MASM22/FMSN30: Linear and Logistic Regression, 7.5 hp
FMSN40: ... with Data Gathering, 9 hp

Lecture 11, spring 2023
Multinomial and ordinal logistic regression, Quantile regression

Mathematical Statistics / Centre for Mathematical Sciences
Lund University

10/5-23

Multinomial logistic regression

Sometimes it is natural to have a categorical Y-variable with more than two categories.

Y_i can take any of the values $k = 0, 1, \ldots, q$ with probabilities $p_{0,i}, \ldots, p_{q,i}$ where $\sum_{k=0}^{q} p_{k,i} = 1$ giving $p_{0,i} = 1 - \sum_{k=1}^{q} p_{k,i}$

Model:

$$Y_i \sim \text{Multinomial}(1, p_{0,i}, \ldots, p_{q,i})$$

Using category 0 as reference, we assume that the log-odds for being in category k instead of in category 0 can be modeled as

$$\ln \frac{p_{1,i}}{p_{0,i}} = \beta_{1,0} + \beta_{1,1} x_{i1} + \ldots + \beta_{1,p} x_{ip} = \mathbf{x}_i \boldsymbol{\beta}_1 \quad \ln \frac{p_i}{1 - p_i} = \mathbf{x}_i \boldsymbol{\beta}$$

$$\vdots$$

$$\ln \frac{p_{q,i}}{p_{0,i}} = \beta_{q,0} + \beta_{q,1} x_{i1} + \ldots + \beta_{q,p} x_{ip} = \mathbf{x}_i \boldsymbol{\beta}_q$$

Rewriting gives the probabilities

$$p_{0,i} = \frac{1}{1 + \sum_{k=1}^{q} e^{\mathbf{x}_i \boldsymbol{\beta}_k}} \qquad p_{0,i} = 1 - p_i = \frac{1}{1 + e^{\mathbf{x}_i \boldsymbol{\beta}}}$$

$$p_{1,i} = \frac{e^{\mathbf{x}_i \boldsymbol{\beta}_1}}{1 + \sum_{k=1}^{q} e^{\mathbf{x}_i \boldsymbol{\beta}_k}} \qquad p_{1,i} = p_i = \frac{e^{\mathbf{x}_i \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i \boldsymbol{\beta}}}$$

$$\vdots$$

$$p_{q,i} = \frac{e^{\mathbf{x}_i \boldsymbol{\beta}_q}}{1 + \sum_{k=1}^{q} e^{\mathbf{x}_i \boldsymbol{\beta}_k}}$$

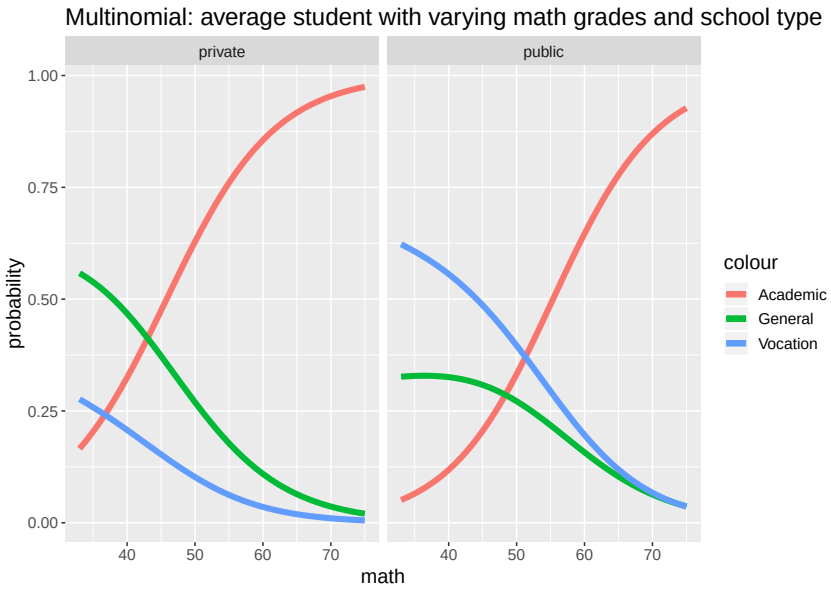
- Estimate all the parameter vectors $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_q$ jointly using Maximum-Likelihood.
- The $\hat{\boldsymbol{\beta}}_k$ are again asymptotically multivariate normal distributed and we can use the Wald test for a specific $\beta_{k,j}$ and construct confidence intervals for both $\beta_{k,j}$ and the linear predictors $\mathbf{x}_i \boldsymbol{\beta}_k$ as before.
- Compare nested models with Likelihood Ratio (Deviance) tests.

