Statistics and learning

Regression

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The regression model

- expresses a random variable Y as a function of random variables $X \in \mathbb{R}^p$ according to:

$$Y = f(X; \beta) + \epsilon,$$

where functional f depends on **unknown parameters** $\beta_1, \ldots, \beta_k$ and the **residual** (or **error**) ϵ is an unobservable rv which accounts for random fluctuations between the model and Y.

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  - if the fit is acceptable, tests on parameters can be performed and the model can be used for **predictions**

Simple linear regression

- A single **explanatory variable** X and an affine relationship to the **dependant variable** Y:

$$E[Y \mid X = x] = \beta_0 + \beta_1 x \text{ or } Y_i = \beta_0 + \beta_1 X_i + \epsilon_i,$$

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- Hence: $E[Y_i] = \beta_0 + \beta_1 x_i$, $\mathrm{Var}(Y_i) = \sigma^2$ and $\mathrm{Cov}(Y_i, Y_j) = 0, \quad \forall i \neq j$.

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- Fitting (or adjusting) the model = estimate β_0, β_1 and σ from the n-sample (x_i, y_i).

Least square estimate

- Seeking values for β_0 and β_1 minimising the sum of quadratic errors:

$$(\hat{\beta}_0, \hat{\beta}_1) = \text{argmin}_{(\beta_0,\beta_1)\in\mathbb{R}^2} \sum \left[y_i - (\beta_0 + \beta_1 x_i)\right]^2$$

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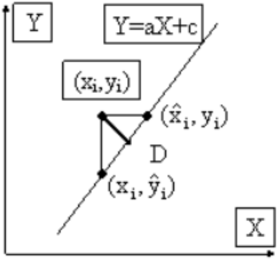

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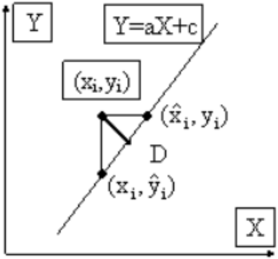

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- In matrix notation (useful later): $Y = X.B + \epsilon$, with $Y = {}^\top(Y_1 \dots Y_n)$, $B = {}^\top(\beta_0, \beta_1)$, $\epsilon = {}^\top(\epsilon_1 \dots \epsilon_n)$ and $X = {}^\top \begin{pmatrix} 1 & \cdots & 1 \\ X_1 & \cdots & X_n \end{pmatrix}$.

Estimator properties

- useful notations: $\bar{x} = 1/n \sum_i x_i$, $\bar{y}$, s_x^2, s_y^2 and $s_{xy} = 1/(n-1) \sum_i (x_i - \bar{x})(y_i - \bar{y})$.

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Theorem

1. *Least Square estimators are* $\hat{\beta}_1 = s_{xy}/s_x^2$ *and* $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$*.*
2. *These estimators are unbiased and efficient.*
3. $s^2 = \frac{1}{n-2} \sum_i \left[y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i) \right]^2$ *is an unbiased estimator of* σ^2*. It is however not efficient.*
4. $\mathrm{Var}(\hat{\beta}_1) = \frac{\sigma^2}{(n-1)s_x^2}$ *and* $\mathrm{Var}(\hat{\beta}_0) = \bar{x}^2 \mathrm{Var}(\hat{\beta}_1) + \sigma^2/n$

Simple Gaussian linear model

- In addition to R1 (centred noise), R2 (equal variance noise) and R3 (uncorrelated noise), we assume (R3') $\forall i \neq j$, ϵ_i and ϵ_j independent and (R4) $\forall i$, $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ or equivalently $y_i \sim \mathcal{N}(\beta_0 + \beta_1 x_i, \sigma^2)$.

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Theorem (Distribution of estimators)

1. $\hat{\beta}_0 \sim \mathcal{N}(\beta_0, \sigma^2_{\hat{\beta}_0})$ *and* $\hat{\beta}_1 \sim \mathcal{N}(\beta_0, \sigma^2_{\hat{\beta}_1})$, *with* $\sigma^2_{\hat{\beta}_0} = \sigma^2 \left(\bar{x}^2 / \sum_i (x_i - \bar{x})^2 + 1/n\right)$ *and* $\sigma^2_{\hat{\beta}_1} = \sigma^2 / \sum_i (x_i - \bar{x})^2$
2. $(n-2)s^2/\sigma^2 \sim \chi^2_{n-2}$
3. $\hat{\beta}_0$ *and* $\hat{\beta}_1$ *are independent of* $\hat{\epsilon}_i$.
4. *Estimators of* $\sigma^2_{\hat{\beta}_0}$ *and* $\sigma^2_{\hat{\beta}_1}$ *are given in 1. by replacing* σ^2 *by* s^2.

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- **Definition**: Determination coefficient $R^2 = \frac{\sum_i (\hat{y_i} - \bar{y})^2}{\sum_i (y_i - \bar{y})^2} = \frac{SSR}{SST} = 1 - \frac{SSE}{SST} = 1 - \frac{\text{Residual Variance}}{\text{Total variance}}$.

