Introduction to Nonparametric Regression

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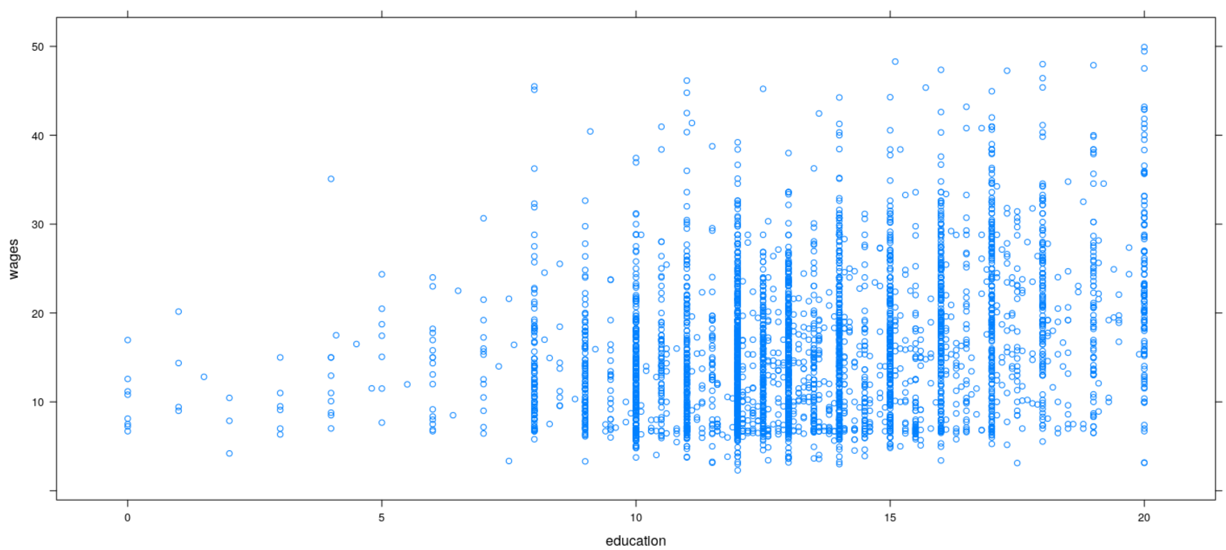
Visualizing distributions

- Recall that the goal of regression is to predict distribution of $\mathbf{Y}|\mathbf{X} = \mathbf{x}$
- How can we assess distribution visually? (e.g., to check normality)
- Usual tools
  - Histograms / density plots
  - Box-and-whisker plots
  - Quantile-quantile plots

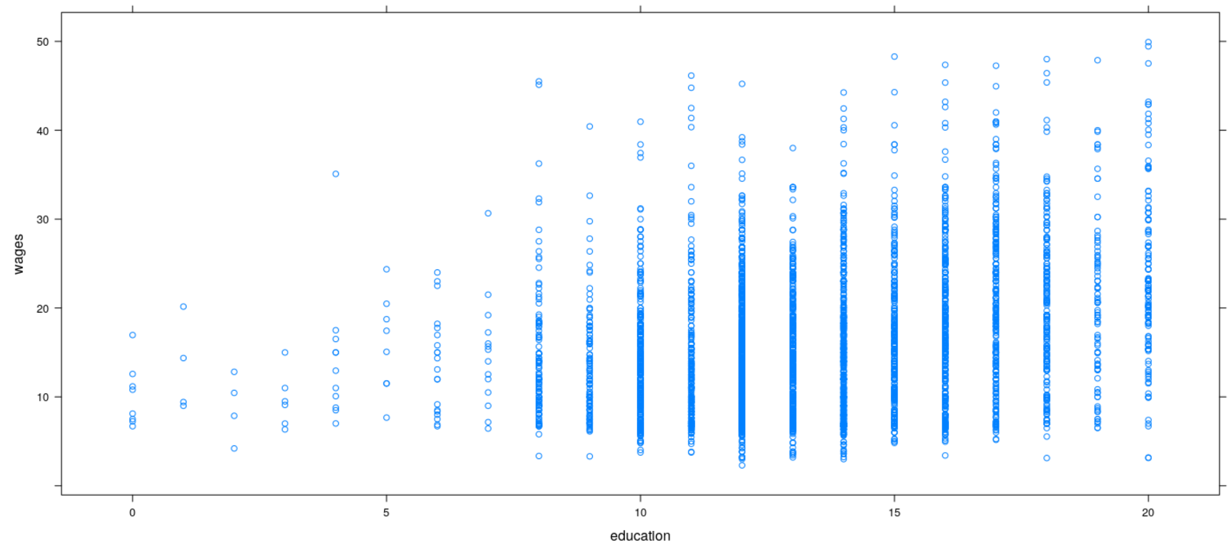
Example: SLID data

```
data(SLID, package = "carData")
xyplot(wages ~ education, data = SLID)
```



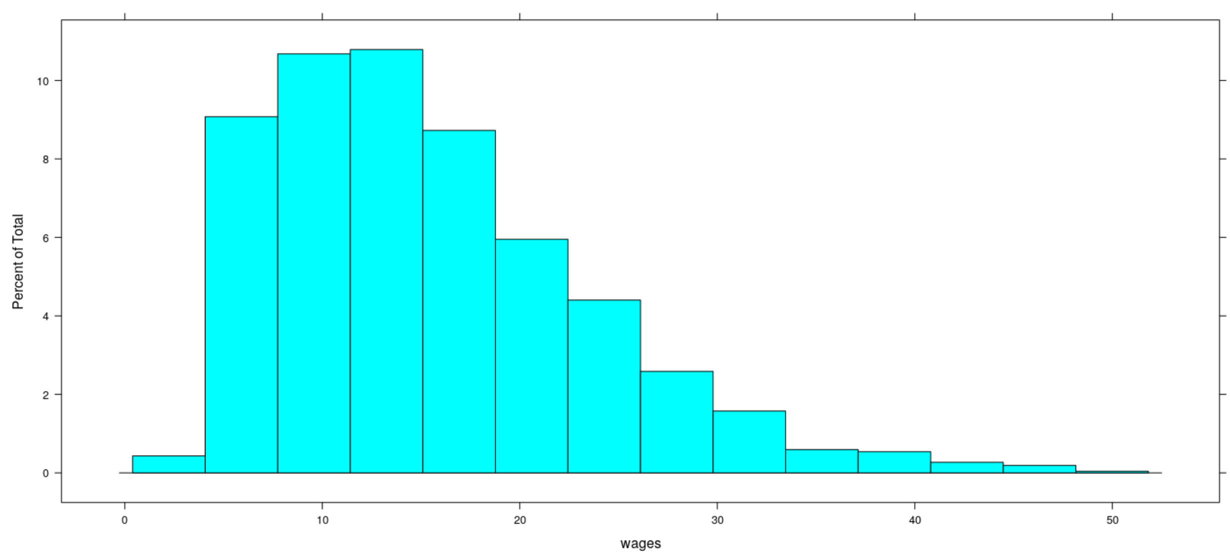
Example: SLID data (rounding education)

```
SLID$education <- round(SLID$education)
xyplot(wages ~ education, data = SLID)
```



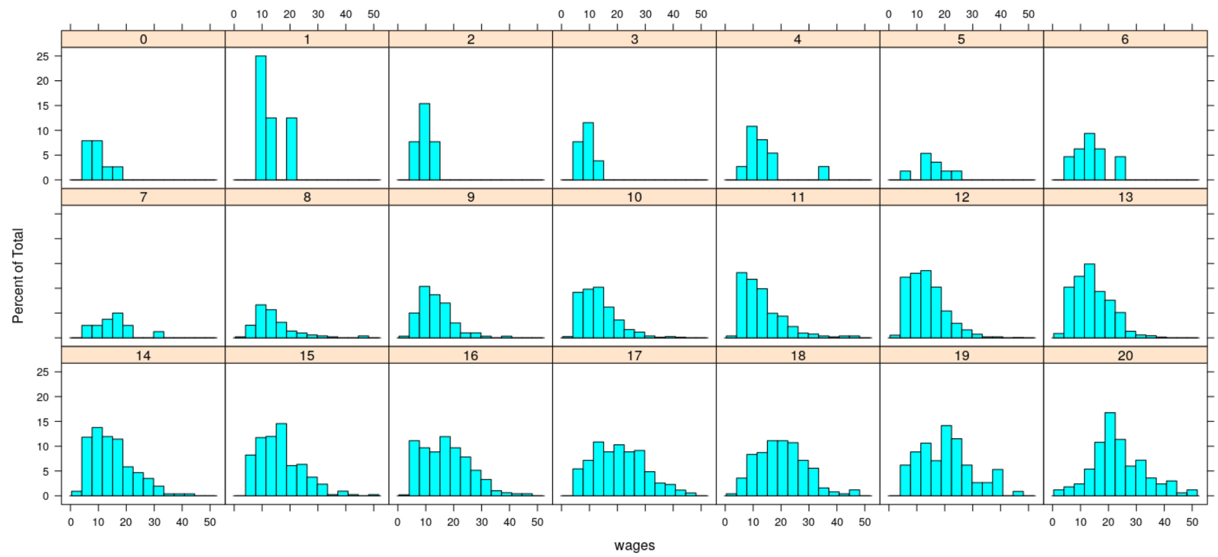
Distribution of wages (overall)

```
histogram( ~ wages, data = SLID)
```

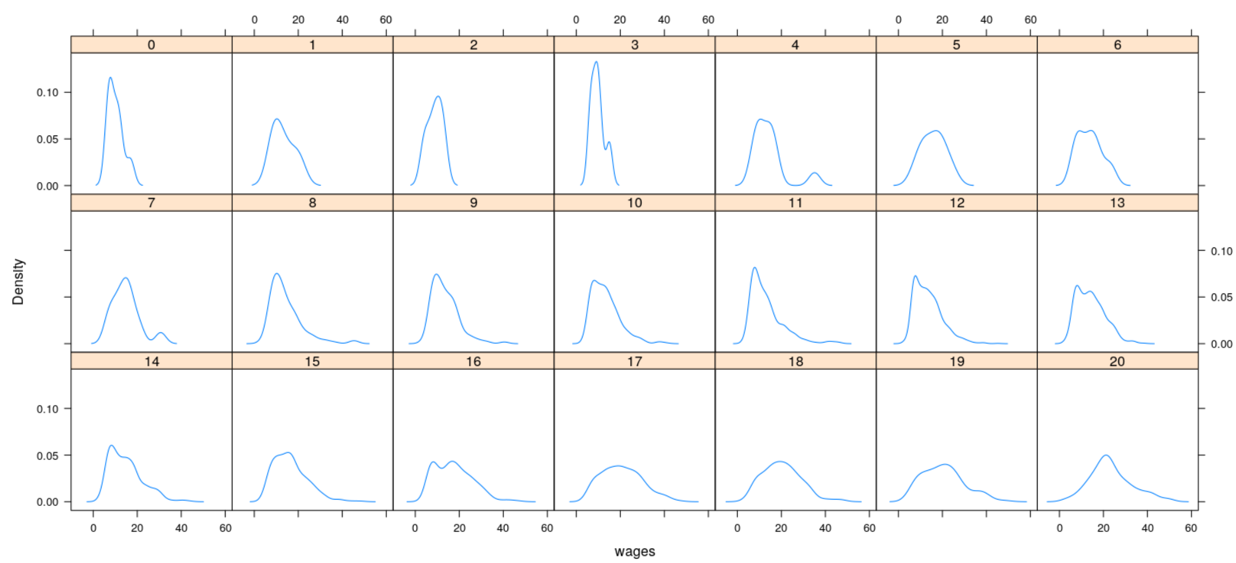


Distribution of wages (conditional on education)

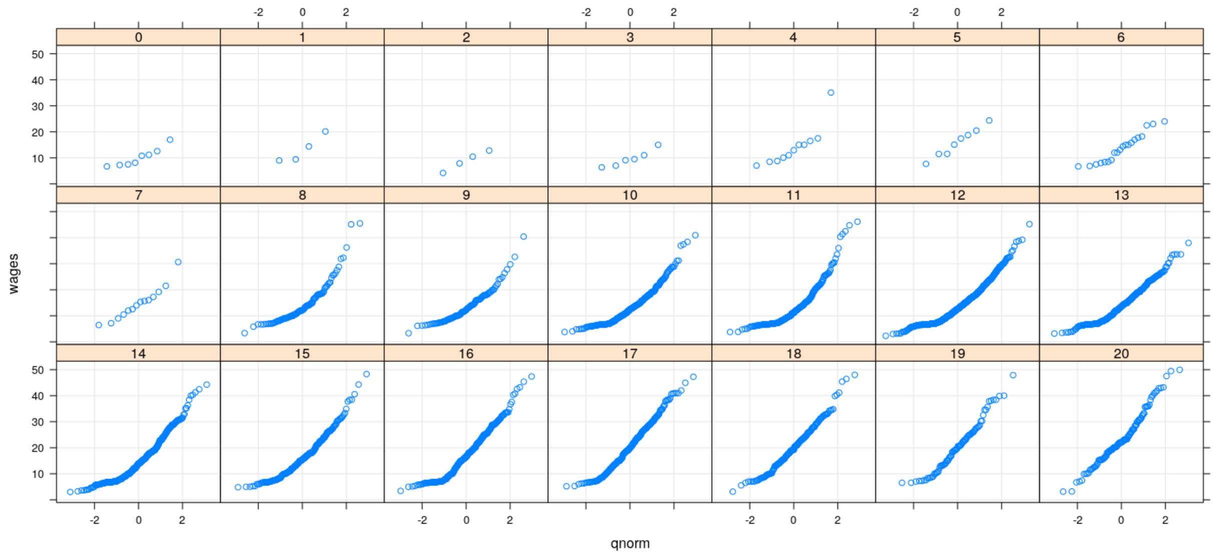
```
histogram( ~ wages | factor(education), data = SLID)
```




```
densityplot( ~ wages | factor(education), data = SLID, plot.points = FALSE)
```

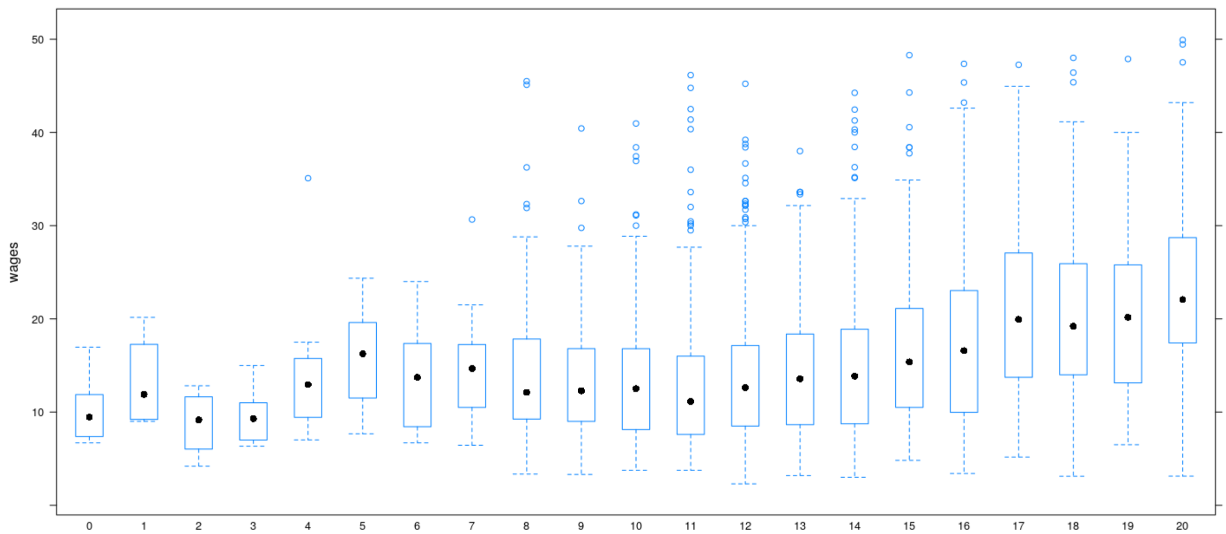



```
qqmath( ~ wages | factor(education), data = SLID, grid = TRUE)
```

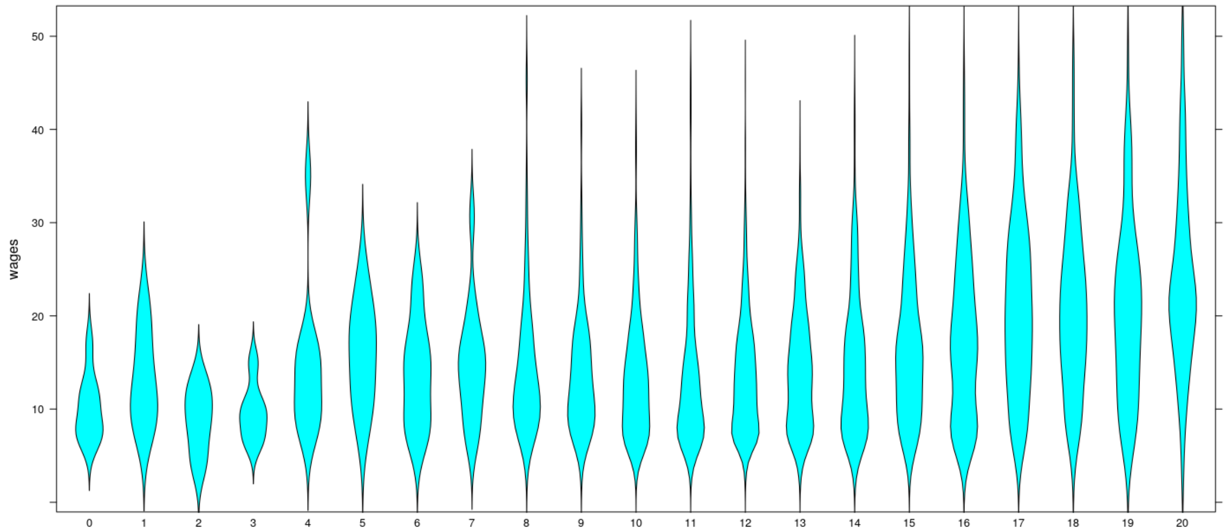


More direct comparison

```
bwplot(wages ~ factor(education), data = SLID)
```




```
bwplot(wages ~ factor(education), data = SLID, panel = panel.violin)
```