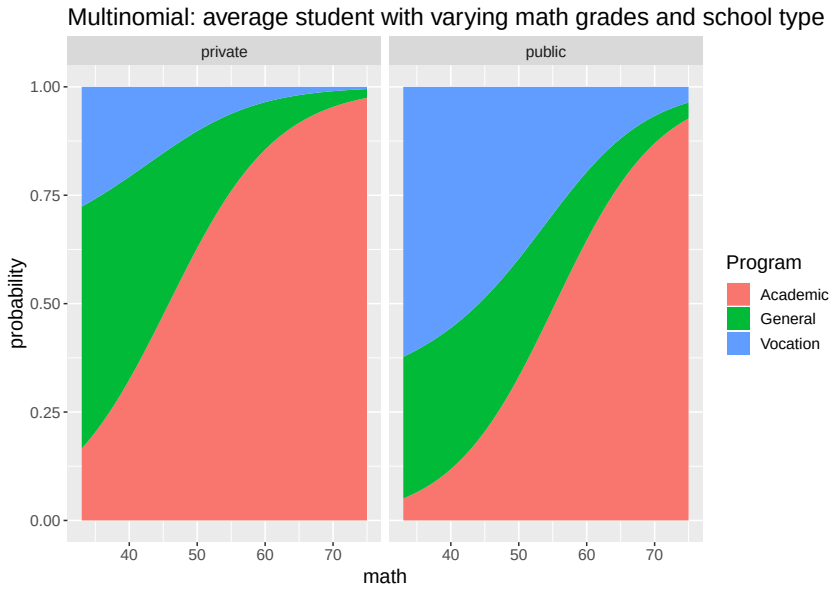
Example: which type of program does a student apply to

- prog: type of program student applies to (Academic, General, Vocation). Dependent categorical variable

	General				Academic				
	$\hat{\beta}_j$	OR	lwr	upr	$\hat{\beta}_j$	OR	lwr	upr	LR
(Intercept)	−5.96 ***	0.00	0.00	0.08	−9.89 ***	0.00	0.00	0.00	
math	0.02 n.s.	1.02	0.95	1.09	0.14 ***	1.15	1.07	1.23	***
socst	0.05 *	1.05	1.00	1.10	0.09 ***	1.10	1.04	1.16	***
science	0.04 n.s.	1.04	0.99	1.10	−0.04 n.s.	0.96	0.91	1.02	***
schtyppublic	0	1	-	-	0	1	-	-	*
schtypprivate	1.35 n.s.	3.85	0.70	21.11	2.00 **	7.36	1.50	36.19	
seslow	1.40 **	4.06	1.39	11.82	1.22 *	3.39	1.13	10.19	
sesmiddle	0	1	-	-	0	1	-	-	*
seshigh	0.51 n.s.	1.66	0.50	5.54	1.21 *	3.34	1.12	9.96	

- LR (deviance) test for differences in β between any of the three programs.
- The odds ratio of applying to Academic, compared to Vocation, increases by 15 % for each 1 unit higher math grade.
- The math grade has no significant effect on the odds ratio of applying to General, compared to Vocation.
- The science grade has no significant effect on the odds ratio when comparing General or Academic to Vocation, but it has a significant effect when comparing General and Academic with each other.


