Lecture 03: Classical Inferential Statistics I: Basics and Confidence Intervals

3.1 Expectation and Covariance Matrix of the Ordinary Least Squares (OLS) Estimator

3.2 Confidence Intervals

▶ Only stochasticity: residual errors ϵ according to $y = X\beta + \epsilon$

► The OLS estimator is linear in *y*:

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$$\hat{\boldsymbol{eta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{y}$$

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= \underline{\boldsymbol{\beta}} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\epsilon}$$

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Expectation value

$$E(\hat{\boldsymbol{\beta}}) = E(\boldsymbol{\beta}) + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'E(\boldsymbol{\epsilon}) = \boldsymbol{\beta}$$

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Expectation value

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The OLS estimator of parameter-linear models is **un-biased** under the mild condition $E(\epsilon) = 0$ for all the data points

- ▶ Gauß-Markow conditions $\rightarrow \epsilon \sim i.i.dN(0,\sigma^2) \rightarrow \hat{\beta}$ is normal distributed
- In this case, the complete error characteristics are specified by the expectation value and the variance-covariance matrix V ²_A

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$$[E(.) \text{ acts only on } \boldsymbol{\epsilon} \rightarrow] = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'E(\boldsymbol{\epsilon}\boldsymbol{\epsilon}')\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$$

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The variance-covariance matrix depends only on the values of the exogenous factors!



Ordinary least squares (OLS) estimator:

$$\hat{\boldsymbol{eta}} = \left(\mathbf{X}' \mathbf{X} \right)^{-1} \mathbf{X}' \boldsymbol{y}$$

Variance-Covariance matrix of the estimation errors (provided the errors are i.i.d.) can be written in terms of the Hesse matrix H of the objective function SSE:

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- Variances of estimation errors: $V(\hat{\beta}_j) = V_{jj}$
- Correlation of estimation errors: $\operatorname{Corr}(\hat{\beta}_j, \hat{\beta}_k) = \frac{V_{jk}}{\sqrt{V_{jj}V_{kk}}}$

▶ Distribution of the normalized estimation errors: $\frac{\beta_i - \beta_i}{\sqrt{V_{i,i}}} \sim N(0,1)$



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Estimation of the residual variance

The above cannot be applied directly since the residual variance σ^2 is unknown and must be estimated by the minimum SSE $S(\hat{\beta})$:

$$\hat{\sigma}^2 = \frac{1}{n-J-1} \sum_i (y_i - \hat{y}(\boldsymbol{x}_i))^2 = \frac{S(\hat{\beta})}{n-J-1}$$

Under the Gauß-Markow assumptions, this can be expressed as the sum of squared Gaussians as follows (derivation for the experts):

$$(n - J - 1)\hat{\sigma}^2 = (\hat{\boldsymbol{y}} - \boldsymbol{y})'(\hat{\boldsymbol{y}} - \boldsymbol{y})$$
$$= (\mathbf{X}\,\hat{\boldsymbol{\beta}} - \boldsymbol{y})'(\mathbf{X}\,\hat{\boldsymbol{\beta}} - \boldsymbol{y})$$
$$= (\mathbf{X}\,\hat{\boldsymbol{\beta}})'(\mathbf{X}\,\hat{\boldsymbol{\beta}}) - (\mathbf{X}\,\boldsymbol{\beta})'\boldsymbol{y} - \boldsymbol{y}'(\mathbf{X}\,\boldsymbol{\beta}) + \boldsymbol{y}'\boldsymbol{y}$$

With following rule for scalar products: a'b = b'a it follows that the two middle terms are equal. Replacing $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'y$ we see that, interestingly, the first term is the negative of each of the two middle terms resulting in

$$(n - J - 1)\hat{\sigma}^2 = \boldsymbol{y}' \left(\boldsymbol{1} - \boldsymbol{X} \left(\boldsymbol{X}' \boldsymbol{X} \right)^{-1} \boldsymbol{X}' \right) \boldsymbol{y}$$

Estimation of the residual variance (ctned)