Pure error model

- Corresponding linear model is called the pure error model (assuming equal variance)

```
fm.linear <- lm(wages ~ education, data = SLID) # for comparison
fm.pe <- lm(wages ~ factor(education), data = SLID)
summary(fm.linear)
```

```

Call:
lm(formula = wages ~ education, data = SLID)

Residuals:
    Min      1Q  Median      3Q     Max 
-17.649  -5.796  -1.005   4.133  34.139 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   5.0829     0.5304   9.584   <2e-16 ***
education     0.7848     0.0388  20.226   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.5 on 4012 degrees of freedom
  (3411 observations deleted due to missingness)
Multiple R-squared:  0.09253,   Adjusted R-squared:  0.09231 
F-statistic: 409.1 on 1 and 4012 DF,  p-value: < 2.2e-16
```

```
summary(fm.pe)
```

```

Call:
lm(formula = wages ~ factor(education), data = SLID)

Residuals:
```

```
    Min      1Q  Median      3Q     Max
-20.393  -5.670  -1.067   4.060  32.834

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)          10.1375     2.6133   3.879 0.000107 ***
factor(education)1    3.1000     4.5264   0.685 0.493470
factor(education)2   -1.3025     4.5264  -0.288 0.773551
factor(education)3   -0.4808     3.9920  -0.120 0.904132
factor(education)4    4.1743     3.4346   1.215 0.224297
factor(education)5    5.7100     3.6958   1.545 0.122429
factor(education)6    3.5995     3.0922   1.164 0.244463
factor(education)7    4.6654     3.2760   1.424 0.154496
factor(education)8    4.2245     2.7043   1.562 0.118327
factor(education)9    3.4266     2.7059   1.266 0.205455
factor(education)10   3.2118     2.6446   1.214 0.224633
factor(education)11   3.1782     2.6529   1.198 0.230994
factor(education)12   3.5089     2.6248   1.337 0.181355
factor(education)13   4.0991     2.6375   1.554 0.120223
factor(education)14   4.7441     2.6335   1.801 0.071714 .
factor(education)15   6.3196     2.6499   2.385 0.017133 *
factor(education)16   7.3000     2.6438   2.761 0.005786 **
factor(education)17  10.5326     2.6545   3.968 7.38e-05 ***
factor(education)18  10.1605     2.6714   3.803 0.000145 ***
factor(education)19  10.3711     2.7322   3.796 0.000149 ***
factor(education)20  13.3853     2.6970   4.963 7.23e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.392 on 3993 degrees of freedom
  (3411 observations deleted due to missingness)
Multiple R-squared:  0.1227,    Adjusted R-squared:  0.1183
F-statistic: 27.93 on 20 and 3993 DF,  p-value: < 2.2e-16
```

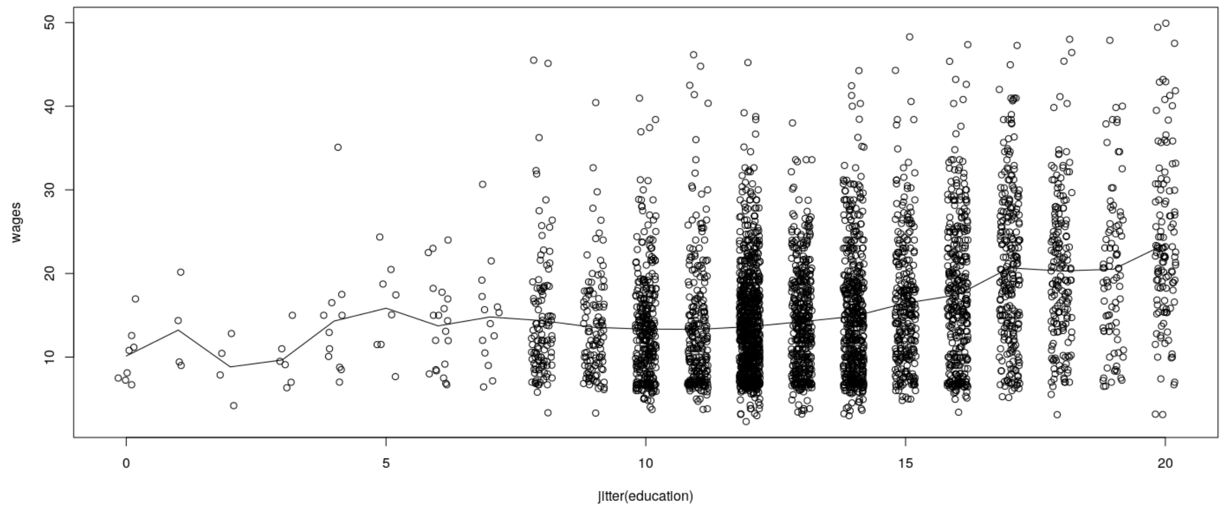
```r
anova(fm.pe)
```

```
Analysis of Variance Table

Response: wages
                    Df Sum Sq Mean Sq F value    Pr(>F)
factor(education)   20  30522 1526.08  27.931 < 2.2e-16 ***
Residuals         3993 218164   54.64
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
anova(fm.linear, fm.pe)
```

```
Analysis of Variance Table

Model 1: wages ~ education
Model 2: wages ~ factor(education)
  Res.Df    RSS Df Sum of Sq      F    Pr(>F)
1   4012 225674
2   3993 218164 19    7510.3 7.2347 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
plot(wages ~ jitter(education), data = SLID)
lines(0:20, predict(fm.pe, newdata = data.frame(education = 0:20)))
```



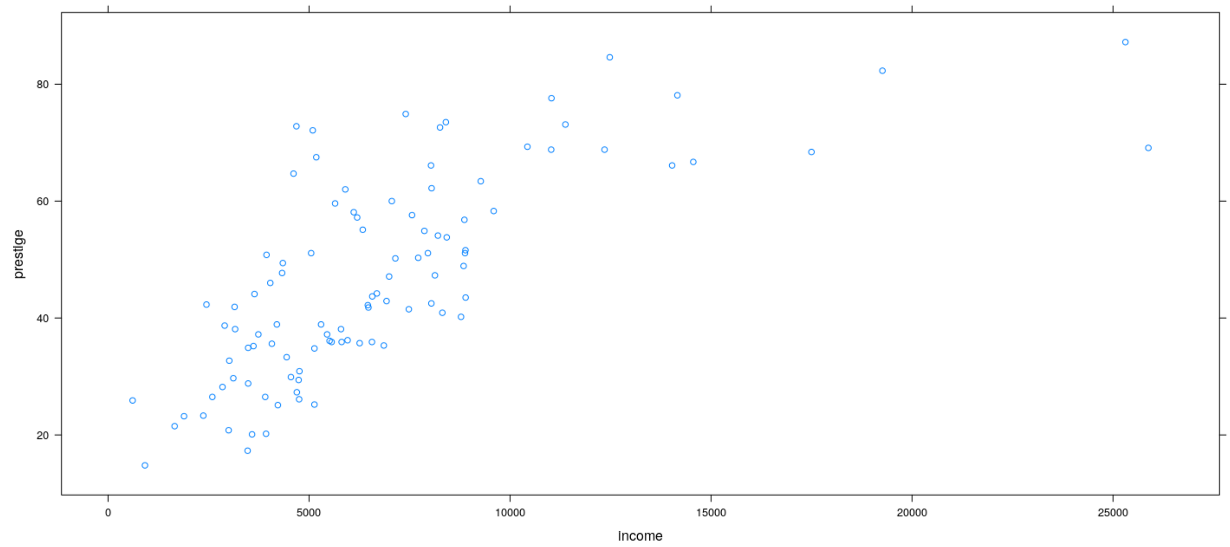
- Such comparison possible when lots of data, few unique covariate values
- Can be used to assess "non-linearity"
- But need graphical tools to assess
  - Skewness
  - Multiple modes
  - "Heavy" tails
  - Unequal variance / spread
- But what can we do when covariate x is continuous?
  - `weight ~ height`
  - `prestige ~ income`

Continuous predictor

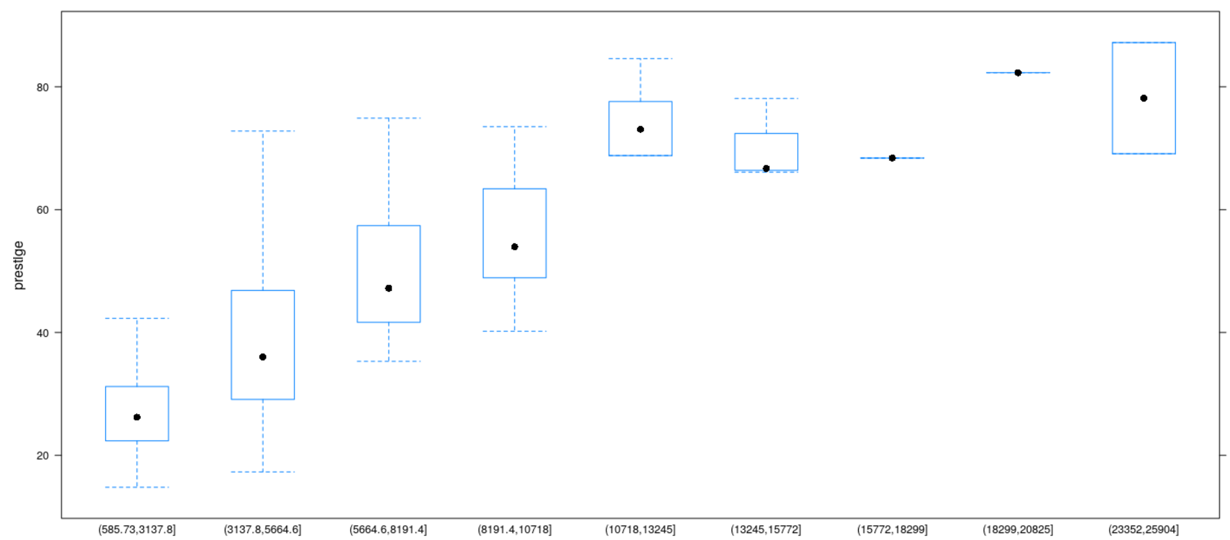
- Even with large datasets, replicated x will be rare
- We can still divide range of x into several bins
- Width of bin represents trade-off (for non-linear relationship)
  - How "locally" we can estimate (bias of estimator)
  - Number of data points (variance of estimator)

Example: Prestige data

```r
data(Prestige, package = "carData")
xyplot(prestige ~ income, data = Prestige)
```

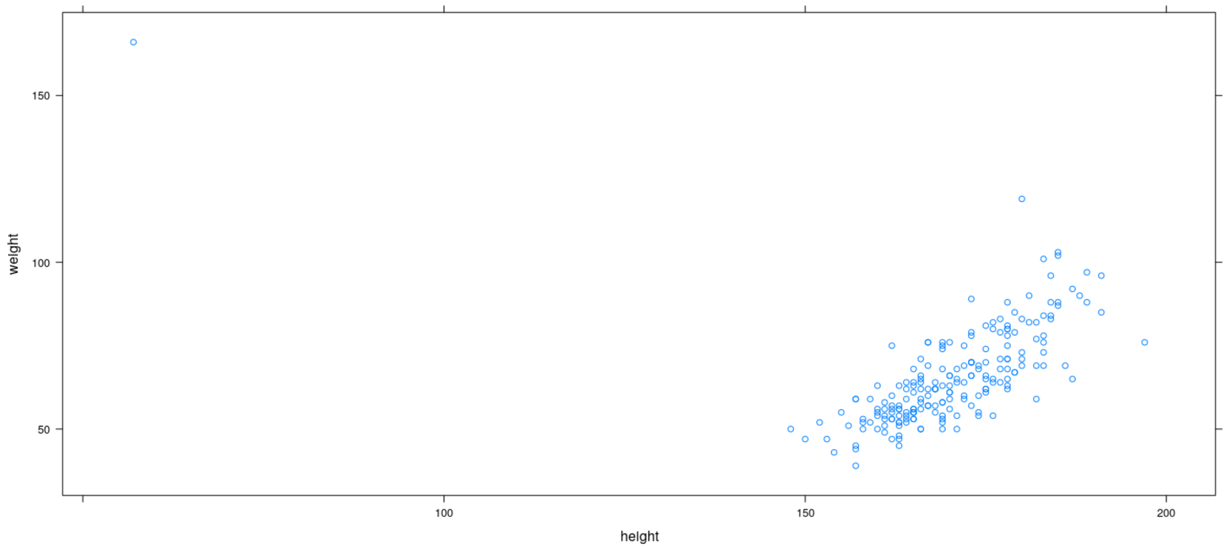



```
bwplot(prestige ~ cut(income, 10, dig.lab = 5), data = Prestige)
```

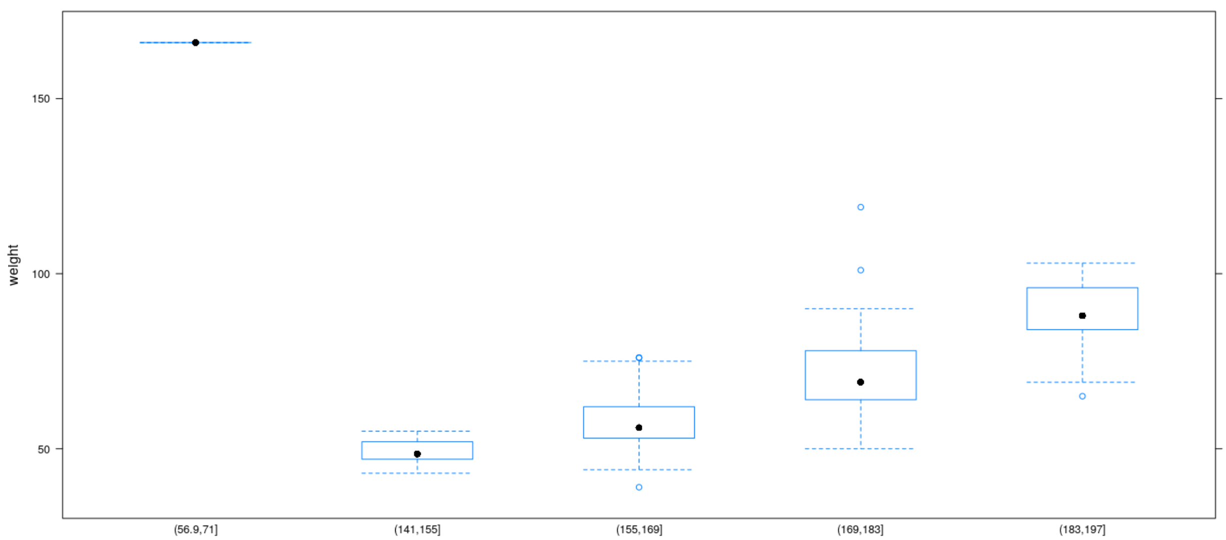


Example: Davis data

```
data(Davis, package = "carData")
xyplot(weight ~ height, Davis)
```

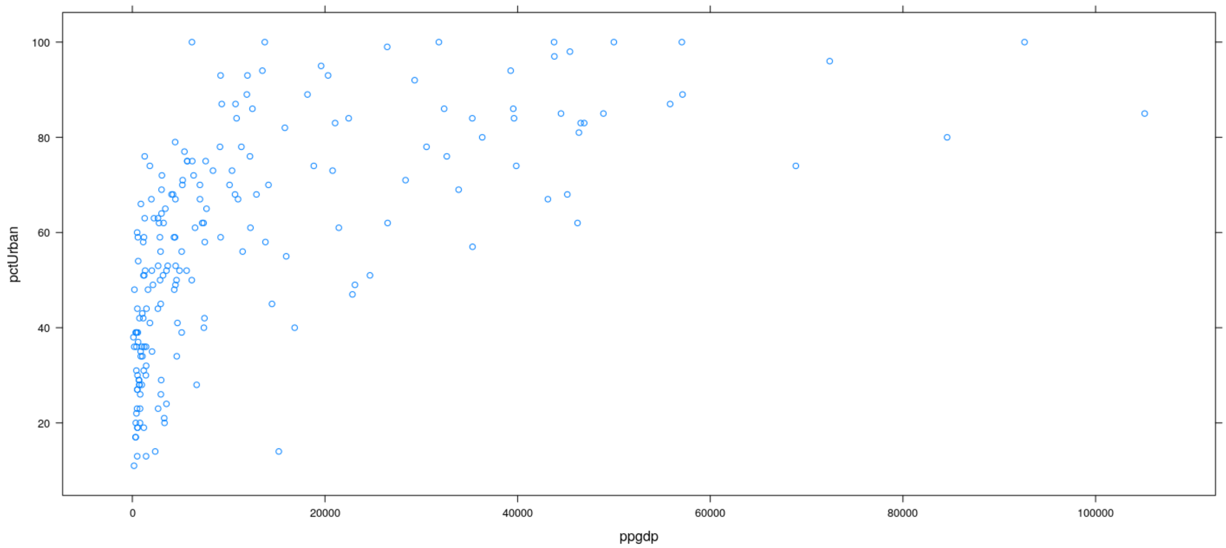



```r
bwplot(weight ~ cut(height, 10), Davis)
```