Multinomial: average student with varying math grades and school type
private
public
1.00
0.75
0.50
0.25
0.00
probability
40
50
60
70
math
colour
Academic
General
Vocation


Multinomial: average student with varying math grades and school type
private
public
1.00
0.75
0.50
0.25
0.00
probability
40
50
60
70
math
Program
Academic
General
Vocation

Model	AIC	BIC	R^2_{D}	$R^2_{\text{D,adj}}$
Null	412.2	418.8	0.0 %	0.0 %
Math	364.2	377.4	12.7 %	12.2 %
Grades	350.7	377.1	18.0 %	16.5 %
Final	343.6	389.7	22.7 %	19.8 %
Full	356.7	435.9	24.4 %	19.0 %

Goodness-of-fit

	predicted				
true	Vocation	Academic	General	Total	Sens(spec)
Vocation	29	17	4	50	$29/50 = 58.0\,\%$
Academic	11	87	7	105	$87/105 = 82.9\,\%$
General	13	22	10	45	$10/45 = 22.2\,\%$
Total	53	126	21	200	
Precision	54.7 %	69.0 %	47.6 %		acc = 63.0 %

Ordinal logistic regression

If Y_i is an ordinal categorical variable, where the categories, $k = 1, \ldots, q$ have a logical order, we should do an ordinal logistic regression instead. We then model the log-odds of being in category k or lower instead of in category $k+1$ or higher.

$$\ln \frac{Pr(Y_i = 1)}{Pr(Y_i > 1)} = \zeta_{1,0} - \beta_1 x_{i1} - \ldots - \beta_p x_{ip} = \zeta_{1,0} - \mathbf{x}_i\boldsymbol{\beta},$$
$$\ln \frac{Pr(Y_i \leq 2)}{Pr(Y_i > 2)} = \zeta_{2,0} - \mathbf{x}_i\boldsymbol{\beta},$$
$$\vdots$$
$$\ln \frac{Pr(Y_i \leq q-1)}{Pr(Y_i = q)} = \zeta_{q-1,0} - \mathbf{x}_i\boldsymbol{\beta}.$$

The linear part $\mathbf{x}_i\boldsymbol{\beta}$ is the same for all categories, only the intercept $\zeta_{k,0}$ changes!

Note: in $\mathbf{x}_i\boldsymbol{\beta}$ we redefine $\boldsymbol{\beta}$ as $(0, \beta_1, \ldots, \beta_p)$ so we can re-use the notation $\mathbf{x}_i$, including 1 in the first column.

- The parameters, $\boldsymbol{\zeta}_0' = (\zeta_{1,0}, \ldots, \zeta_{q-1,0})$ and $\boldsymbol{\beta}$ are estimated using Maximum-likelihood and are asymptotically normally distributed.
- The probabilities for each of the categories have to be calculated recursively:

$$\ln \frac{1-\hat{p}_{q,i}}{\hat{p}_{q,i}} = \hat{\zeta}_{q-1,0} - \mathbf{x}_i\hat{\boldsymbol{\beta}} \Rightarrow \hat{p}_{q,i} = \frac{1}{1+\mathrm{e}^{\hat{\zeta}_{q-1,0}-\mathbf{x}_i\hat{\boldsymbol{\beta}}}}$$

$$\frac{\hat{Pr}(Y_i \leq k-1)}{\hat{Pr}(Y_i > k-1)} = \frac{\sum_{j=1}^{k-1}\hat{p}_{j,i}}{\sum_{j=k}^{q}\hat{p}_{j,i}} = \frac{1-\sum_{j=k}^{q}\hat{p}_{j,i}}{\sum_{j=k}^{q}\hat{p}_{j,i}} = \mathrm{e}^{\hat{\zeta}_{k-1,0}-\mathbf{x}_i\hat{\beta}} \Rightarrow$$

$$\sum_{j=k}^{q}\hat{p}_{j,i} = \frac{1}{1+\mathrm{e}^{\hat{\zeta}_{k-1,0}-\mathbf{x}_i\hat{\boldsymbol{\beta}}}} \Rightarrow$$

$$\hat{p}_{k,i} = \frac{1}{1+\mathrm{e}^{\hat{\zeta}_{k-1,0}-\mathbf{x}_i\hat{\boldsymbol{\beta}}}} - \sum_{j=k+1}^{q}\hat{p}_{j,i}, \text{ for } k = 1, \ldots, q-1$$

- LR test for nested models. AIC, BIC and Confusion matrices for non-nested models.