Finally, we replace the observed endogeneous data vector y by the model $y = \mathbf{X}\beta + \epsilon$ Notice: the true and, according to the Gauß-Markow assumptions, immutable parameter vector β is used here!:

$$\begin{split} (n-J-1)\hat{\sigma}^2 &= (\mathbf{X}\,\boldsymbol{\beta} + \boldsymbol{\epsilon})' \left(\mathbf{1} - \mathbf{X}\,(\mathbf{X}\,'\mathbf{X}\,)^{-1}\mathbf{X}\,'\right) (\mathbf{X}\,\boldsymbol{\beta} + \boldsymbol{\epsilon}) \\ &= \boldsymbol{\epsilon}'(\mathbf{1} - \mathbf{X}\,(\mathbf{X}\,'\mathbf{X}\,)^{-1}\mathbf{X}\,')\boldsymbol{\epsilon} \\ &+ 2(\mathbf{X}\,\boldsymbol{\beta})'(\mathbf{1} - \mathbf{X}\,(\mathbf{X}\,'\mathbf{X}\,)^{-1}\mathbf{X}\,')\boldsymbol{\epsilon} + \boldsymbol{\beta}'\mathbf{X}\,'(\mathbf{1} - \mathbf{X}\,(\mathbf{X}\,'\mathbf{X}\,)^{-1}\mathbf{X}\,')\boldsymbol{\epsilon} \end{split}$$

After doing the simplification, we realize that the second and third term are each equal to zero, so we have the final result

$$(n-J-1)\hat{\sigma}^2 = \boldsymbol{\epsilon}'(\mathbf{1} - \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')\boldsymbol{\epsilon}$$

With the Gauß-Markow-assumptions, this is proportional to a sum of (n-J-1) squared Gaussians, i.e., a $\chi^2(n-J-1)$ distributed random variable

Results if the variance needs to be estimated

Estimated variance-covariance matrix:

$$\hat{\mathbf{V}}_{\hat{\boldsymbol{\beta}}} = 2\hat{\sigma}^{2}\mathbf{H}^{-1} = \hat{\sigma}^{2}\left(\mathbf{X}'\mathbf{X}\right)^{-1}$$

The normalized approximate estimation errors are student-t distributed (a Gaussian in the numerator and the square root of a χ² distributed random variable in the denominator):

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{V}_{jj}}} \sim T(n - 1 - J)$$

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Multivariate distribution function of $\hat{\boldsymbol{\beta}}$

The distribution of the errors $\Delta \hat{\beta} = \hat{\beta} - \beta$ obeys a multivariate normal distribution:

$$f_{\hat{\boldsymbol{\beta}}}(\Delta \hat{\boldsymbol{\beta}}) \propto \exp\left[-\frac{1}{2}\Delta \hat{\boldsymbol{\beta}}' \mathbf{V}^{-1} \Delta \hat{\boldsymbol{\beta}}\right] = \exp\left[-\frac{\Delta \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} \Delta \hat{\boldsymbol{\beta}}}{2\sigma_{\epsilon}^{2}}\right]$$

Relation to the maximum-likelihood-method (\rightarrow Lecture 07:) Expand the SSE $S(\beta)$ around $\hat{\beta}$ to second order:

$$S(\boldsymbol{\beta}) - S(\hat{\boldsymbol{\beta}}) \approx \frac{1}{2} \Delta \hat{\boldsymbol{\beta}}' \mathbf{H} \ \Delta \hat{\boldsymbol{\beta}} = \Delta \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} \ \Delta \hat{\boldsymbol{\beta}}$$

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and with the estimated residual variance $\hat{\sigma}_{\epsilon}^2 = S(\hat{oldsymbol{eta}})/(n-J-1)$

$$\hat{f}_{\hat{\beta}}(\beta) \propto \exp\left[-\frac{(n-J-1)}{2}\left(\frac{S(\beta)}{S(\hat{\beta})}-1\right)\right]$$

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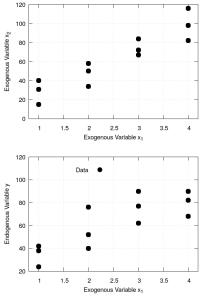
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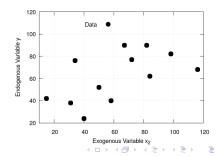
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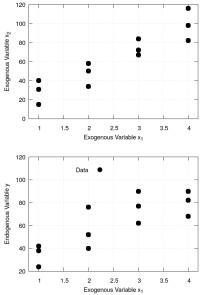


The example of Lecture 02:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

- Exogenous factors: x₀ = 1, x₁: proxy for quality [# stars]; x₂: price [€/night].
- Endogenous variable: booking rate [%]
- The demand is positively correlated with both the quality and the price

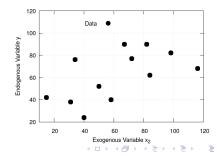


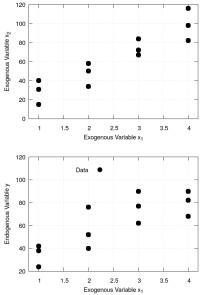


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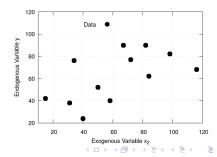