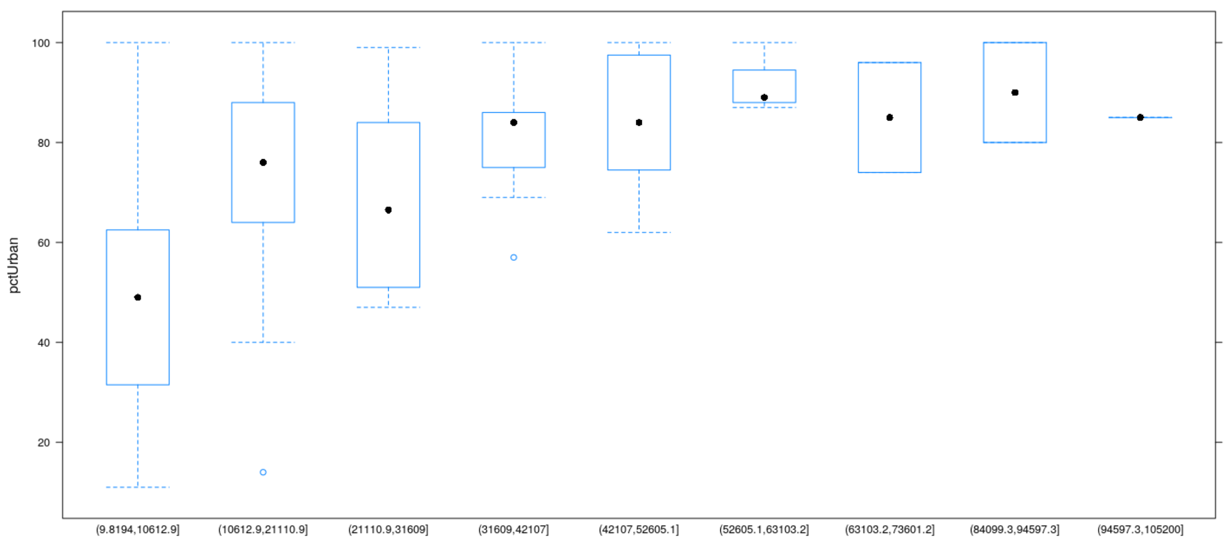


Example: UN data

```r
data(UN, package = "carData")
xyplot(pctUrban ~ ppgdp, UN)
```



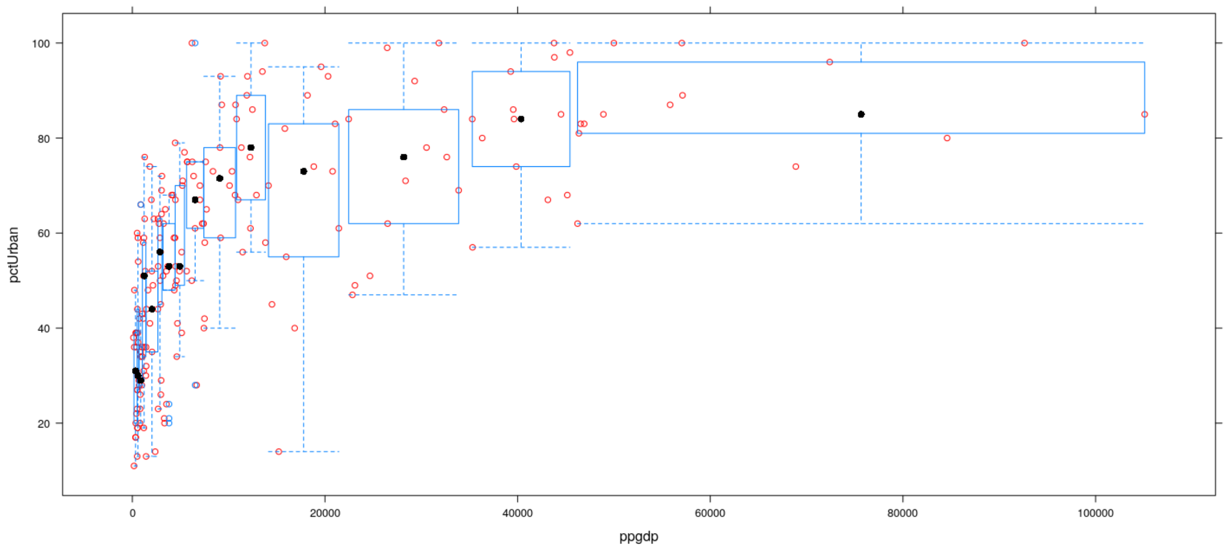

```
bwplot(pctUrban ~ cut(ppgdp, 10, dig.lab = 6), UN)
```



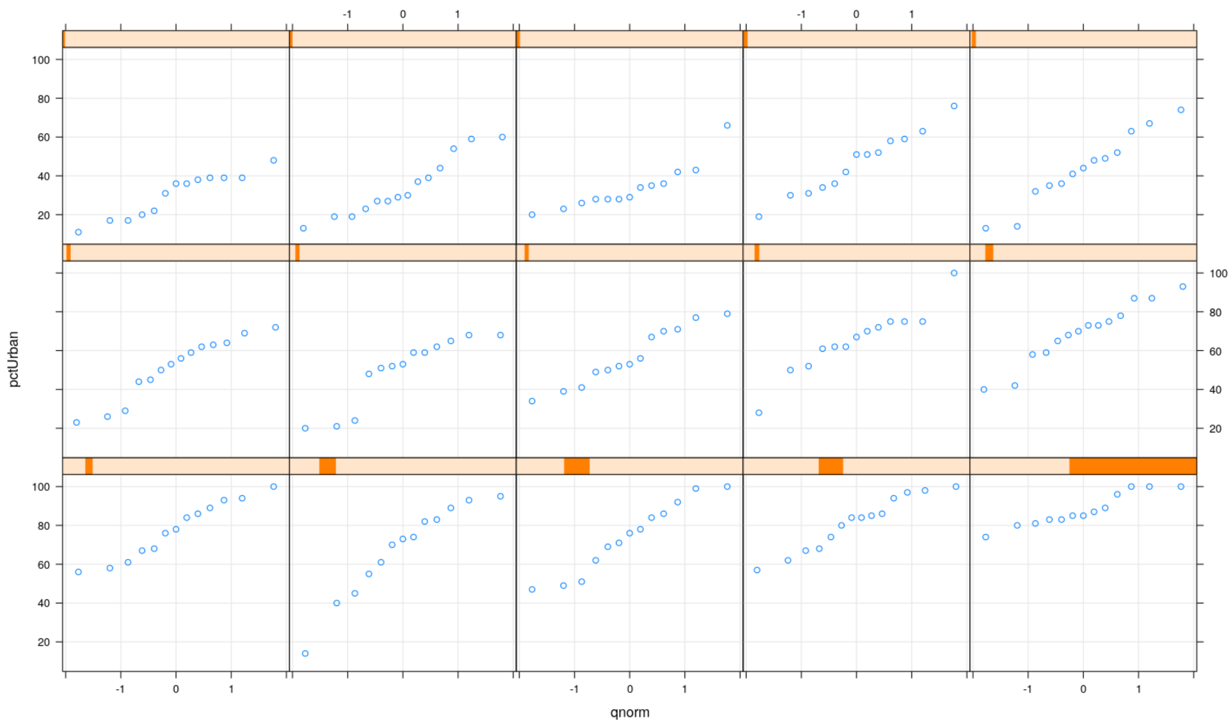
Choice of bin width - constant vs variable

- Constant bin width means some bins could have very few data, or even be empty
- Generally better to define bins with fixed number of data points
  - Decide number of bins
  - Bin boundaries are defined by quantiles

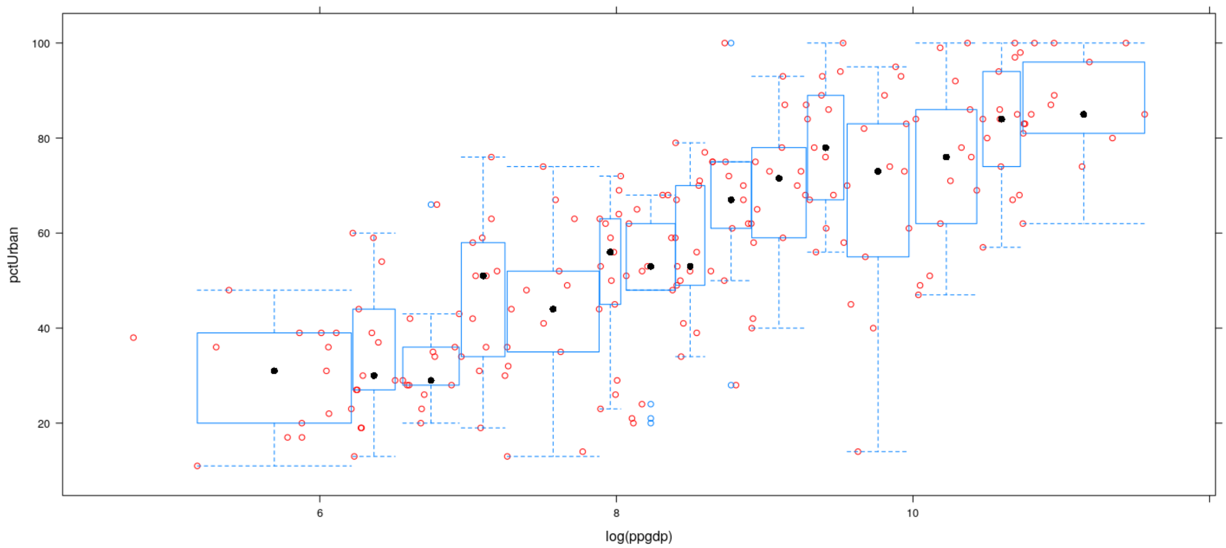
Example: UN data — box and whisker plots



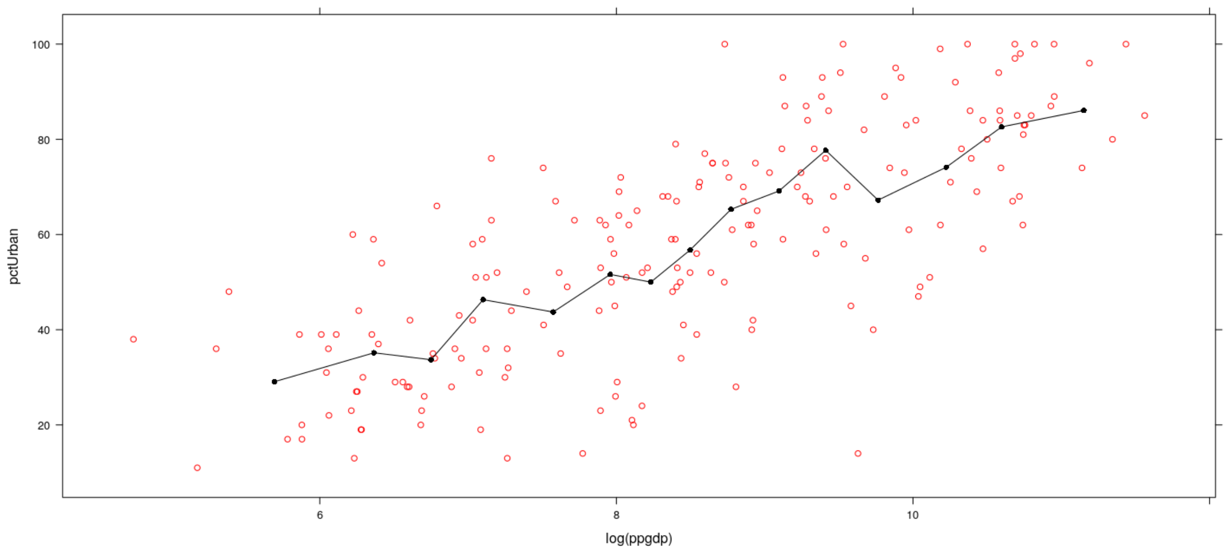
Example: UN data — Q-Q plots



Example: UN data — log-transformed GDP



Assessing linearity



- Can summarize distribution in each bin my mean or median (and possibly standard deviation to assess non-constant variance)

Estimating conditional mean: a local binning approach

- Model: $Y_i = f(x_i) + \varepsilon_i$
- Interested in estimating $f(x) = E(Y|x)$ for various x

- Approach: Estimate $f(x)$ locally by fitting mean or linear regression within bin
- Window size represents trade-off
  - Larger window means more data points
  - More data points means lower variance
  - But larger window means larger bias
- Specifically, estimate is biased if f is non-linear, or if x is not uniformly distributed

Bias-variance trade-off — large data

- Any reasonable method should at least be *consistent*
- In other words, if we want to estimate $E(Y|x)$, we should have

$$\hat{E}_n(Y|x) \to E(Y|x) \text{ as } n \to \infty$$

- Suppose for sample size n, we define $\sqrt{n}$ bins, each containing $\sqrt{n}$ points.
- Clearly, as $n \to \infty$,
  - number of bins $\to \infty$
  - width of each bin $\to 0$ (with some assumptions about x)
  - number of data points in each bin $\to \infty$

If $f(x) = E(Y|x)$ is "smooth", then for x_i in the same bin as x_0,

$$f(x_i) = f(x_0) + f'(x_0)(x_i - x_0) + h(x_i)(x_i - x_0)$$

where $h(\cdot)$ is such that $\lim_{x \to x_0} h(x) = 0$ (Taylor's Theorem)

$Y_i = f(x_i) + \varepsilon_i$, so for x_i in the same bin as x_0,

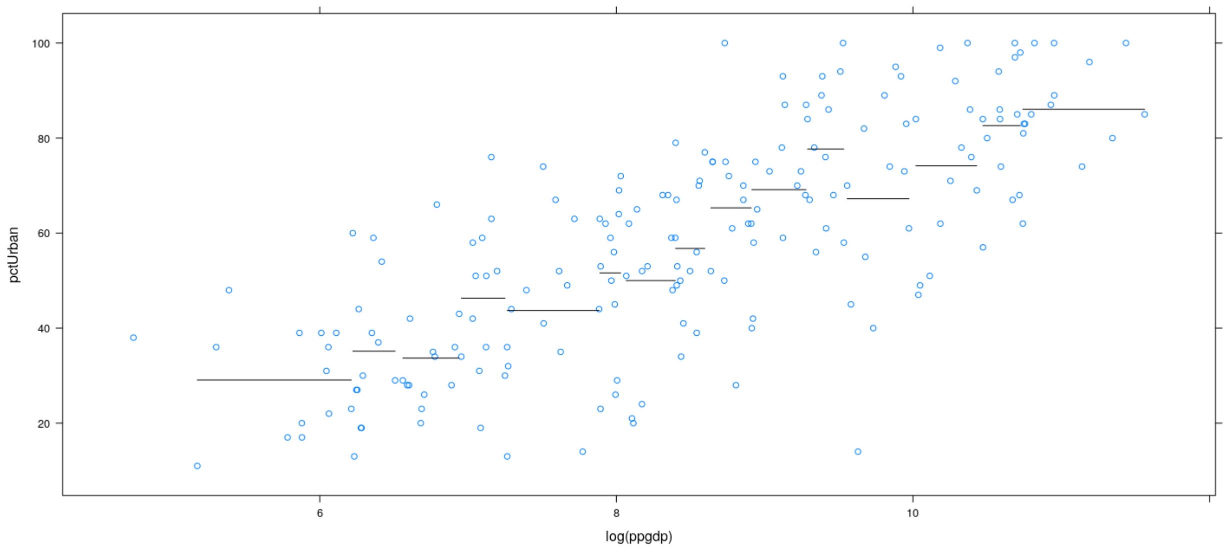
$$Y_i = f(x_0) + f'(x_0)(x_i - x_0) + h(x_i)(x_i - x_0) + \varepsilon_i$$

and so

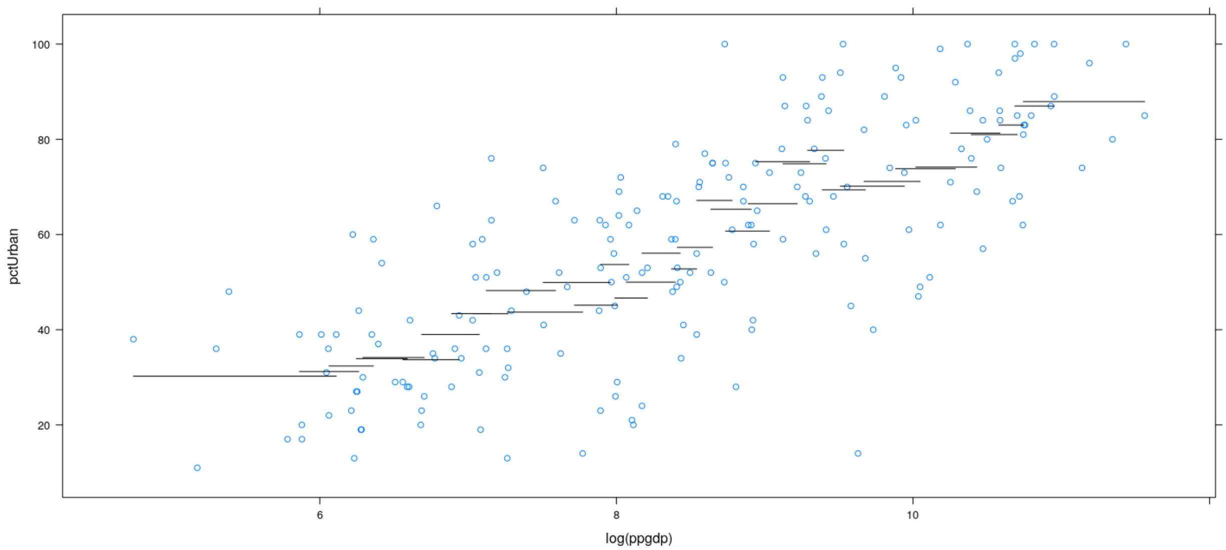
$$\bar{Y}(x_0) = f(x_0) + f'(x_0)(\bar{x} - x_0) + \bar{\varepsilon} + \frac{1}{n} \sum_i h(x_i)(x_i - x_0)$$

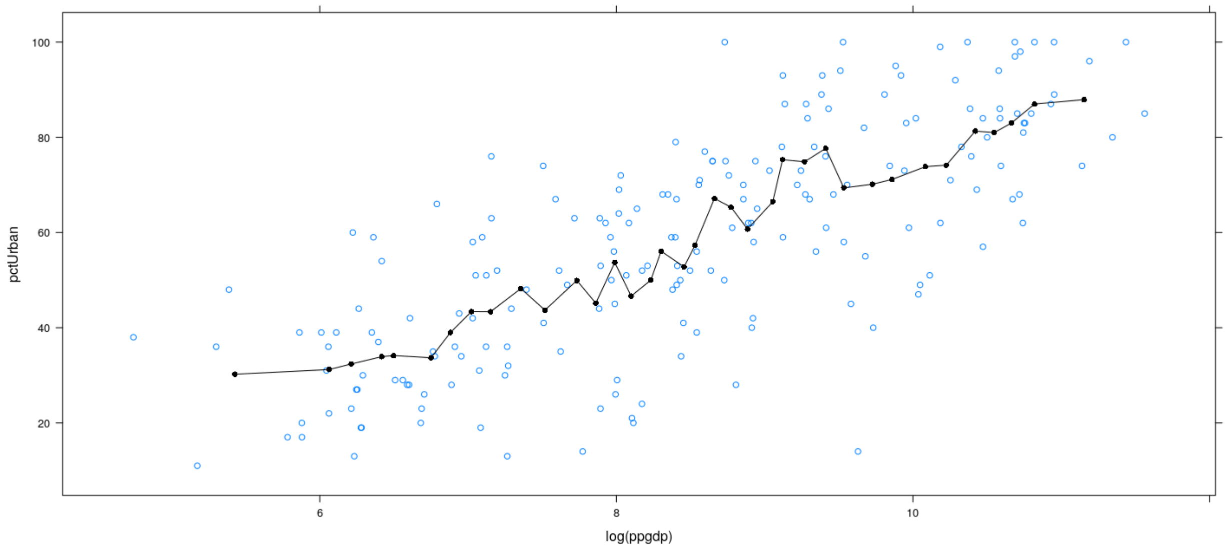
As $n \to \infty$, $x_i, \bar{x} \to x_0$, so $\bar{Y}(x_0) \to f(x_0)$