Example: How likely is a student to apply to graduate school?

We have Y_i with $q = 3$ ordered categories: "unlikely", "somewhat likely", "very likely". The potential x-variables are

- `pared` = at least one parent has a graduate degree (no/yes),
- gpa = student's grade point average (continuous).

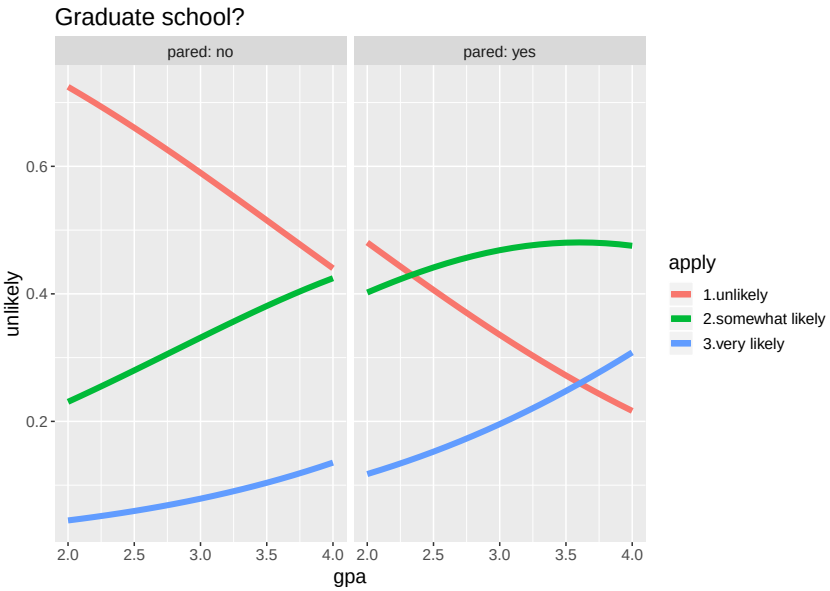
Model

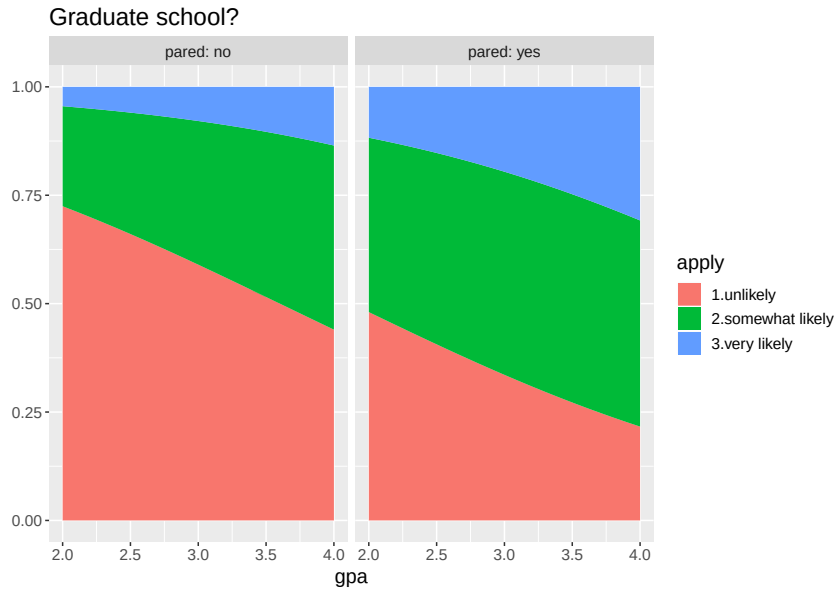
$$\ln \frac{Pr(Y_i = \text{unlikely})}{Pr(Y_i = \text{somewhat or very likely})} = \zeta_{1,0} - \mathbf{x}_i\boldsymbol{\beta},$$
$$\ln \frac{Pr(Y_i = \text{unlikely or somewhat likely})}{Pr(Y_i = \text{very likely})} = \zeta_{2,0} - \mathbf{x}_i\boldsymbol{\beta}$$

where $\mathbf{x}_i\boldsymbol{\beta} = \beta_1 \cdot \text{pared} + \beta_2 \cdot \text{gpa}$.