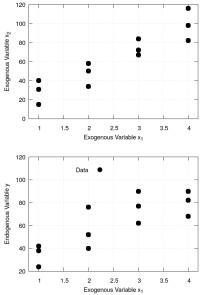


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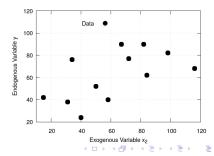




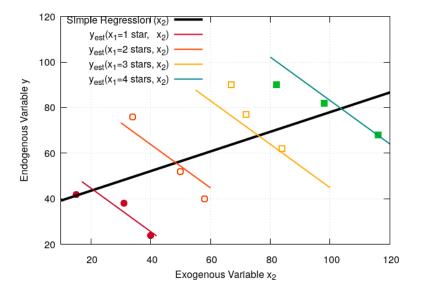
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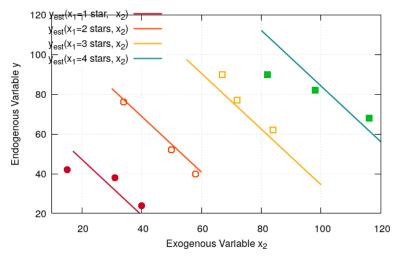
Residual errors for fitted parameters



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Effect of mis-fit parameters I: small effect if β_1 and β_2 have opposite misfits

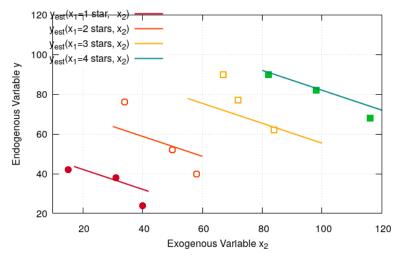




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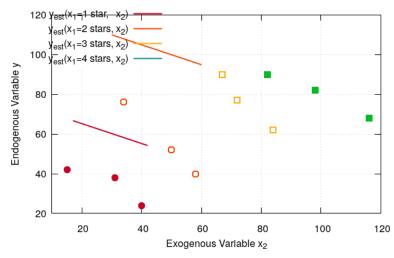
Effect of mis-fit parameters II: small effect if β_1 and β_2 have opposite misfits





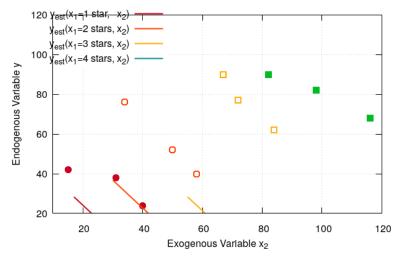
Effect of mis-fit parameters III: large effect if β_1 and β_2 have both positive misfits





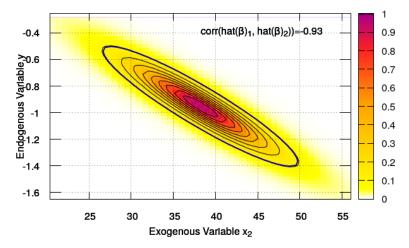
Effect of mis-fit parameters IV: large effect if β_1 and β_2 have both negative misfits





All this results in a negative correlation between the estimation errors for β_1 and β_2

Density hat(f) (hat(β)₁, hat(β)₂) | β ₁=38.21, β ₂=-0.95



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- Model: $y = \beta_0 + \epsilon := \mu + \epsilon$
- System matrix: $\mathbf{X} = (1, 1, ..., 1)'$
- OLS estimator:

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$$(\mathbf{X}'\mathbf{X})^{-1} = \frac{1}{n}, \quad \mathbf{X}'\mathbf{y} = \sum_{i} y_{i} = n\bar{y},$$
$$\hat{\beta}_{0} = \hat{\mu} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \bar{y}$$

► Variance:
$$V_{00} = V(\hat{\mu}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1} = \frac{\sigma^2}{n}$$
, $\hat{V}_{00} = \frac{\hat{\sigma}^2}{n}$

• Distribution of the estimator (if $\epsilon \sim i.i.dN(\mu, \sigma^2)$)

$$\begin{array}{ll} \displaystyle \frac{\hat{\beta}_0 - \beta_0}{\sqrt{V_{00}}} & = & \displaystyle \frac{\bar{y} - \mu}{\sigma} \sqrt{n} \sim N(0, 1), \\ \displaystyle \frac{\hat{\beta}_0 - \beta_0}{\sqrt{V_{00}}} & = & \displaystyle \frac{\bar{y} - \mu}{\hat{\sigma}} \sqrt{n} \sim T(n - 1) \end{array}$$