Example: UN data

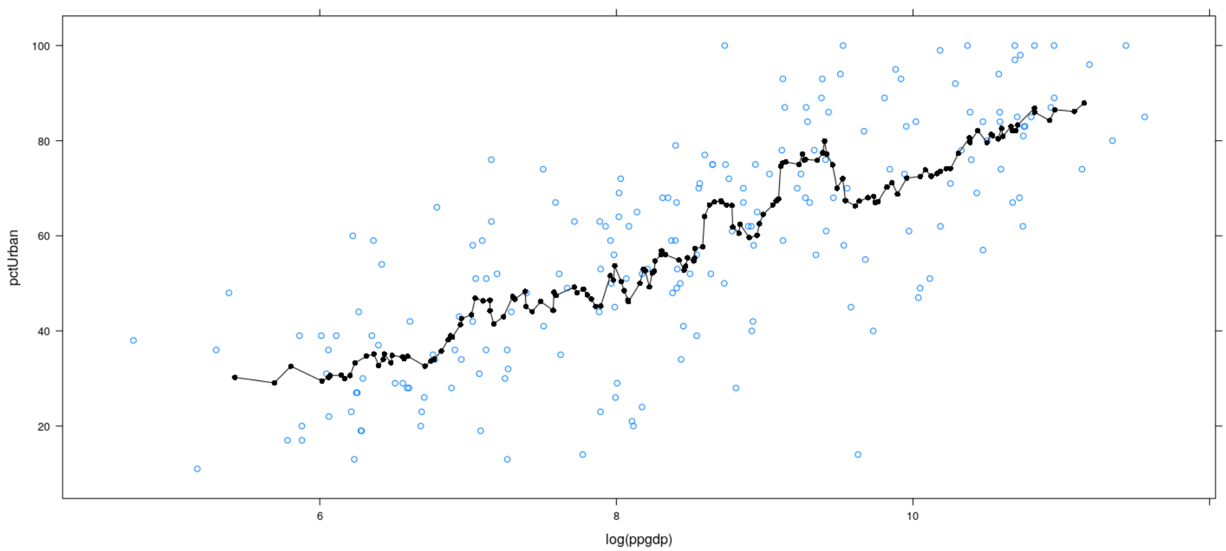


Example: UN data – overlapping bins

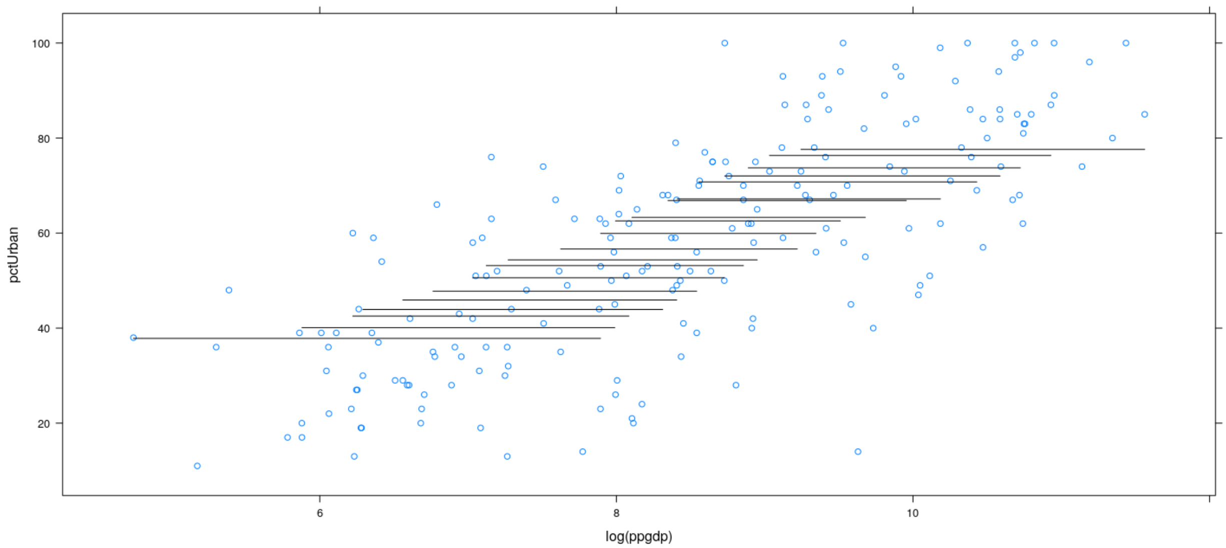


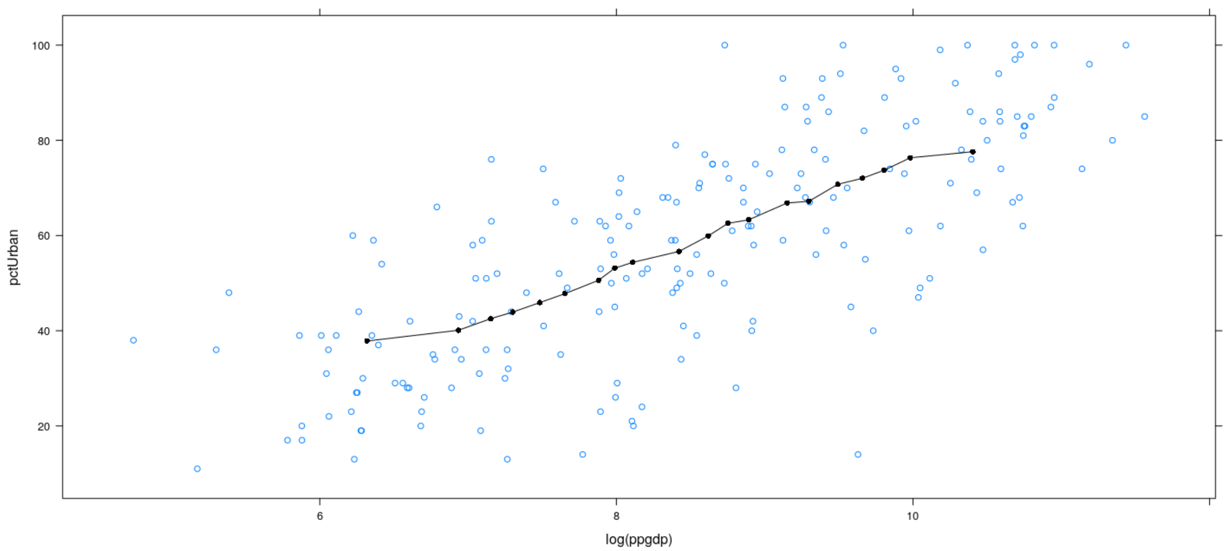


Example: UN data – more bins



Example: UN data – wider bins





Locally linear regression

- Instead of $\bar{Y}$, we could fit a linear regression model in each bin

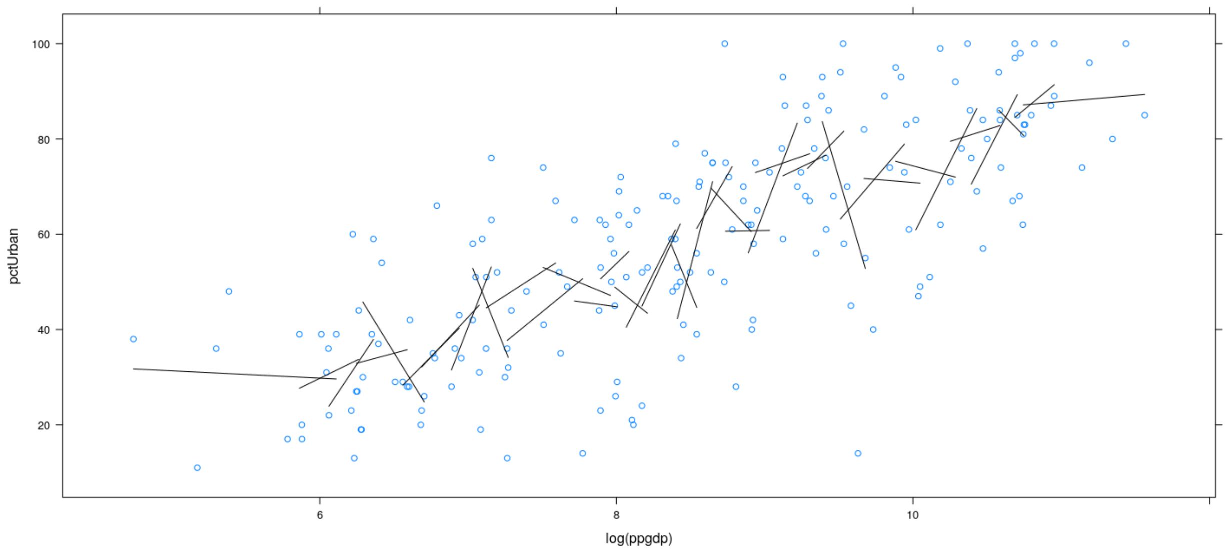
$$\hat{Y}(x_0) = \hat{\alpha}$$

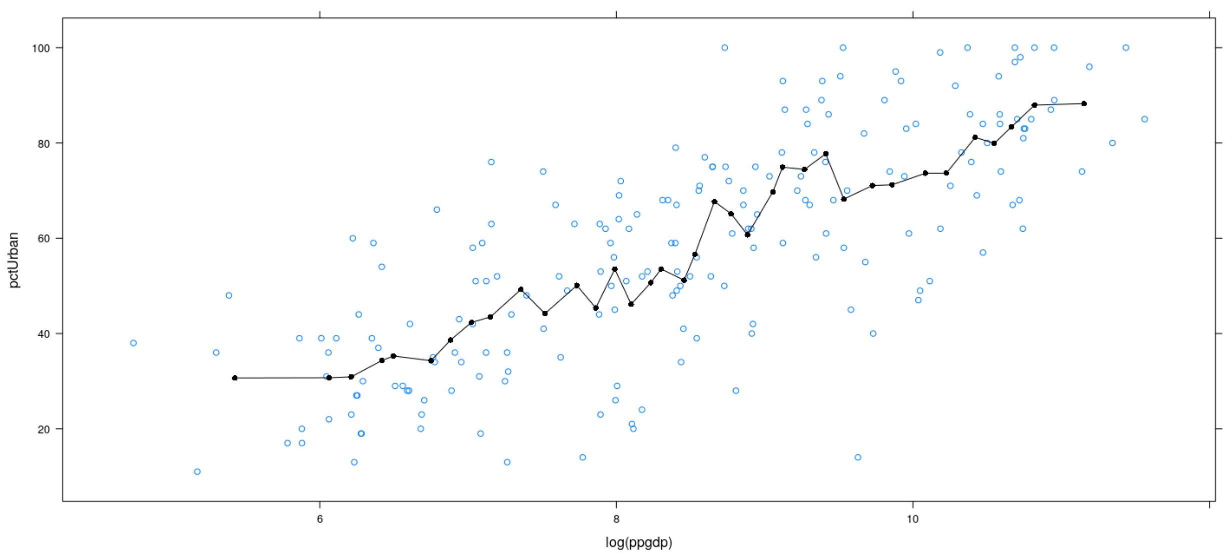
where $\hat{\alpha}$ and $\hat{\beta}$ are estimated by fitting the linear regression model (for all x_i in the same bin as x_0)

$$Y_i = \alpha + \beta(x_i - x_0) + \varepsilon_i$$

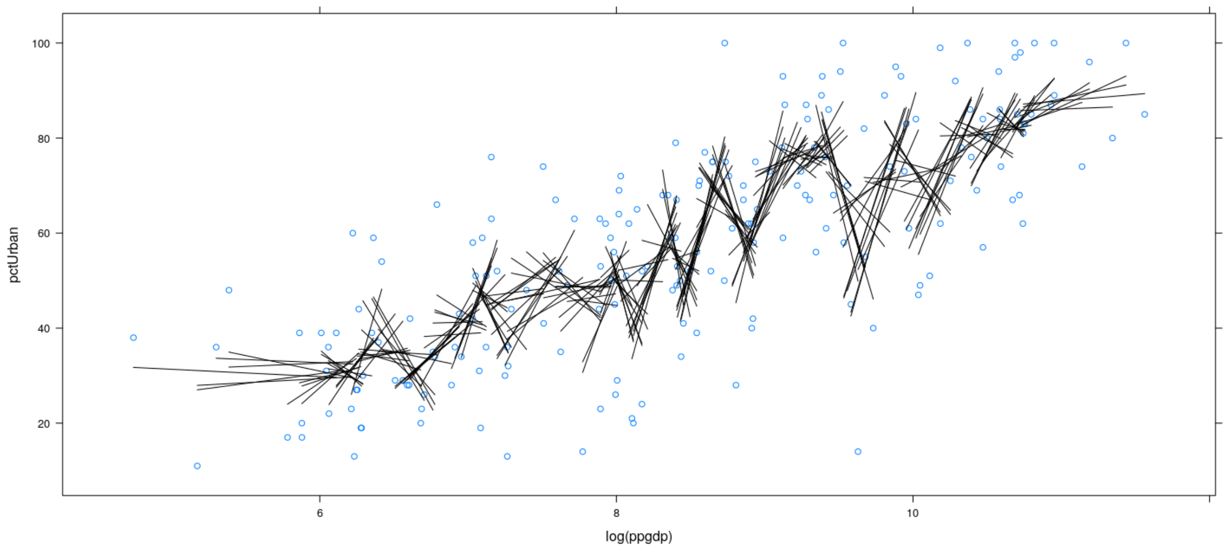
- In general, the model could be a d-th *"degree"* polynomial
  - $d = 0$: local mean
  - $d = 1$: locally linear fit
  - $d = 2$: locally quadratic fit
- Tuning parameter *"span"* : proportion of full data in each bin

