
+             n.points = 1000, range = bounds)
+ }

> take_sm <- with(nhanes,
+                  compute_smoother(sys_mean, dia_mean, taking_aspirin))
> nott_sm <- with(nhanes,
+                  compute_smoother(sys_mean, dia_mean, !taking_aspirin))
```

Taking
Not taking

43
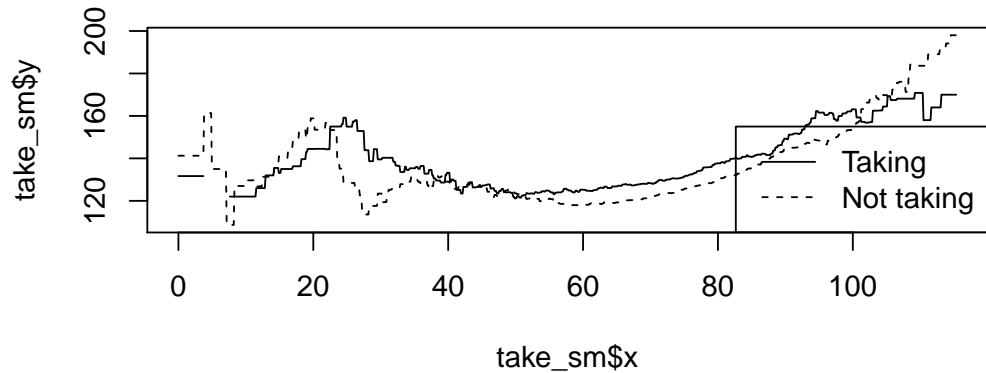
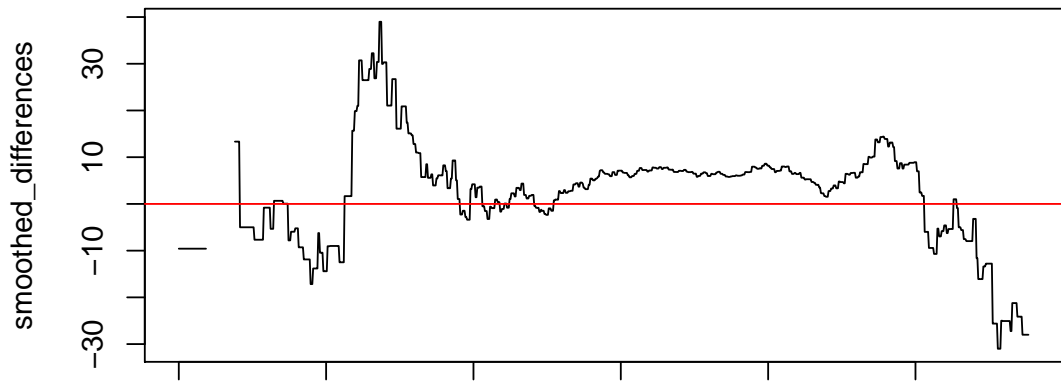## Difference Function

We probably want to know if

$$\mu_1(x) > \mu_0(x) \Rightarrow \mu_1(x) - \mu_0(x) > 0$$

```
> smoothed_differences <- take_sm$y - nott_sm$y
```

Confidence intervals for differences

```
> mu_diff <- function(data, index) {
+   xstar <- data[index, ]
+
+   s1 <- with(xstar,
+               compute_smoother(sys_mean, dia_mean, taking_aspirin))
+
+   s2 <- with(xstar,
+               compute_smoother(sys_mean, dia_mean, !taking_aspirin))
+
+   return(s1$y - s2$y)
+ }
```

```
> mu_boot <- boot(nhanes,
+   mu_diff,
+   strata = nhanes$taking_aspirin, R = 100)
> point_ci <- apply(mu_boot$t, 2,
+                   quantile, probs = c(0.025, 0.975), na.rm = TRUE)
```

95% confidence CIs for difference of mean fns
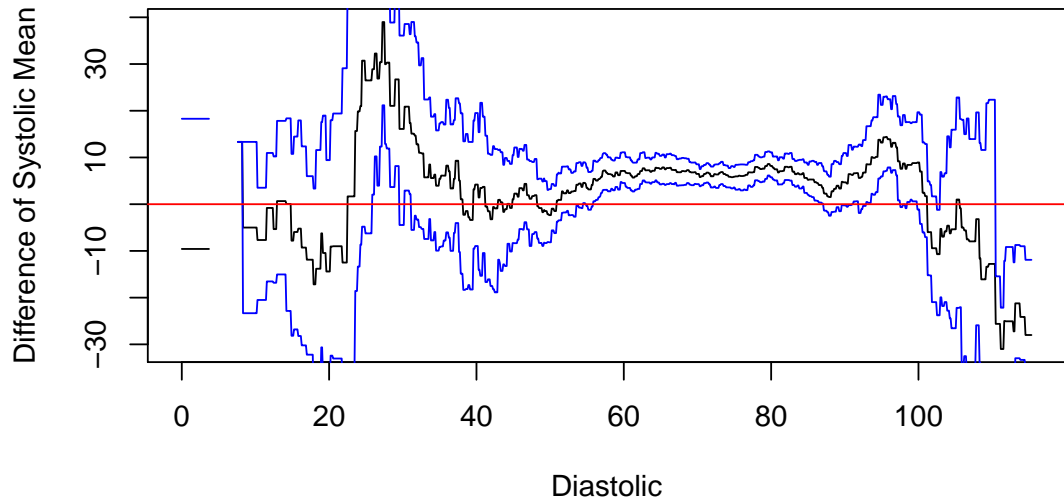
Smoothed Mean Function Summary

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$$Y = \mu(x) + \epsilon, \, \mathsf{E}\left(\epsilon = 0\right) \iff \mathsf{E}\left(Y \mid x\right) = \mu(x)$$

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- Added uncertainty using bootstrap (could have assumed constant variance as well)