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Special case 2: Simple linear regression

• Model (with $x_1 = x$): $y = \beta_0 + \beta_1 x + \epsilon$

System matrix:

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \quad \mathbf{X}'\mathbf{X} = \begin{pmatrix} n & n\bar{x} \\ n\bar{x} & \sum x_i^2 \end{pmatrix}$$

• OLS estimator (with $s_x^2 = 1/n(\sum x_i^2 - n\bar{x}))$:

$$\left(\mathbf{X}'\mathbf{X} \right)^{-1} = \frac{1}{ns_x^2} \left(\begin{array}{cc} \frac{\sum x_i^2}{n} & -\bar{x} \\ -\bar{x} & 1 \end{array} \right), \quad \mathbf{X}'\mathbf{y} = \left(\begin{array}{c} n\bar{y} \\ \sum x_iy_i \end{array} \right)$$

$$\hat{\beta}_1 = \left(-\frac{\bar{x}}{ns_x^2}, \frac{1}{ns_x^2}\right) \left(\begin{array}{c}n\bar{y}\\\sum x_iy_i\end{array}\right) = \frac{\sum_i x_iy_i - n\bar{x}\bar{y}}{\sum x_i^2 - n\bar{x}} = \frac{s_{xy}}{s_x^2},$$
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Simple linear regression (ctnd)

Variance-covariance matrix (assuming w/o loss of generality $\bar{x} = 0$):

$$\mathbf{V}(\hat{\boldsymbol{\beta}}) = \sigma^2 \left(\mathbf{X}' \mathbf{X} \right)^{-1} = \sigma^2 \left(\begin{array}{cc} \frac{1}{n} & 0\\ 0 & \frac{1}{ns_x^2} \end{array} \right)$$

• Variance of the estimator $\hat{y}(x)$ (x is deterministic):

$$V(\hat{y}(x)) = V(\hat{\beta}_0 + \hat{\beta}_1 x) = V_{00} + x^2 V_{11} + 2x V_{01} = \frac{\sigma^2}{n} \left(1 + \frac{x^2}{s_x^2} \right)$$

• Distribution of the estimator for y(x):

$$\hat{y}(x) \sim N\big(y(x), V(\hat{y}(x))\big)$$

If σ^2 has to be estimated by $\hat{\sigma}^2$, the normalized estimators for β_0 , β_1 and y(x) are $\sim T(n-2)$.

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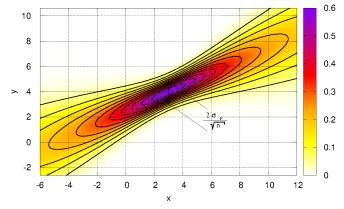
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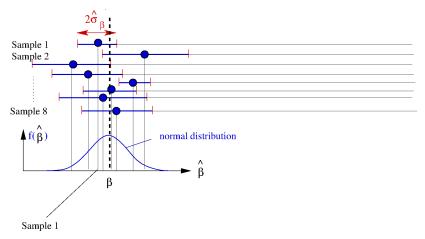
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Probability density for $\hat{y}(x)$ for simple linear regression

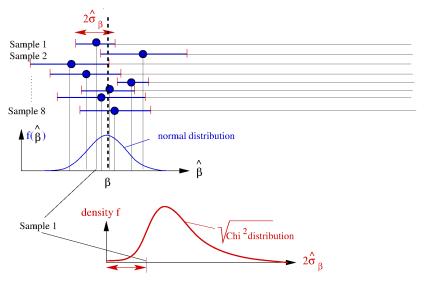


- ▶ If the Gauß-Markov assumptions apply, the model estimation errors $\hat{y}(x) y(x)$ are Gaussian distributed
- The expectation and variance depends on x; the standard error is hyperbola-shaped.