Variable	Param.	Est,	e^{est}	95 % CI(e^{β_j})	
pared	β_1	1.046	2.85	1.69	4.81
gpa	β_2	0.604	1.83	1.12	3.02
unlikely vs somewhat or very	$\zeta_{1,0}$	2.176	8.81		
unlikely or somewhat vs very	$\zeta_{2,0}$	4.272	71.64		

- A student where neither parent has a graduate degree and who had 0 as grade point average, has a probability to answer "unlikely" that is $\mathrm{e}^{\zeta_{1,0}} = 8.81$ times as large as the probability to answer something more positive, i.e, the odds is 8.81.
- If at least one parent has a graduate degree, the probability to answer "unlikely" is only $\mathrm{e}^{\zeta_{1,0}-\beta_1} = \frac{\mathrm{e}^{\zeta_{1,0}}}{\mathrm{e}^{\beta_1}} = \frac{8.81}{2.85} = 3.10$ times as large.
- If he also has a grade point average of 3, the probability to answer "unlikely" is $\mathrm{e}^{\zeta_{1,0}-\beta_1-3\beta_2} = \frac{\mathrm{e}^{\zeta_{1,0}}}{\mathrm{e}^{\beta_1+3\beta_2}} = \frac{8.81}{2.85 \cdot 1.84^3} = 0.51$ times as large.
- If $\beta_j > 0$, increasing the value of x_j increases the probability of giving a more positive answer.


Graduate school?
pared: no
pared: yes
unlikely
0.6
0.4
0.2
2.0
2.5
3.0
3.5
4.0
gpa
apply
1.unlikely
2.somewhat likely
3.very likely


Graduate school?
pared: no
pared: yes
1.00
0.75
0.50
0.25
0.00
2.0
2.5
3.0
3.5
4.0
gpa
apply
1.unlikely
2.somewhat likely
3.very likely

Model	AIC	BIC	R^2_{D}	$R^2_{\text{D,adj}}$
Null	745.2	753.2	0.0 %	0.0 %
Final	725.1	741.0	3.3 %	3.0 %
Full	727.0	747.0	3.3 %	2.9 %

Confusion matrix

Final model	predicted				
true	unlikely	somewhat	very	total	sens.
unlikely	201	19	0	220	91.4 %
somewhat	110	30	0	140	21.4 %
very	27	13	0	40	0.0 %
total	338	62	0	400	
prec.	59.5 %	48.84 %	—		57.8 %

Distribution free methods

For the entire course we assumed that our data were samples from some specific distribution:

- Normally distributed responses $\rightarrow$ linear regression;
- binary responses $\rightarrow$ Bernoulli/binomial distributions $\rightarrow$ logistic regression;
- ... and other members from the exponential family $\rightarrow$ GLMs.

It is implicit that when we say "we assume a certain distribution" we should use diagnostic methods to verify that the assumption holds.

For example by using QQ-plots, to compare sample quantiles with the exact quantiles from an hypothesized distribution.

Now we consider a methodology which is "distribution free".

Quantiles

General case: The α-quantile y_α is defined as $Pr(Y > y_\alpha) = \alpha$.
Regression: The α-quantile $y_{i\alpha}$ is defined as $Pr(Y_i > y_{i\alpha} \,|\, \mathbf{x}_i) = \alpha$.

Linear regression

With $Y_i = \mathbf{x}_i\boldsymbol{\beta} + \epsilon_i$ where $\epsilon_i \sim N(0, \sigma^2)$ we have $y_{i\alpha} = \mathbf{x}_i\boldsymbol{\beta} + \lambda_\alpha \cdot \sigma$.
Estimated by the prediction interval. Requires that ϵ_i really are $N(0, \sigma^2)$.
[here λ_α is the α-quantile from N(0,1)]