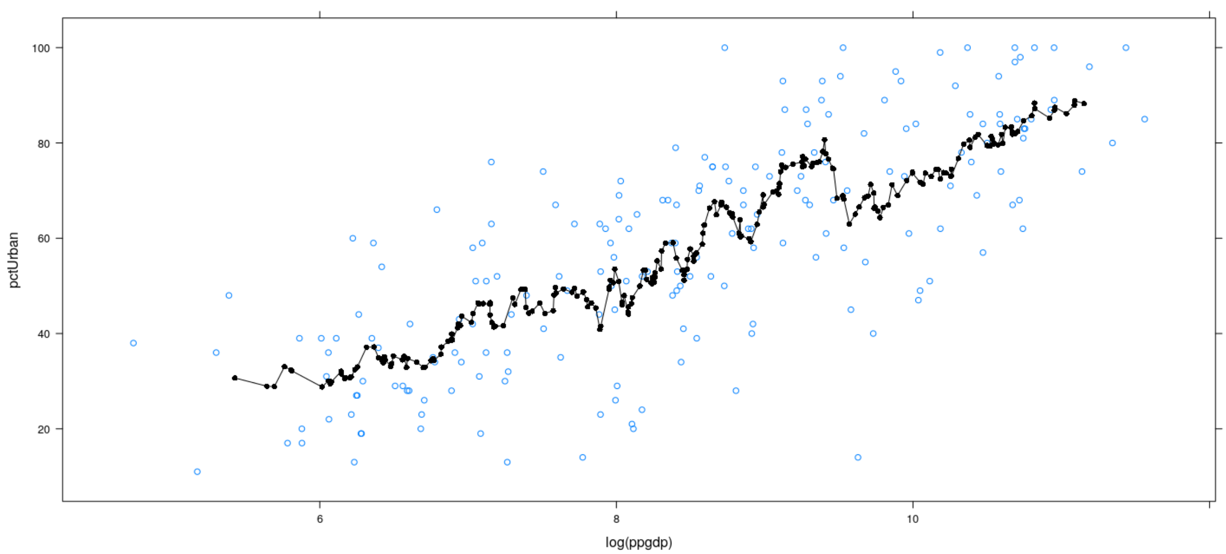
Example: UN data – locally linear



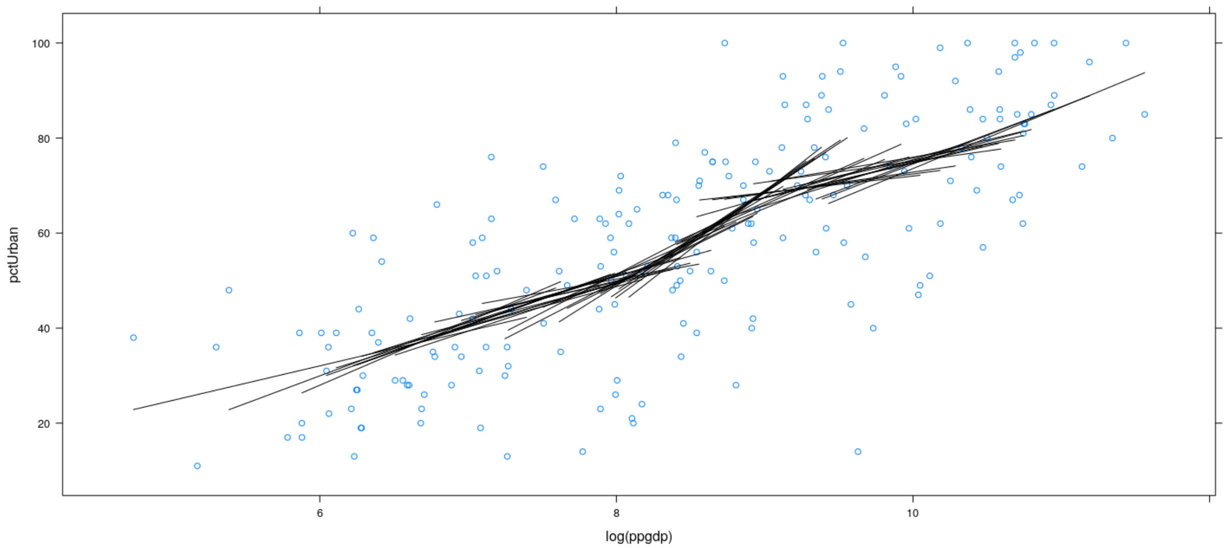


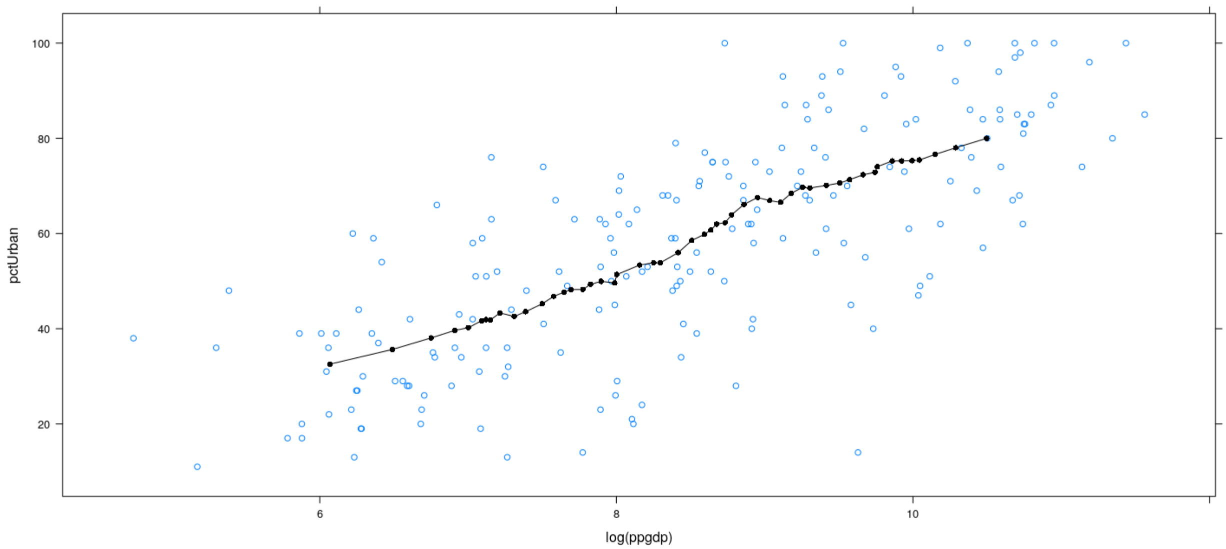
Example: UN data – locally linear with more bins





Example: UN data – locally linear with wider bins





Adding weights

- Larger span gives
  - Wider bins
  - Smoother estimate of $f(x) = E(Y|x)$
  - But more data points per bin (less "local")
- One solution is to add *weights* (give more weightage to x_i near x_0)
- Weighted mean: $\hat{Y} = \frac{\sum w_i Y_i}{\sum w_i}$

- Weighted regression: Normal equations are given by

$$\mathbf{X}^T\mathbf{W}\mathbf{X}\widehat{\beta} = \mathbf{X}^T\mathbf{W}\mathbf{y}$$

  where $\mathbf{W}^{-1}$ is a diagonal matrix of inverse weights $1/w_i^2$ (higher weight means less uncertainty).

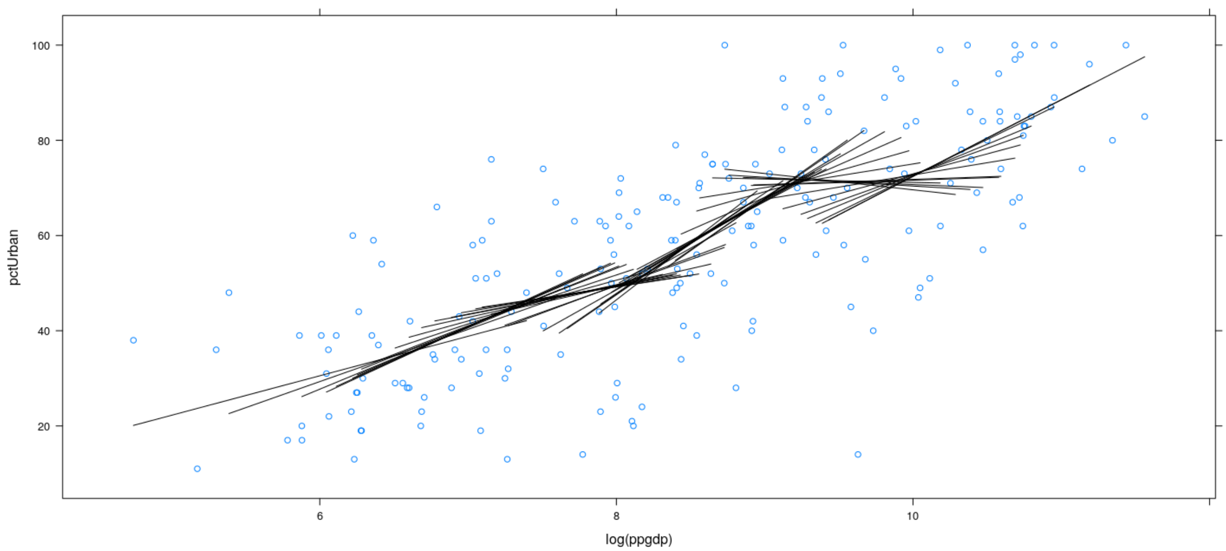
- For example,

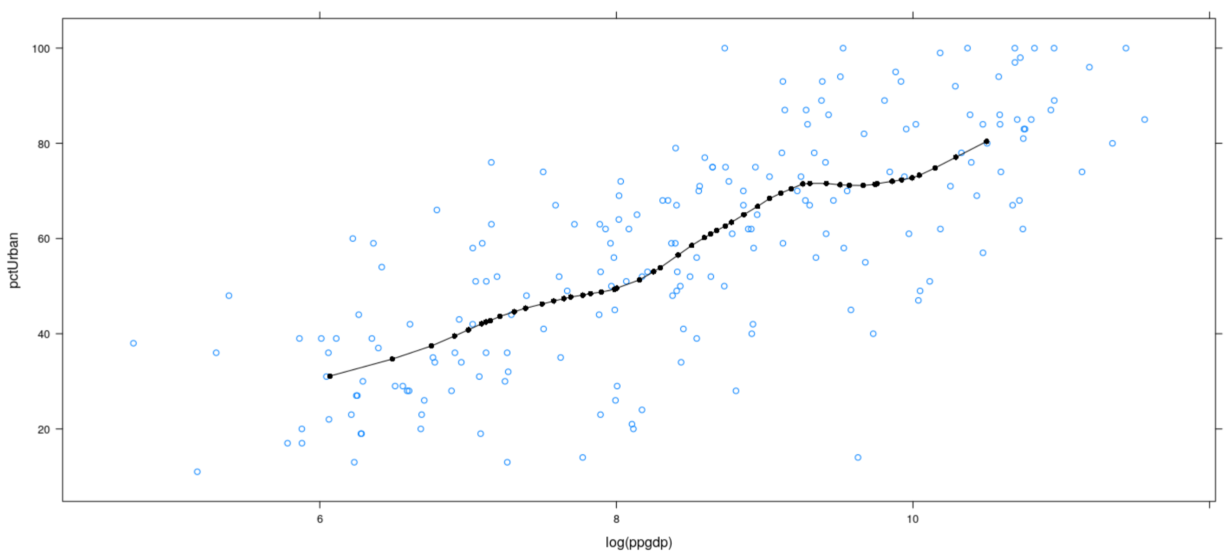
$$w_i = k((x_i - x_0)/h),$$

  where

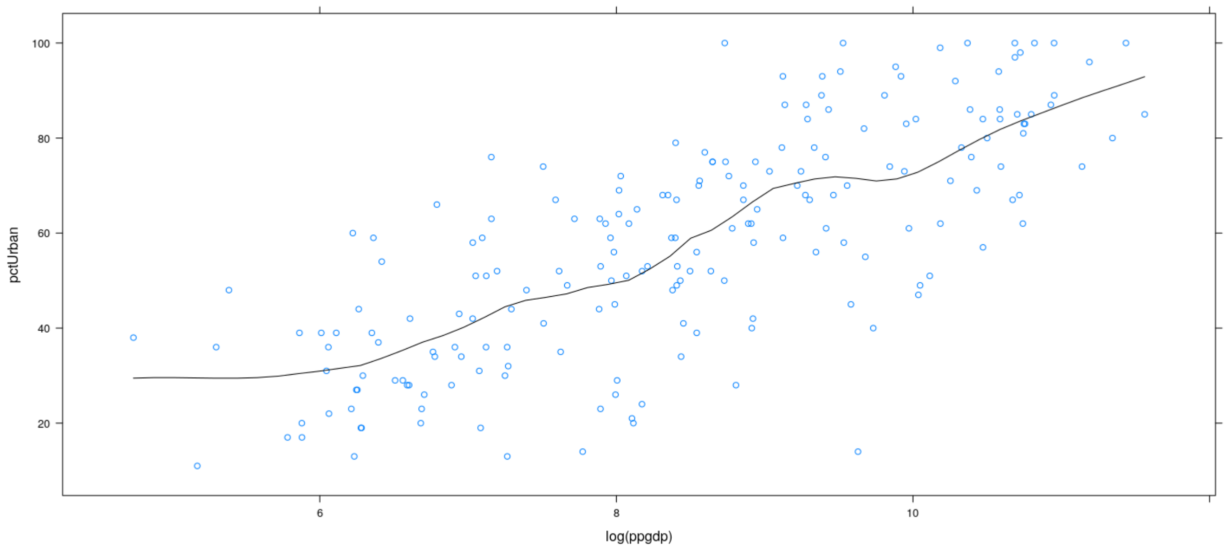
  - $2h$ is the bin width
  - $k(\cdot)$ is a symmetric weight function that is highest at 0 and decreases (usually to 0 at $\pm h$)

Example: UN data – locally weighted linear regression





Example: UN data – LOWESS



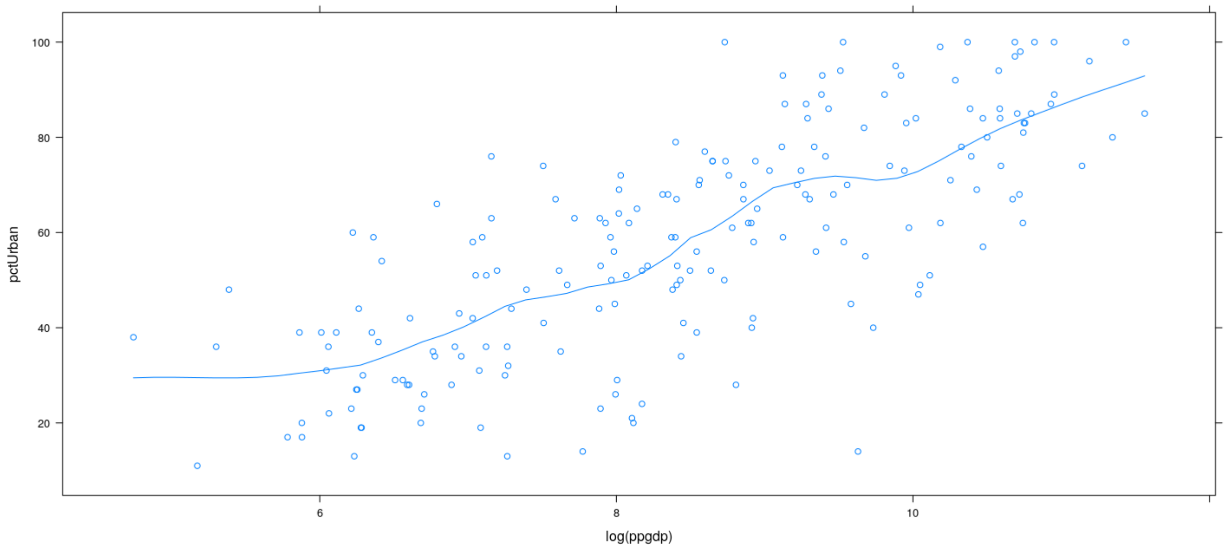

```
xyplot(pctUrban ~ log(ppgdp), data = UN, col.line = "black",
       type = c("p", "smooth"), span = 0.27, degree = 1, family = "gaussian")
```

LOWESS

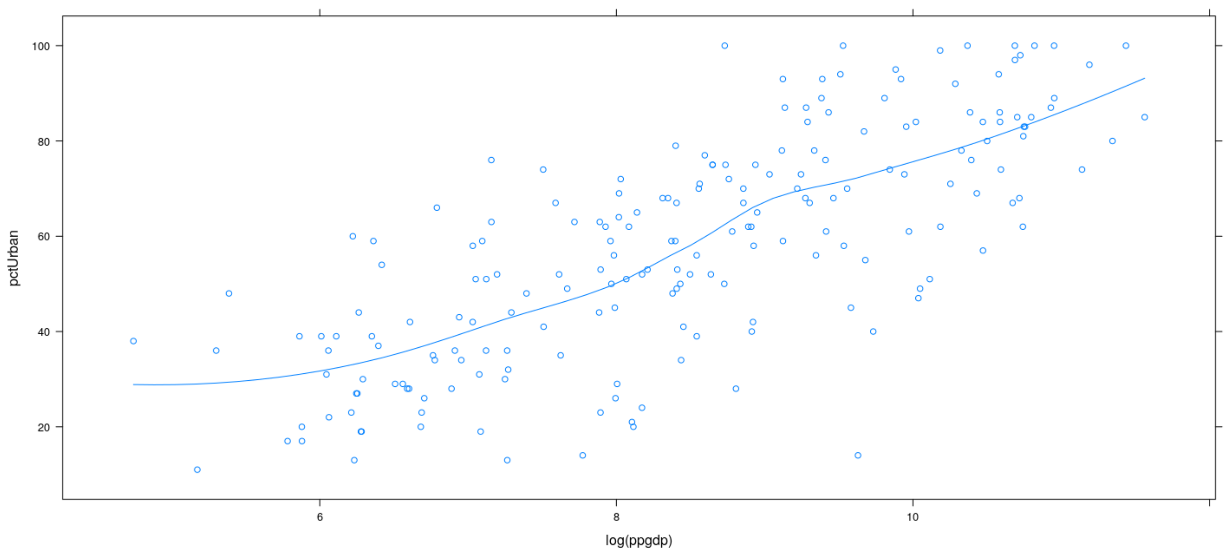
- Stands for "LOcally WEighted Scatterplot Smoother"
- Can be viewed as k nearest neighbour weighted local polynomial regression
- Main control parameters are `span` and `degree`
- Optionally provides estimates of standard error
- By default also provides "robust" estimates

Example: UN data – LOWESS

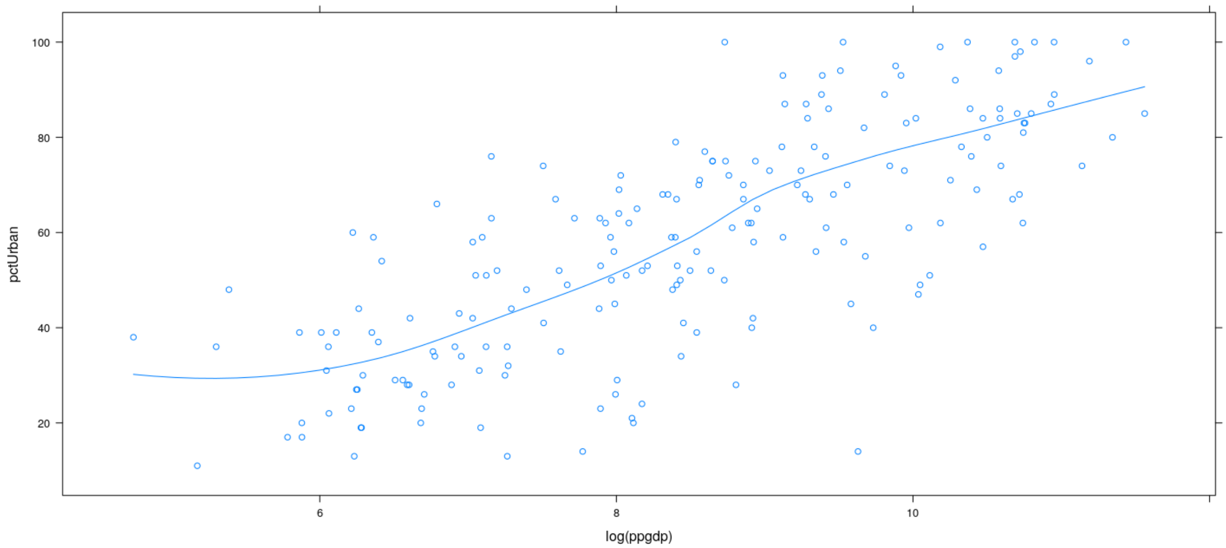
```
xyplot(pctUrban ~ log(ppgdp), data = UN, type = c("p", "smooth"),
       span = 0.27, degree = 1, family = "gaussian")
```




```r
xyplot(pctUrban ~ log(ppgdp), data = UN, type = c("p", "smooth"),
       span = 2/3, degree = 2, family = "gaussian")
```