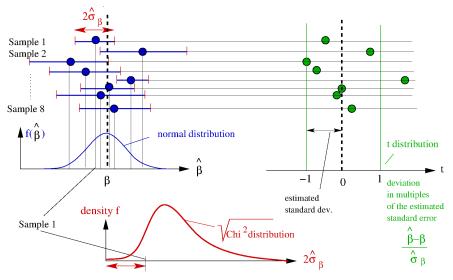
3.2. Confidence Intervals: where the Student-t distribution comes from



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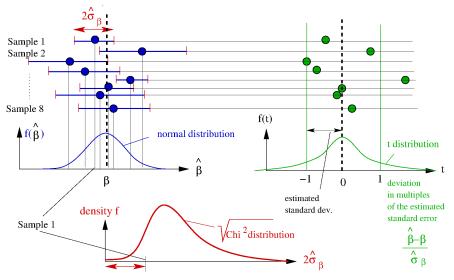


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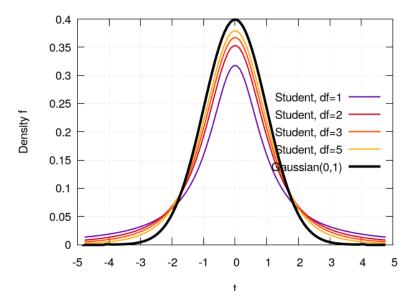


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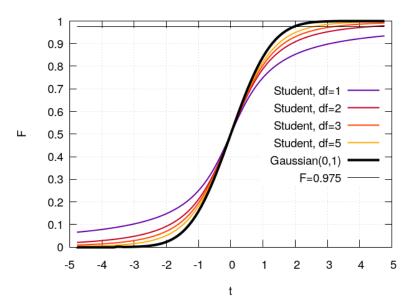


Densities of standard normal vs. Student-t distribution



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Distributions of standard normal vs. Student-t-distribution



Calculation of the confidence intervals (CI)

$$\mathsf{Cl}_{\beta_j}^{(\alpha)}:\beta_j\in\left[\,\hat\beta_j-\Delta\hat\beta_j,\hat\beta_j+\Delta\hat\beta_j\,\right],\quad \Delta\hat\beta_j=t_{1-\alpha/2}^{(n-J-1)}\hat\sigma_{\hat\beta_j}.$$

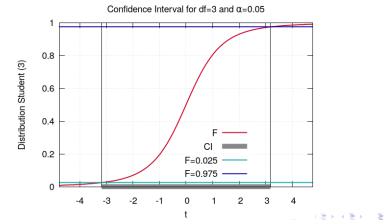
• $t_{1-\alpha/2}$: Quantile (inverse of) the distribution function

Equation CI "uncertainty principle": Higher sensitivity implies higher α error.

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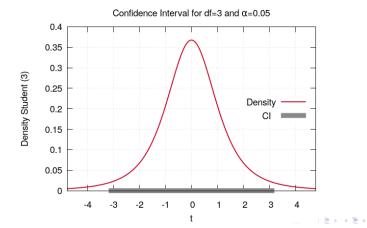


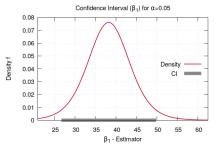
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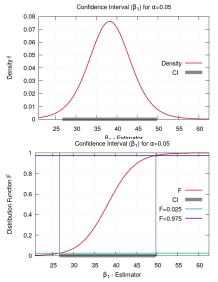


Model: $y(\boldsymbol{x}) = \sum_{j} \beta_{j} x_{j} + \epsilon$

Factors: $x_0 = 1, x_1$: #stars, x_2 : price

Confidence interval (CI):

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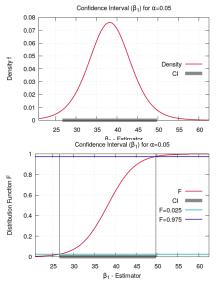
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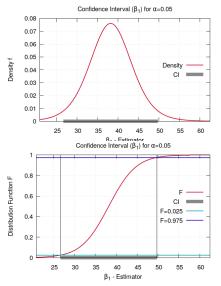
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Factors: $x_0 = 1, x_1$: #stars, x_2 : price

Confidence interval (CI):

$$\begin{split} \beta_1 &\in \left[\hat{\beta}_1 - \Delta \hat{\beta}_1^{(\alpha)}, \hat{\beta}_1 + \Delta \hat{\beta}_1^{(\alpha)}\right] \\ \Delta \hat{\beta}_1^{(\alpha)} &= t_{1-\alpha/2}^{(n-3)} \sqrt{\hat{V}(\hat{\beta}_1)} \\ \hat{V}(\hat{\beta}_1) &= \hat{\sigma}_{\epsilon}^2 \left[\left(\mathbf{X}'\mathbf{X}\right)^{-1} \right]_{11} \\ \hat{\sigma}_{\epsilon}^2 &= \frac{1}{n-3} \sum_{i=1}^n \left(\hat{y}_i - y_i \right)^2 \end{split}$$

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