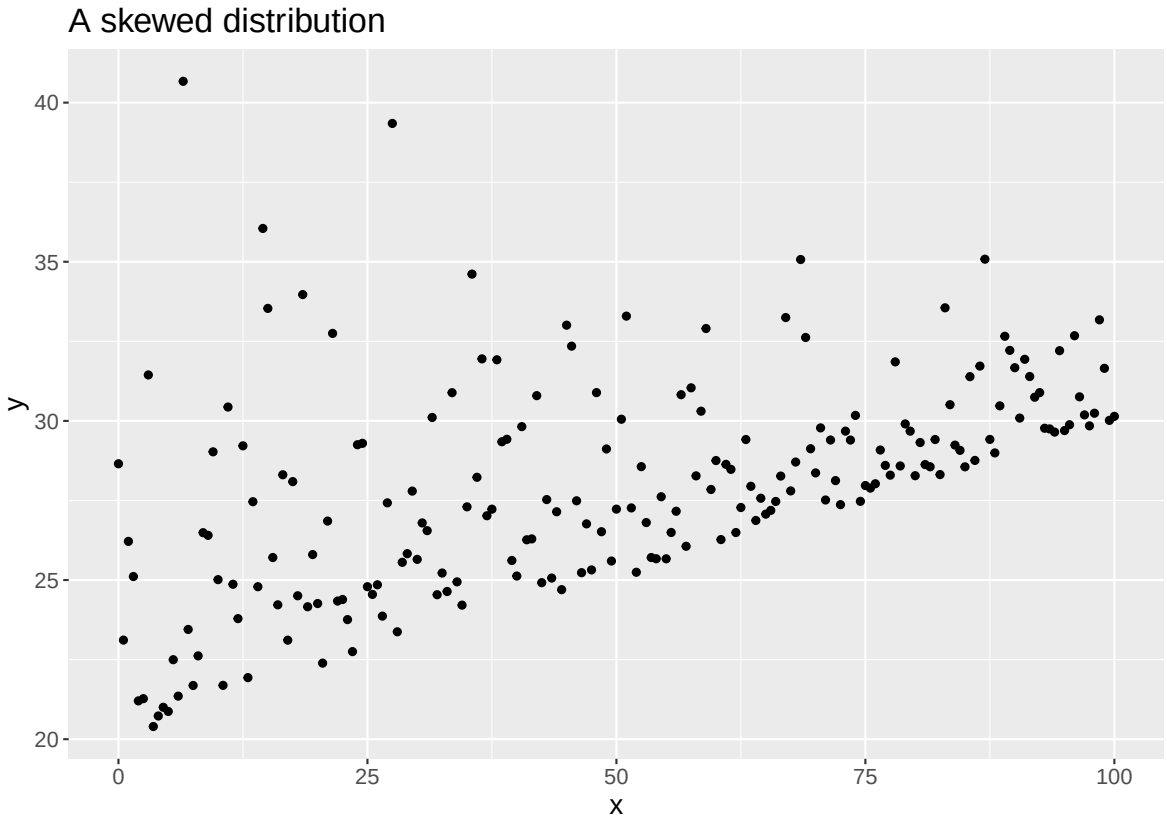
Poisson regression

With $Y_i \sim Po(\mathrm{e}^{\mathbf{x}_i\boldsymbol{\beta}})$ we can use the quantiles in the (estimated) Poisson distribution.

Other distributions

As long as we know ("pretend to know") the distribution type and can estimate all its parameters we can use its quantiles.
What if we don't know the distribution type?

Example:



Skewed distribution with larger variability for lower expected values.
Difficult to find a transformation.

Quantile as solution to minimization problem

- Sample mean as a solution to minimization: $\hat{\mu} = \bar{y}$ solves

$$\min_{\mu} \sum_{i=1}^{n} (y_i - \mu)^2$$

- Median (i.e. 50% quantile) $\hat{m} = \text{median}(y_1, \ldots, y_n)$ solves:

$$\min_{m} \sum_{i=1}^{n} |y_i - m| \qquad \text{(robust to outliers!)}$$

- generic empirical quantile y_α corresponding to a probability α solves:

$$\min_{y_\alpha} \left\{ (1-\alpha) \sum_{y_i > y_\alpha} |y_i - y_\alpha| + \alpha \sum_{y_i \leq y_\alpha} |y_i - y_\alpha| \right\}$$

and is *robust to outliers*.