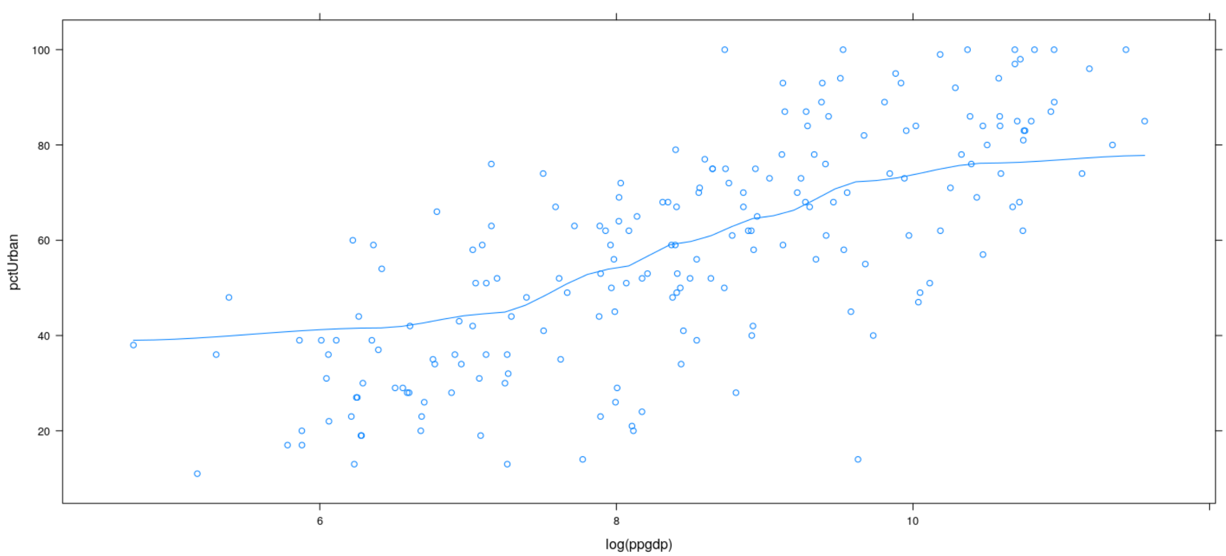



```r
xyplot(pctUrban ~ log(ppgdp), data = UN, type = c("p", "smooth"),
       span = 2/3, degree = 2, family = "symmetric")
```



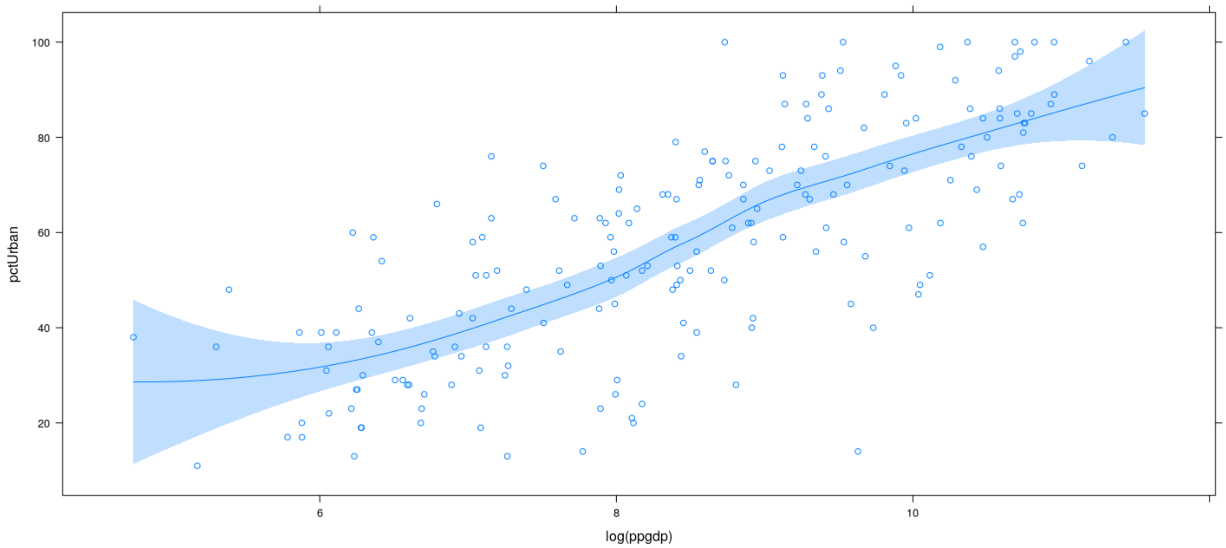
Example: UN data – LOWESS with local mean

```
xyplot(pctUrban ~ log(ppgdp), data = UN, type = c("p", "smooth"),
       span = 2/3, degree = 0, family = "symmetric")
```



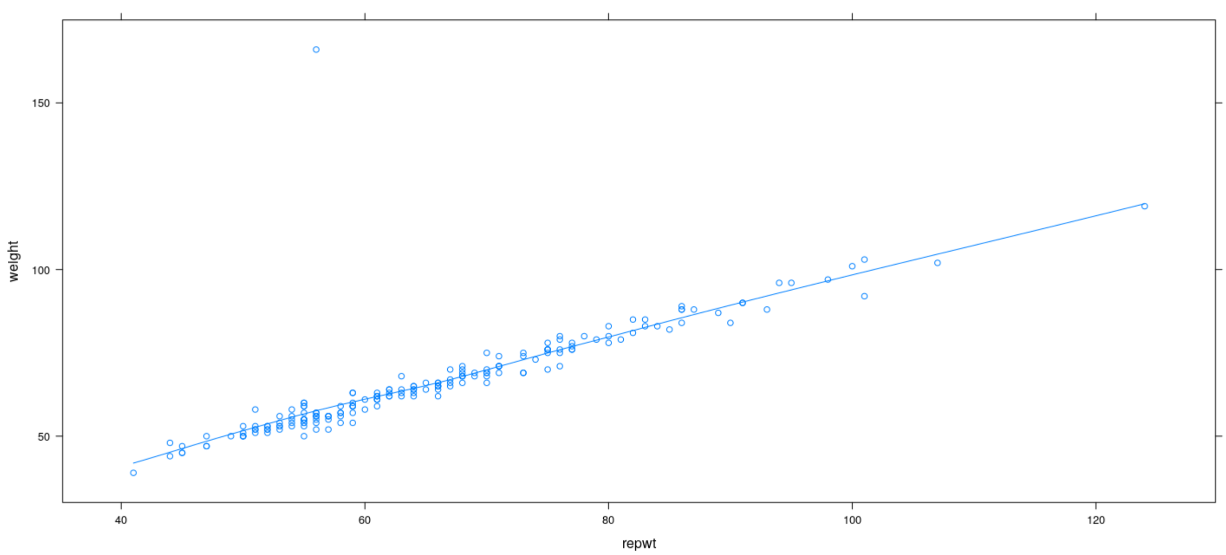
Example: UN data – LOWESS with confidence band

```
library(latticeExtra)
xyplot(pctUrban ~ log(ppgdp), data = UN) + layer(panel.smoother(x, y, method = "loess", se = TRUE))
```



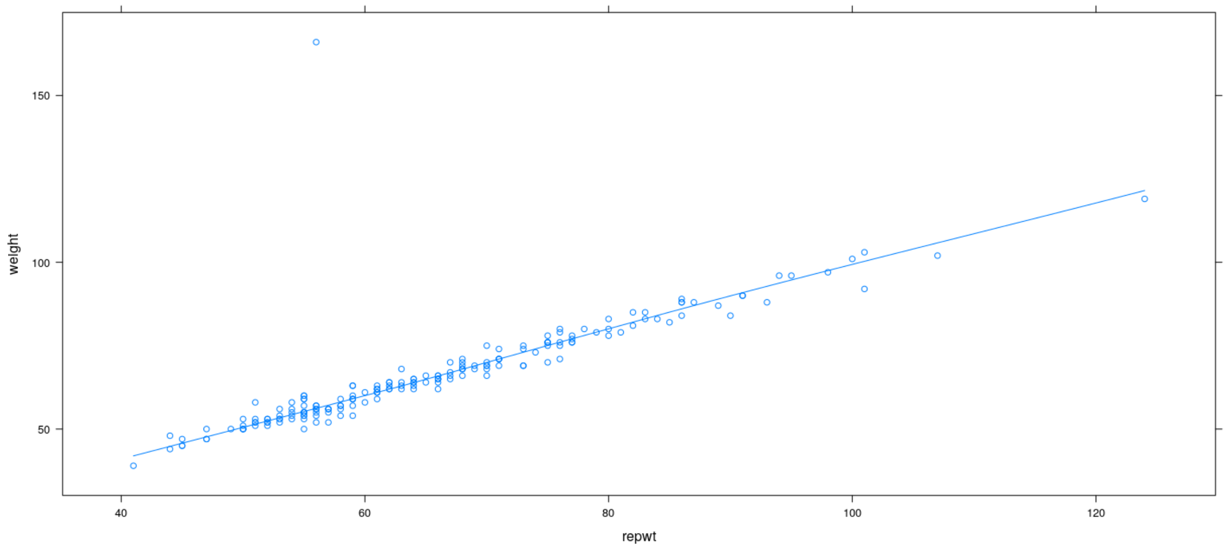
Example: Davis data – LOWESS with least squares

```
xyplot(weight ~ repwt, data = Davis, type = c("p", "smooth"), family = "gaussian") # non-robust
```



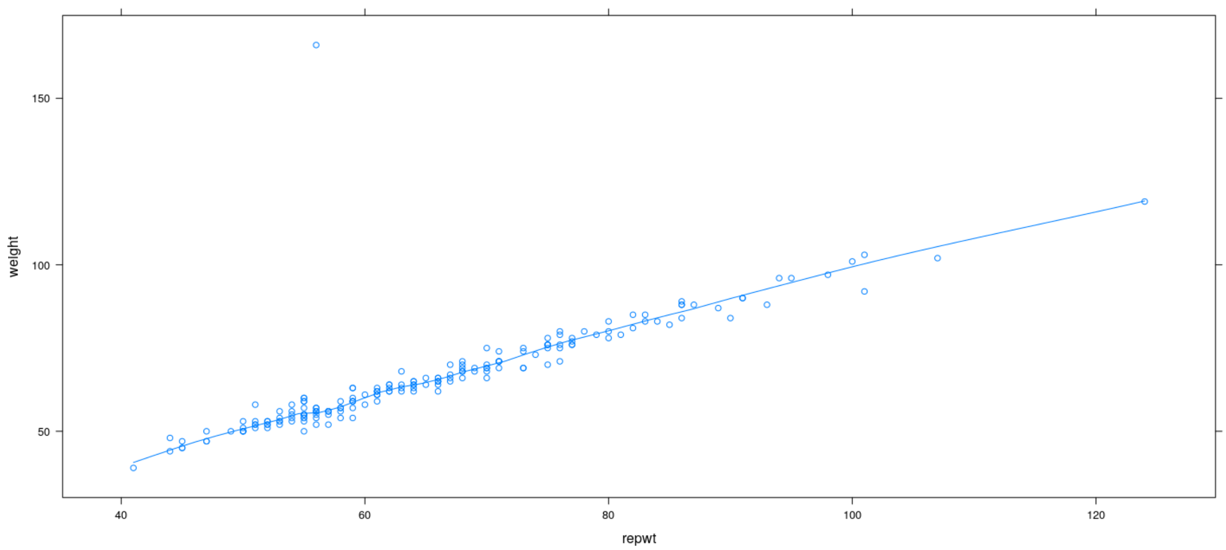
Example: Davis data – LOWESS with robust regression

```
xyplot(weight ~ repwt, data = Davis, type = c("p", "smooth"), family = "symmetric") # robust
```



Example: Davis data – effect of `span`

```
xyplot(weight ~ repwt, data = Davis, type = c("p", "smooth"), span = 1/6)
```



Choice of `span` in LOWESS

- The `span` (proportion of data in each bin) is an important tuning parameter
- How do we choose `span`?
- Generally speaking, cross-validation is often a useful strategy for choosing tuning parameters

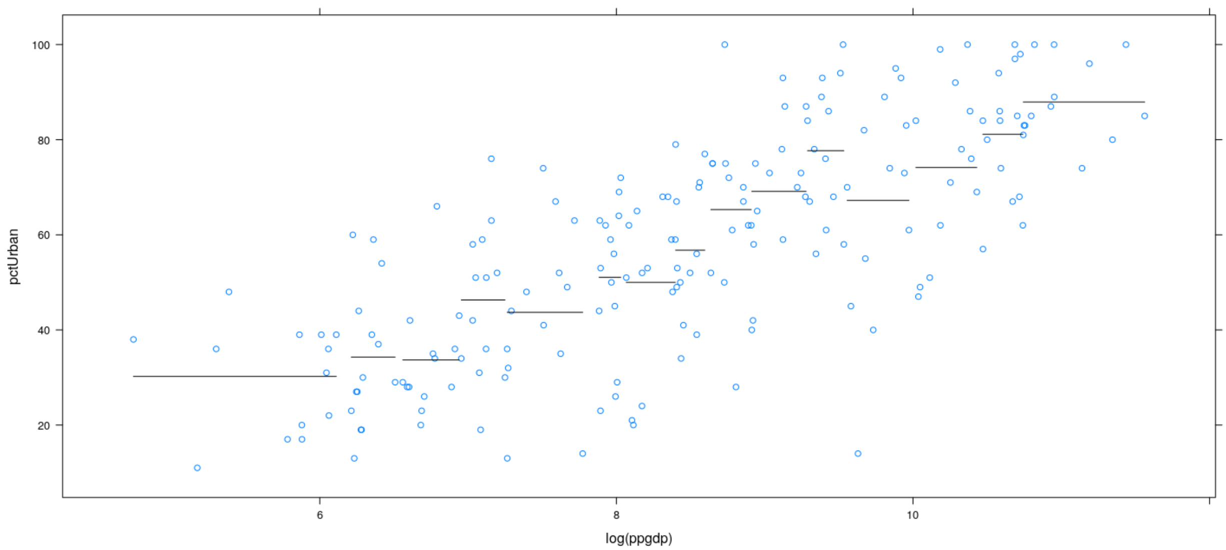
- Choose `span` to minimize

$$\sum_{i=1}^{n}(Y_i - \hat{Y}_{i(-i)})^2$$

- This is equivalent to maximixing predictive R^2
- Next assignment!

Parametric "smooth" regression

- The linear model is actually more flexible than it first seems
- Recall our previous example:



- This can be viewed as a piecewise constant $f(x)$
- Choose breakpoints ("knots") $-\infty = t_0 < t_1 < t_2 < \cdots < t_k = +\infty$
- Define $Z_{ji} = 1\{X_i \in (t_{j-1}, t_j]\}$ for $j = 1, 2, \ldots, k$
- Fit linear model $\mathbf{y} = \mathbf{Z}\beta + \varepsilon$ — this will give piecewise constant $\hat{f}$

Pieceise constant regression

- Implementation in R

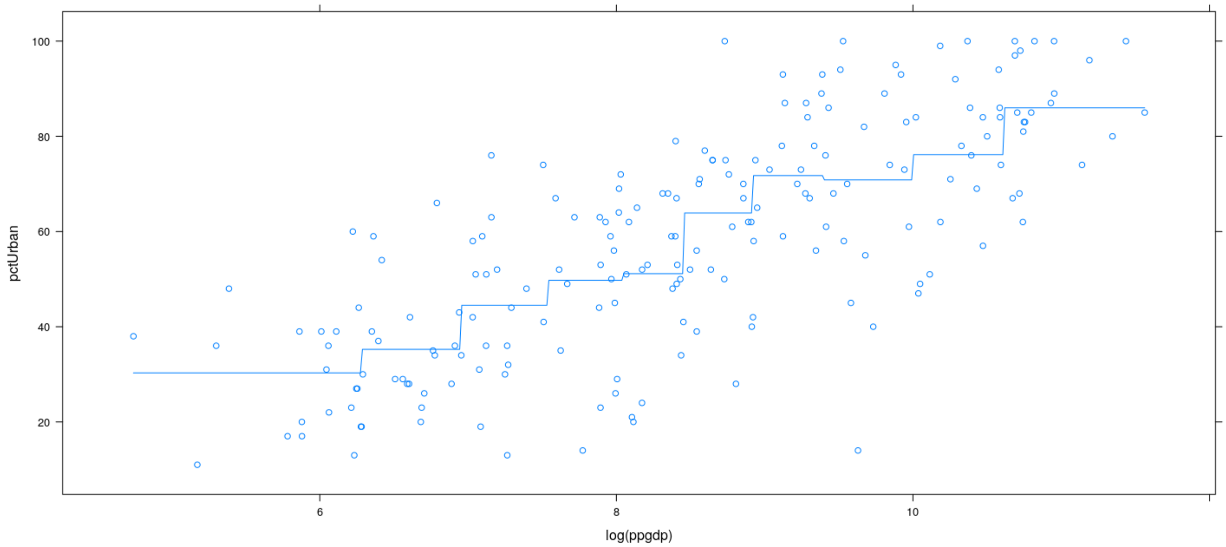
```
pconst <- function(x, knots)
{
    Z <- matrix(0, length(x), length(knots) - 1)
    for (j in seq_len(length(knots)-1))
        Z[, j] <- ifelse(knots[j] < x & x <= knots[j+1], 1, 0)
    Z
}
lgdp.knots <- c(-Inf,
```

```
                quantile(log(UN$ppgdp), probs = seq(0.1, 0.9, by = 0.1), na.rm = TRUE),
                Inf)
```

- Fitting a model

```
fm <- lm(pctUrban ~ 0 + pconst(log(ppgdp), knots = lgdp.knots))
```

```
xplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", se = FALSE, n = 500, form = y ~ 0 + pconst(x, knots = lgdp
```

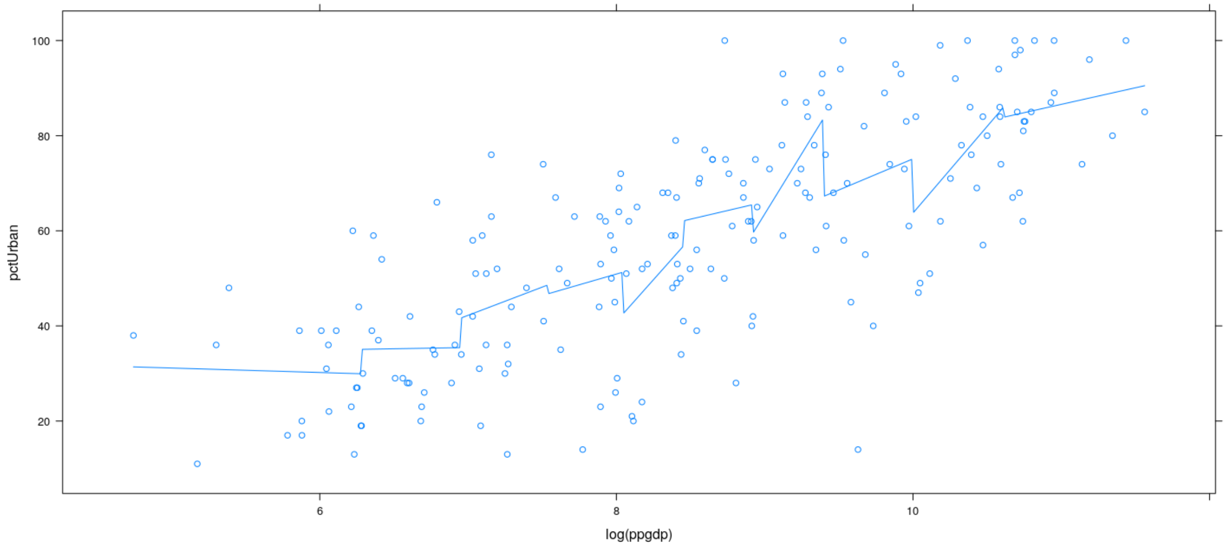


Piecewise linear regression

- Knots $-\infty = t_0 < t_1 < t_2 < \cdots < t_k = +\infty$
- $f(x) = \alpha_j + \beta_j x$ for $x \in (t_{j-1}, t_j]$ for $j = 1, 2, \ldots, k$
- Define $Z_{ji} = 1\{X_i \in (t_{j-1}, t_j]\}$ for $j = 1, 2, \ldots, k$
- Additionally, define $\tilde{Z}_{ji} = Z_{ji} x_i$ for $j = 1, 2, \ldots, k$

```
plinear <- function(x, knots)
{
    Z <- pconst(x, knots)
    cbind(Z, Z * x)
}
```

```
xyplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", se = FALSE, n = 500, form = y ~ 0 + plinear(x, knots = lg
```



Piecewise linear interpolating regression

This is the *best* (least squares) piecewise linear $f(x)$ of the form

$$f(x) = \alpha_j + \beta_j x$$

for $x \in (t_{j-1}, t_j]\,,\, j = 1, 2, \dots, k$.

- But we would prefer f to be continuous
- Requires $\alpha_j + \beta_j t_j = \alpha_{j+1} + \beta_{j+1} t_j$ for $j = 1, 2, \dots, k-1$

Equivalent formulation

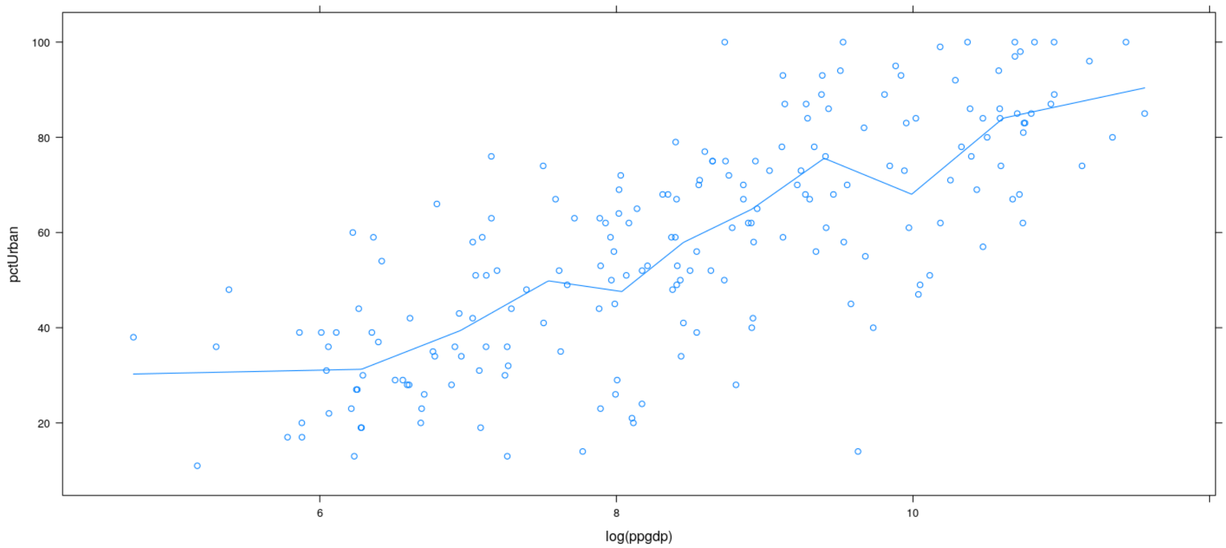
$$f(x) = \delta_0 + \gamma_0 x + \sum_{j=1}^{k-1} \gamma_j (x - t_j)_+$$

where $x_+ = \max\{0, x\}$

```
plincont <- function(x, knots)
{
    Z <- matrix(0, length(x), length(knots)-1)
    Z[,1] <- x
    for (j in seq_len(length(knots)-2)) Z[, j+1] <- pmax(x - knots[j+1], 0)
    Z
}
```

Piecewise linear regression

```
xyplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", se = FALSE, n = 500, form = y ~ 1 + plincont(x, knots = l
```



Natural generalization: piecewise quadratic interpolation

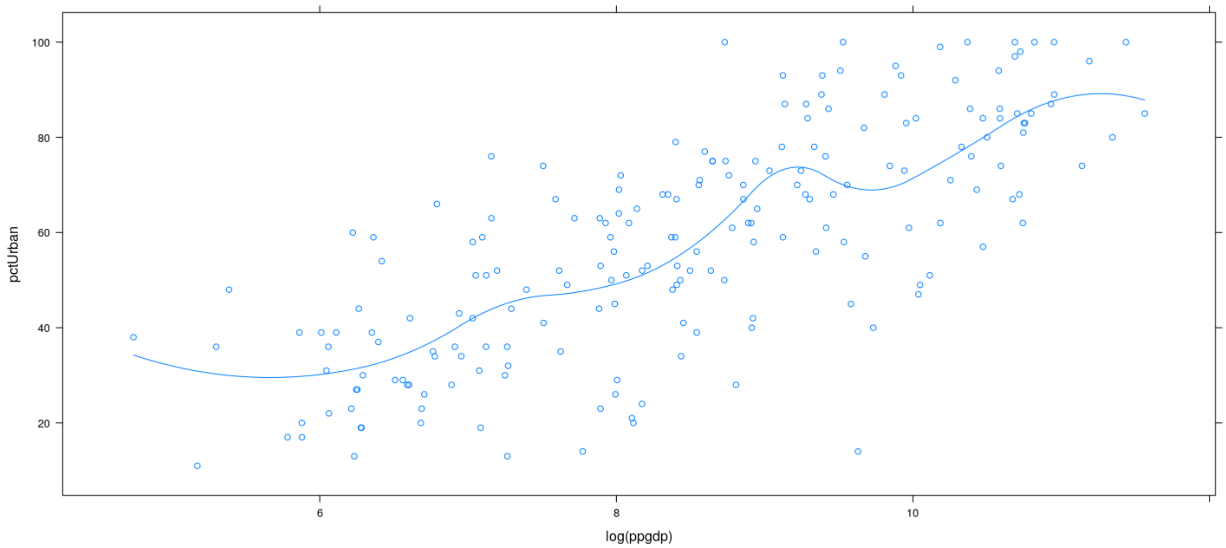
(with matching first derivatives)

$$f(x) = \alpha_0 + \alpha_1 x + \beta_0 x^2 + \sum_{j=1}^{k-1} \beta_j (x - t_j)_+^2$$

where $x_+ = \max\{0, x\}$

```
pquadint <- function(x, knots)
{
    Z <- plincont(x, knots)
    cbind(x, Z^2)
}
```

```
xyplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", se = FALSE, n = 500, form = y ~ 1 + pquadint(x, knots = lg
```



Further generalization: piecewise cubic interpolation

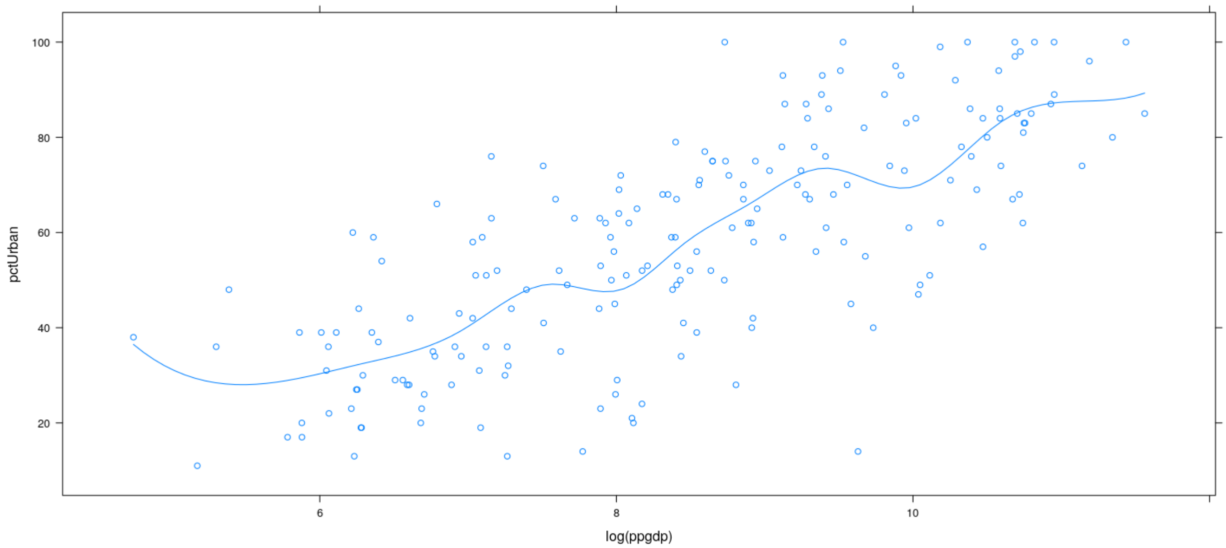
(with matching second derivatives)

$$f(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \beta_0 x^3 + \sum_{j=1}^{k-1} \beta_j (x - t_j)_+^3$$

where $x_+ = \max\{0, x\}$

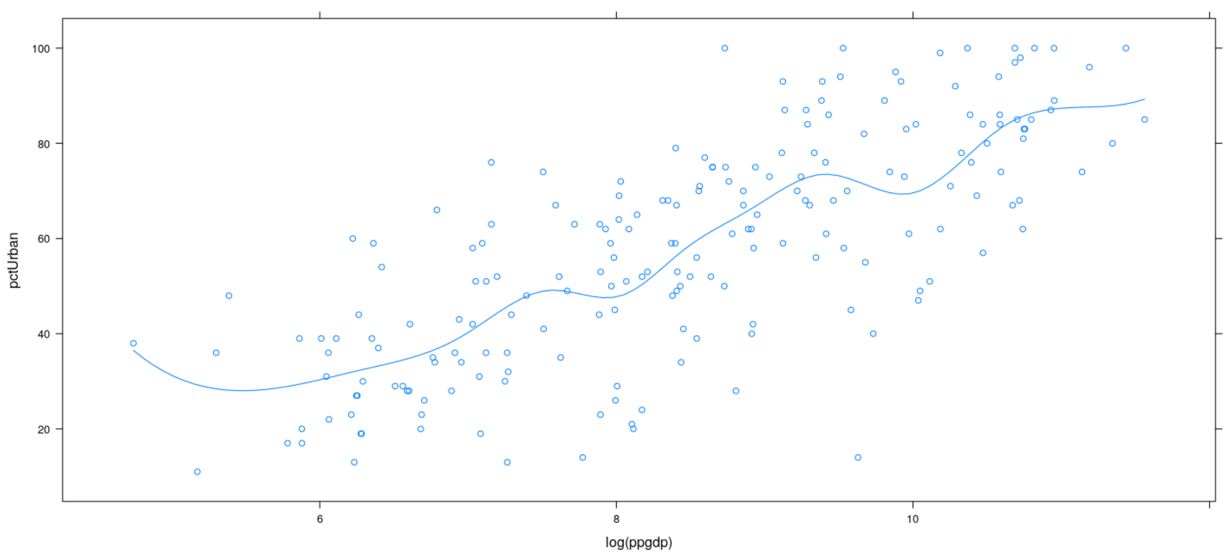
```
pcubint <- function(x, knots)
{
    Z <- plincont(x, knots)
    cbind(x, x^2, Z^3)
}
```

```
xyplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", se = FALSE,
                         form = y ~ 1 + pcubint(x, knots = lgdp.knots)))
```



Also known as cubic spline regression

```
library(splines)
xyplot(pctUrban ~ log(ppgdp), data = UN) +
    layer(panel.smoother(x, y, method = "lm", form = y ~ bs(x, knots = lgdp.knots[2:10]), se = FALSE))
```



Regression with basis functions: background

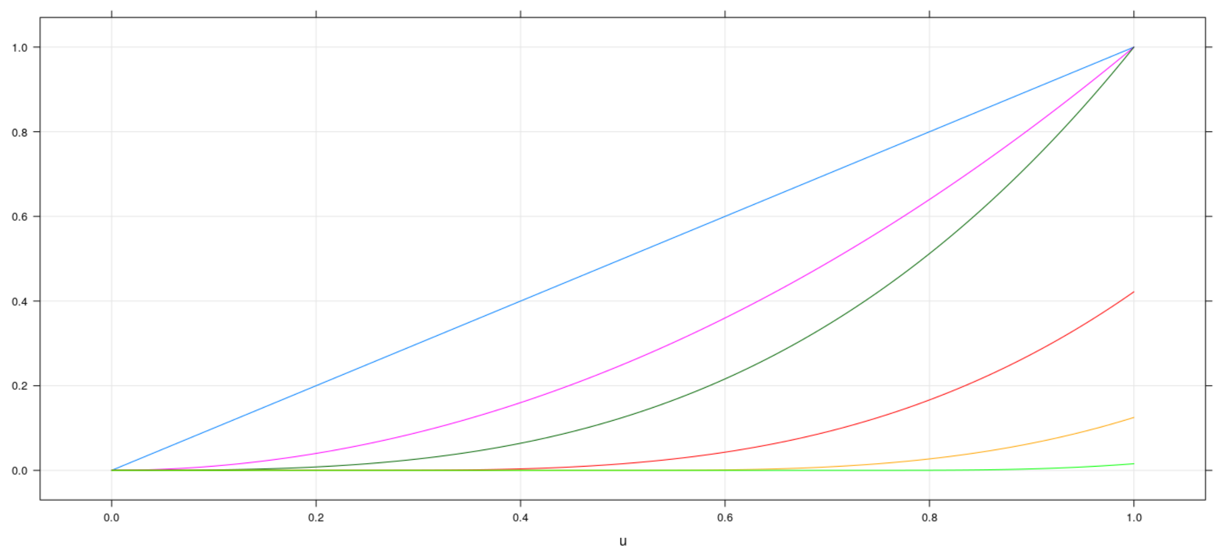
- Goal: Estimate best (least squares) $\hat{f}$ within some class of functions
- Example: "Interpolating splines" — piecewise cubic polynomials with continuous second derivatives
- All the examples we have seen are *vector spaces* (for a fixed set of knots)

- To find $\hat{f}$ using a linear model, we need to find a *basis*
- One example (for cubic interpolating splines) is

$$\{1, x, x^2, x^3\} \cup \{(x - t_j)_+^3 : j = 1, ..., k - 1\}$$

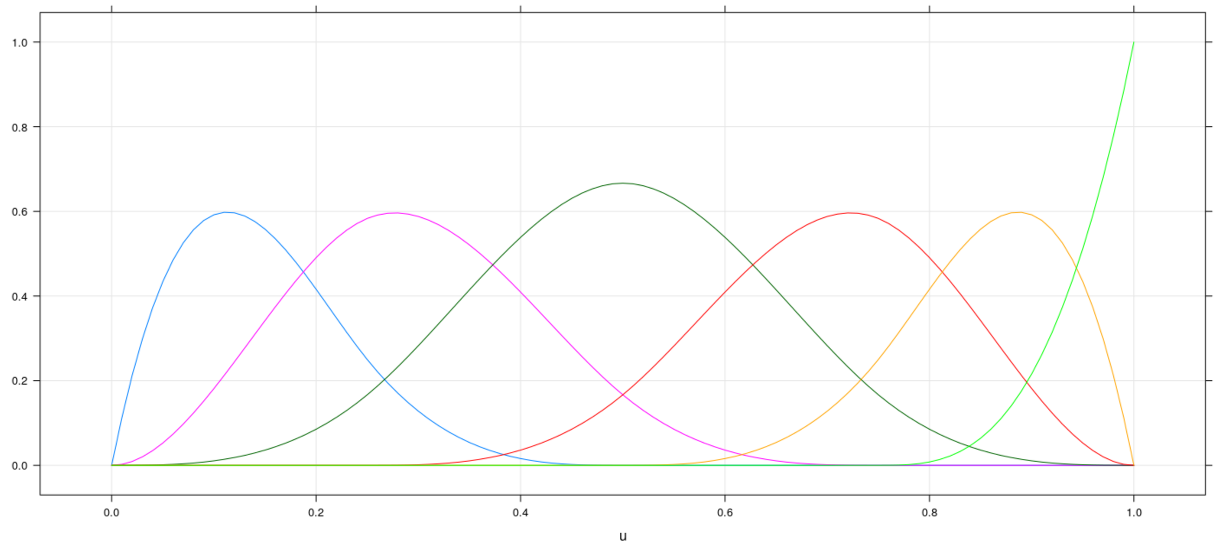
Plot of cubic spline basis functions

```
u <- seq(0, 1, length = 101)
m <- as.data.frame(pcubint(u, knots = c(-Inf, c(0.25, 0.5, 0.75, Inf))))
names(m) <- paste0("f", seq_len(ncol(m)))
xyplot(f1 + f2 + f3 + f4 + f5 + f6 ~ u, data = cbind(u, m), type = "l", ylab = NULL, grid = TRUE)
```



Alternative basis for cubic splines

```
u <- seq(0, 1, length = 101)
m <- as.data.frame(bs(u, knots = c(0.25, 0.5, 0.75)))
names(m) <- paste0("f", seq_len(ncol(m)))
xyplot(f1 + f2 + f3 + f4 + f5 + f6 ~ u, data = cbind(u, m), type = "l", ylab = NULL, grid = TRUE)
```