Quantile regression

Set $y_{i\alpha} = \mathbf{x}_i\boldsymbol{\beta}_\alpha$ where $Pr(Y_i > y_{i\alpha} \,|\, \mathbf{x}_i) = \alpha$.
Replace Least-squares $(Y_i - \mu_i)^2$ by

$$\rho_\alpha(Y_i - y_{i\alpha}) = \begin{cases} (1-\alpha) \cdot |Y_i - y_{i\alpha}| & \text{if } Y_i > y_{i\alpha}, \\ \alpha \cdot |Y_i - y_{i\alpha}| & \text{if } Y_i \leq y_{i\alpha}. \end{cases}$$

and minimize $\sum_{i=1}^{n} \rho_\alpha(Y_i - \mathbf{x}_i\boldsymbol{\beta}_\alpha)$ with respect to $\boldsymbol{\beta}_\alpha = \begin{pmatrix} \beta_{0\alpha} \\ \beta_{1\alpha} \\ \vdots \\ \beta_{p\alpha} \end{pmatrix}$

Symbol $\boldsymbol{\beta}_\alpha$ is meant to emphasize that it is not an estimate based on least squares or maximum likelihood (in the latter case it would not be possible as we do not specify the distribution for observed data).

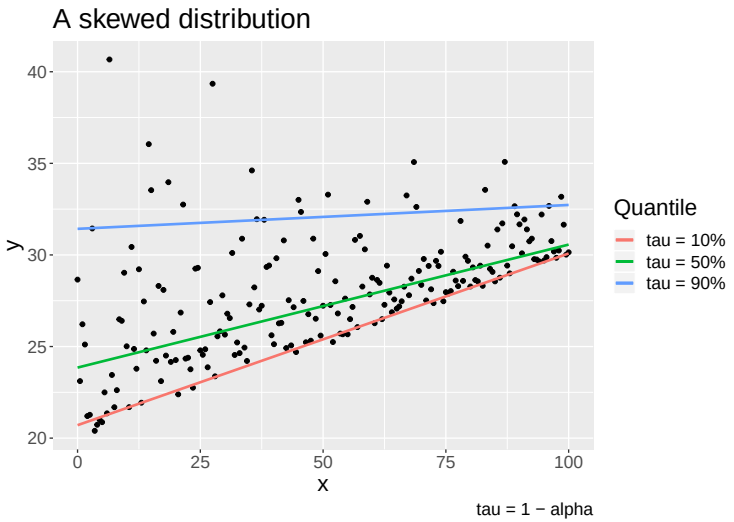
Features

- the resulting α-quantile regression line is such that, for given covariates $\mathbf{x}_i$, a proportion of approximately α data points lies above the fitted value

$$y_{i\alpha} = \beta_{0\alpha} + \beta_{1\alpha}x_{i1} + \cdots + \beta_{p\alpha}x_{ip}$$

  and a proportion $1 - \alpha$ lies below.
- In R: install the package `quantreg`, then `library(quantreg)`
- `rq(y ~ x, data = data, tau = c(0.1, 0.5, 0.9))` where $\tau = 1 - \alpha$ is a list of quantiles.
- `anova(model)` tests if the lines are parallel, i.e. H_0: $\beta_{j,\alpha_1} = \ldots = \beta_{j,\alpha_m}$ for $j = 1, \ldots, p$.
- Use $D_0 - D =$ `-2*(logLik(model.red) - logLik(model.full))` $> \chi^2_{0.05}(k)$ to compare models for a specific τ.

Example (cont)