Basis splines in R

- Available as the `bs()` function in package `splines` (degree 3, "cubic", by default)
- Usually specify `df` rather than explicit knots (tuning parameter providing flexibility)

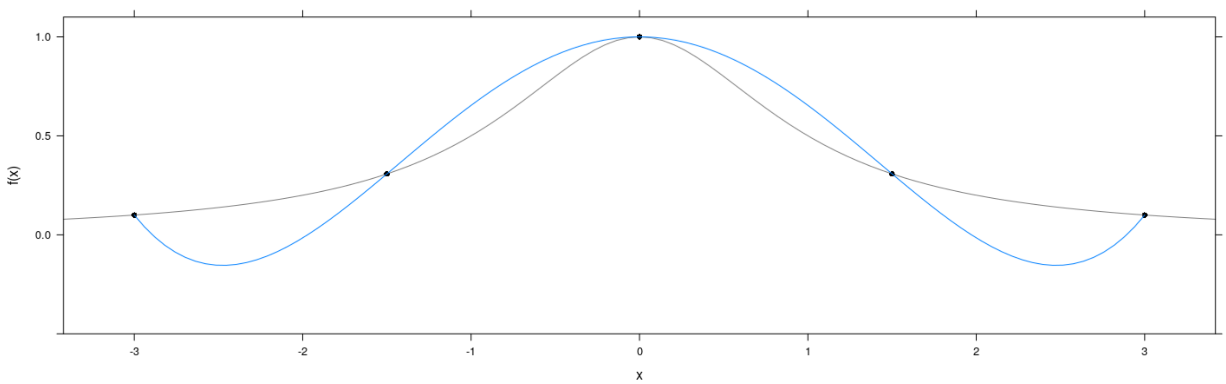
```
summary(lm(pctUrban ~ 1 + bs(log(ppgdp), df = 6), data = UN)) # fitting a B-spline model
```

```

Call:
lm(formula = pctUrban ~ 1 + bs(log(ppgdp), df = 6), data = UN)

Residuals:
    Min      1Q  Median      3Q     Max 
-58.942  -9.267   0.426  11.094  38.561 

Coefficients:
                        Estimate Std. Error t value Pr(>|t|)    
(Intercept)               34.688     13.254   2.617 0.009573 ** 
bs(log(ppgdp), df = 6)1  -11.885     20.810  -0.571 0.568600    
bs(log(ppgdp), df = 6)2    2.469     13.466   0.183 0.854691    
bs(log(ppgdp), df = 6)3   21.769     14.884   1.463 0.145226    
bs(log(ppgdp), df = 6)4   44.026     14.446   3.048 0.002631 ** 
bs(log(ppgdp), df = 6)5   46.601     16.149   2.886 0.004354 ** 
bs(log(ppgdp), df = 6)6   59.317     16.645   3.564 0.000462 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 15.65 on 192 degrees of freedom
  (14 observations deleted due to missingness)
Multiple R-squared:  0.5674,	Adjusted R-squared:  0.5539 
F-statistic: 41.98 on 6 and 192 DF,  p-value: < 2.2e-16
```

Why splines?

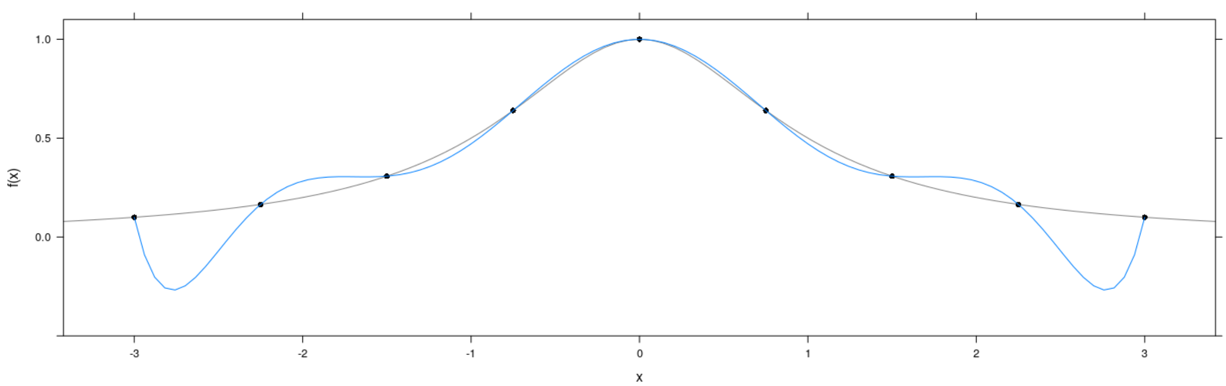
- Consider the problem of interpolation through k points
- Obvious approach: Fit a polynomial

```
f <- function(x) 1 / (1 + x^2)
degree <- 4
x <- seq(-3, 3, length = degree + 1)
xyplot(f(x) ~ x, col = 1, pch = 16, ylim = c(-0.5, 1.1)) +
    layer_(panel.curve(f, type = "l", col = "grey50")) +
        layer(panel.smoother(x, y, method = "lm", form = y ~ poly(x, degree), se = FALSE))
```



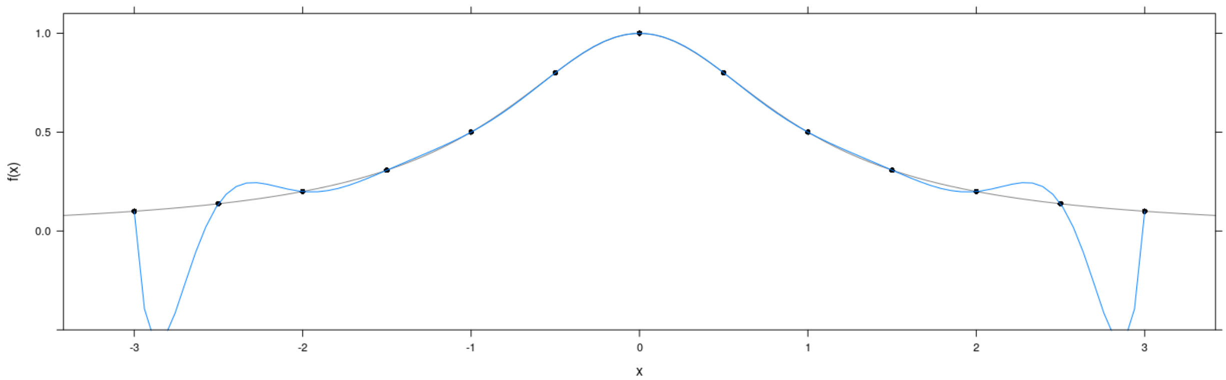
- Consider the problem of interpolation through k points
- Obvious approach: Fit a polynomial

```
f <- function(x) 1 / (1 + x^2)
degree <- 8
x <- seq(-3, 3, length = degree + 1)
xyplot(f(x) ~ x, col = 1, pch = 16, ylim = c(-0.5, 1.1)) +
    layer_(panel.curve(f, type = "l", col = "grey50")) +
        layer(panel.smoother(x, y, method = "lm", form = y ~ poly(x, degree), se = FALSE))
```



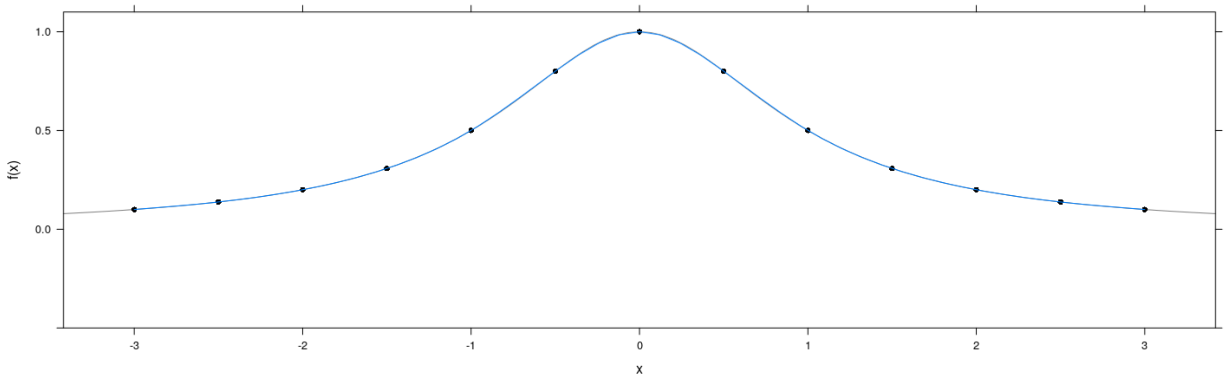
- Consider the problem of interpolation through k points
- Obvious approach: Fit a polynomial — Runge's phenomenon

```
f <- function(x) 1 / (1 + x^2)
degree <- 12
x <- seq(-3, 3, length = degree + 1)
xyplot(f(x) ~ x, col = 1, pch = 16, ylim = c(-0.5, 1.1)) +
    layer_(panel.curve(f, type = "l", col = "grey50")) +
        layer(panel.smoother(x, y, method = "lm", form = y ~ poly(x, degree), se = FALSE))
```



- Consider the problem of interpolation through k points
- Alternative: Fit a cubic spline

```
f <- function(x) 1 / (1 + x^2)
degree <- 12
x <- seq(-3, 3, length = degree + 1)
xyplot(f(x) ~ x, col = 1, pch = 16, ylim = c(-0.5, 1.1)) +
    layer_(panel.curve(f, type = "l", col = "grey50")) +
        layer(panel.lines(predict(interpSpline(x, y))))
```



An interesting property of interpolating splines

Consider finding $f : [a,b] \to \mathbb{R}$ interpolating the points $\{(x_i, y_i) : x_i \in [a,b]\}$ that minimizes

$$\int_a^b (f''(t))^2 dt \qquad \text{(roughness penalty)}$$

in the class of functions with continuous second derivative

- The solution is a "natural" cubic spline
- "Natural" because the solution is linear outside the range of the knots

Smoothing splines

A non-parametric regression approach motivated by this:

Find f to minimize (given $\lambda > 0$)

$$\sum_i (y_i - f(x_i))^2 + \lambda \int_a^b (f''(t))^2 dt$$

- The solution is a "natural" cubic spline
- λ represents a tuning parameter (smoothness vs flexibility)
- λ is usually chosen by a form of cross-validation
- The mathematical analysis of smoothing splines is relatively complicated (will not discuss)

Smoothing splines in R

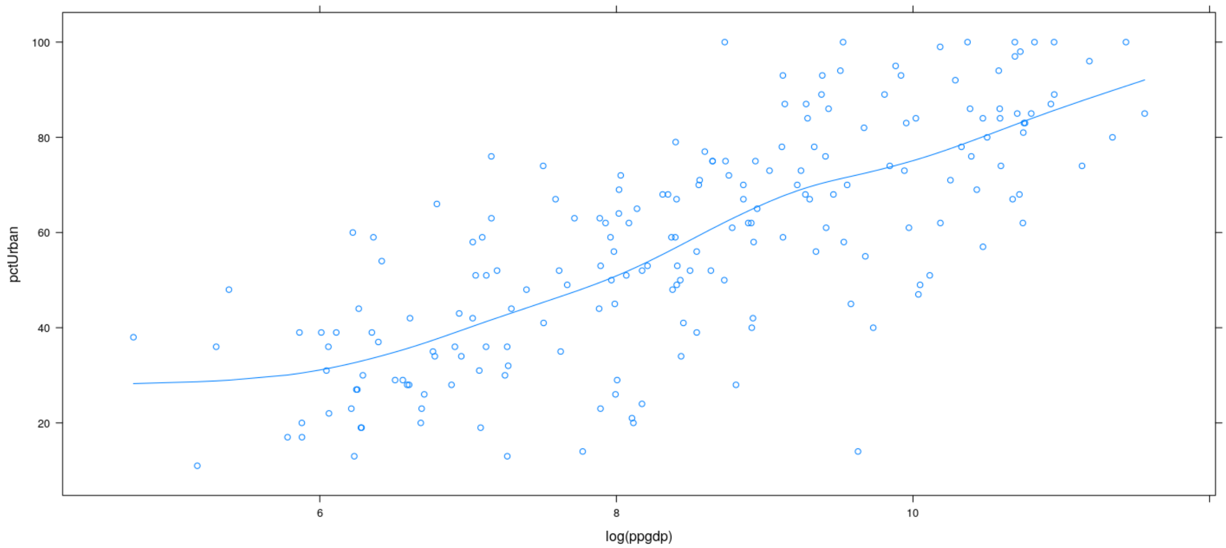
```
UN.sub <- subset(UN, !is.na(ppgdp) & !is.na(pctUrban)) # cannot handle NA
fm.ss <- with(UN.sub, smooth.spline(log(ppgdp), pctUrban, df = 6)) # lambda controlled by df
fm.ss
```

```
Call:
smooth.spline(x = log(ppgdp), y = pctUrban, df = 6)

Smoothing Parameter  spar= 1.034826  lambda= 0.004116211 (12 iterations)
Equivalent Degrees of Freedom (Df): 6.000823
Penalized Criterion (RSS): 46566.24
GCV: 1031.185
```

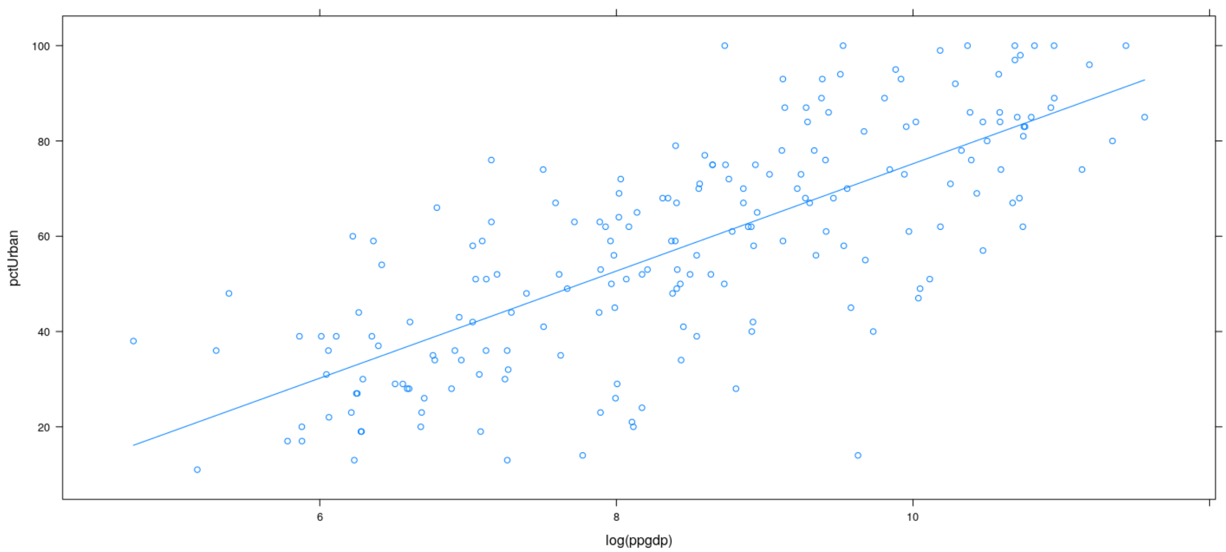
```
fm.ss.gcv <- with(UN.sub, smooth.spline(log(ppgdp), pctUrban)) # lambda chosen by GCV
fm.ss.gcv
```

```
Call:
smooth.spline(x = log(ppgdp), y = pctUrban)

Smoothing Parameter  spar= 1.499952  lambda= 9.443731 (25 iterations)
Equivalent Degrees of Freedom (Df): 2.030403
Penalized Criterion (RSS): 47818.1
GCV: 986.3203
```

```
xyplot(pctUrban ~ log(ppgdp), data = UN) + layer(panel.lines(predict(fm.ss)))
```




```r
xyplot(pctUrban ~ log(ppgdp), data = UN) + layer(panel.lines(predict(fm.ss.gcv)))
```



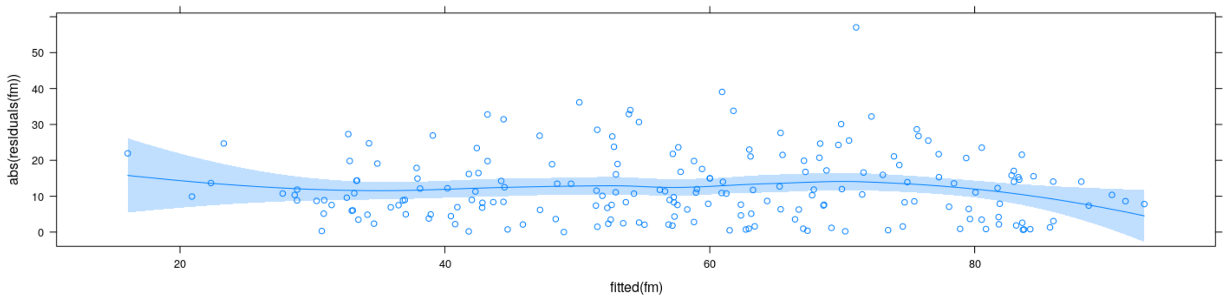
Summary: smooth regression for non-linear expectation function

- Focuses on estimating $f(x) = E(Y|X = x)$
- Several methods available, both non-parametric and parametric
- Usually involves tuning parameter that needs to be chosen
- Can be used to visually diagnose non-linearity of $f(x)$

What about non-constant variance?

- Assume constant variance
- Define $\hat{\varepsilon}_i = y_i - \hat{f}(x_i)$
- Expect $E(|\hat{\varepsilon}_i|) \propto \sigma$

```
fm <- lm(pctUrban ~ log(ppgdp), data = UN)
xyplot(abs(residuals(fm)) ~ fitted(fm)) + layer(panel.smoother(x, y, method = "loess"))
```



Summary: smooth regression for non-linear expectation function

- Focuses on estimating $f(x) = E(Y|X = x)$
- Several methods available, both non-parametric and parametric
- Usually involves tuning parameter that needs to be chosen
- Can be used to visually diagnose non-linearity of $f(x)$
- Can also be used to diagnose heteroscedasticity