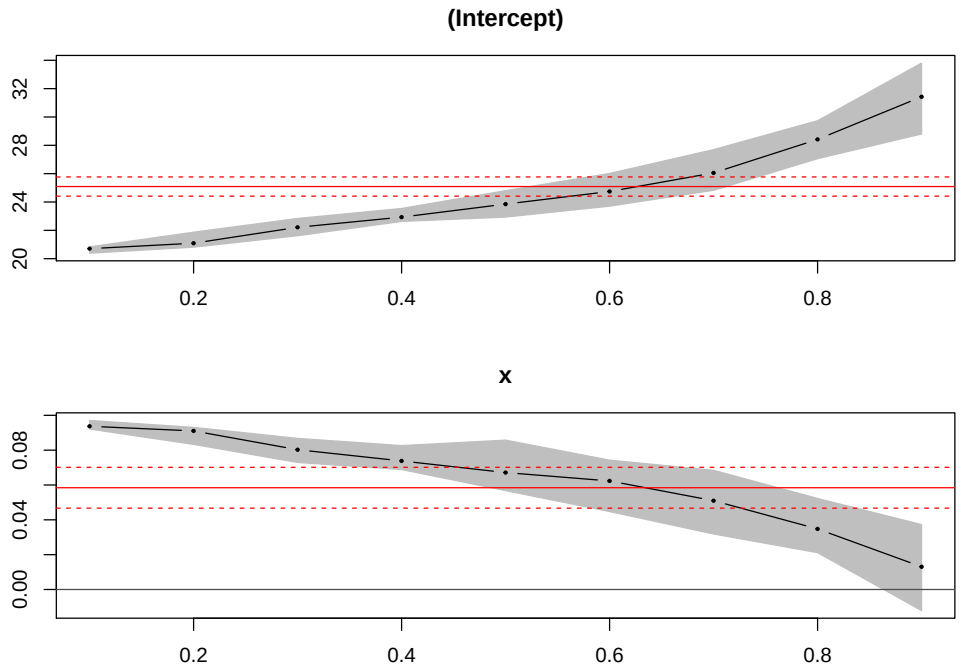


- Test for parallel lines, H$_0$: $\beta_{1,0.1} = \beta_{1,0.5} = \beta_{1,0.9}$, gives F-value $= 14.64 > F_{0.05,2,601} = 3.01$ (P-value $= 6 \cdot 10^{-7} < 0.05$). The lines are not parallel.
- H$_0$: $\beta_{1,0.1} = 0$ cannot be rejected and its AIC is very similar to the null model, i.e., the line is horizontal.

	Null model		
	$\tau = 0.1, \alpha = 0.9$	$\tau = \alpha = 0.5$	$\tau = 0.9, \alpha = 0.1$
Intercept ($\hat{\beta}_{0,\alpha}$)	23.9	28.1	32.2
AIC	1156.729	1071.145	1174.435
	Model		
	$\tau = 0.1, \alpha = 0.9$	$\tau = \alpha = 0.5$	$\tau = 0.9, \alpha = 0.1$
Intercept ($\hat{\beta}_{0,\alpha}$)	20.7 (20.4, 20.8)	23.9 (22.9, 24.8)	31.4 (28.8, 33.8)
Slope ($\hat{\beta}_{1,\alpha}$)	0.094 (0.092, 0.097)	0.067 (0.057, 0.086)	0.013 (-0.012, 0.037)
AIC	860.4221	962.9234	1174.0644
LR-test Model vs Null model	$D_0 - D = 298.3$	$D_0 - D = 110.2$	$D_0 - D = 2.37$
Reject if $> \chi^2_{0.05}(1) = 3.84$	sign.	sign.	n.s.

Parameters changing with α

```
plot(summary(rq(..., tau = seq(0.1, 0.9, 0.1))))
```



- Black dots show increasing intercepts and decreasing slopes for varying $\tau = 1 - \alpha$ levels. Grey areas are the corresponding 95 % confidence bands.
- Horizontal red lines are the least squares estimates with 95 % confidence intervals, assuming all quantiles have the same slope.

- You cannot compared nested models using `anova()`.
- You cannot use `step` for forward/backward/stepwise selection.
- `AIC()` can only handle one model at a time and will give AIC for each separate tau. `BIC()` does not work.
- No R^2 or pseudo R^2.
- Advantages of QR:
  - does not require assumptions on the distribution of Y,
  - more robust to outliers than least squares (quantiles do not change that much in presence of outliers).
- Disadvantages of QR: due to lack of distribution assumptions the estimated asymptotic variance of $\hat{\boldsymbol{\beta}}_{\boldsymbol{\alpha}}$ does **not** attain minimal variance (Cramer-Rao bound), unlike maximum likelihood estimates (MLE).