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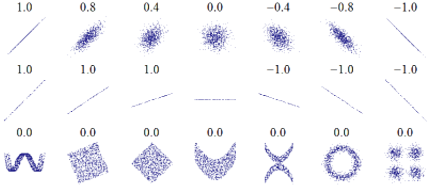
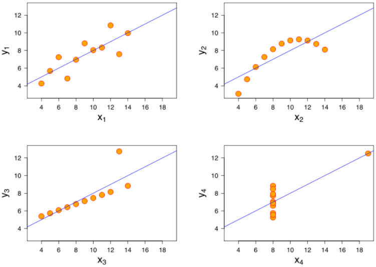
$\rightarrow$ Always use scatterplots to interpret linear model adequacy



same $R^2 = 0.667$



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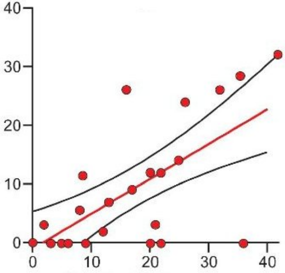
- The precision varies according to the x^* value you want to predict:



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- Parameter estimation: $\mathrm{argmin}_\beta \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_i^j - \beta_0 \right)^2 \Leftrightarrow \mathrm{argmin}_\beta \sum_i \hat{\epsilon_i}^2 \Leftrightarrow \mathrm{argmin}_\beta \|Y - X\beta\|_2^2$.

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- **Theorem** The Least Square Estimator of β is $\hat{\beta} = ({}^\top X X)^{-1}\, {}^\top X\, Y$.

Properties of the least square estimate

Theorem

The estimator $\hat{\beta}$ previously defined is s.t.

1. $\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2({}^\top X X)^{-1})$ *and*
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Theorem

$\hat{Y} = X\hat{\beta}$*: predicted values. Then* $\hat{Y} = H\,Y$*, with* $H = X\,({}^\top X\,X)^{-1}\,{}^\top X$*;* $\epsilon = Y - \hat{Y} = (Id - H)\,Y$*. Note that* H *is the orthogonal projection on* $\mathrm{Vect}(X) \subset \mathbb{R}^n$*. We have:*

1. $\mathrm{Cov}(\hat{Y}) = \sigma^2 H$,
2. $\mathrm{Cov}(\epsilon) = \sigma^2(Id - H)$ *and*
3. $\hat{\sigma^2} = \frac{\|\epsilon^2\|}{n-p-1}$.

Practical uses

- CI for β_j: $[\hat{\beta}_j + / - t_{n-p-1;1-\alpha/2}\sigma_{\hat{\beta}_j}]$, with $t_{n-p-1;1-\alpha/2}$ a Student-quantile and $\sigma_{\hat{\beta}_j}$ the squareroot of the j^{th} element of $\mathrm{Cov}(\hat{\beta})$.

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- Confidence region for $\beta = (\beta_0 \dots \beta_p)$:

$$R_{1-\alpha}(\beta) = \left\{ z \in \mathbb{R}^{p+1} | \, {}^{\top}(z - \hat{\beta}) \, {}^{\top}X \, X \, (z - \hat{\beta}) \leq (p+1)s^2 f_{k;n-p-1;1-\alpha} \right\}.$$

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- CI for previsions on y^*:

$$[y^* + / - t_{n-p-1;1-\alpha/2} s \left(1 +^\top x^* (^\top X\, X)^{-1}\right)^{1/2}].$$

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- test by ANOVA: $F = \frac{SSR/p}{SSE/(n-p-1)}$ has a Fisher distribution with $p, (n-p-1)$ df. Since testing (H0) $\beta_1 = \ldots = \beta_p = 0$ has little interest (rejected asa one of the variable is linked to Y), one can test (H0') $\beta_{i_1} = \ldots = \beta_{i_q} = 0$, with $q < p$ and $\frac{(SSR-SSR_q)/q}{SSE/(n-p-1)}$ has a Fisher distribution with $q, (n-p-1)$ df.

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- Application: variable selection for model interpretation: backward (remove 1 by 1 least significative with t-test), forward (include 1 by 1 most significative with F-test), stepwise (variant of forward).

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- to detect collinearity, compute $VIF(x_j) = \frac{1}{1-R_j^2}$, with R_j^2 the determination coefficient of x_j regressed againt $x \setminus \{x_j\}$. Perfect orthogonality is $VIF(x_j) = 1$ and the stronger the collinearity, the larger the value for $VIF(x_j)$.

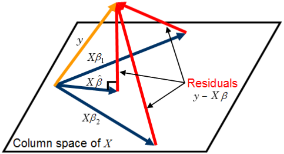
Collinearity and model selection

- detecting colinearity between the x_i's. Inverting ${}^\top X\,X$ if $\det({}^\top X\,X) \approx 0$ is difficult. Moreover, the inverse will have a huge variance !
- to detect collinearity, compute $VIF(x_j) = \frac{1}{1-R_j^2}$, with R_j^2 the determination coefficient of x_j regressed againt $x \setminus \{x_j\}$. Perfect orthogonality is $VIF(x_j) = 1$ and the stronger the collinearity, the larger the value for $VIF(x_j)$.
- Ridge regression introduces a bias but reduces the variance (keeps all variables). Lasso regression does the same but also does a selection on variables. Issue here: penalty term to tune...

Last generalisations

Multiple outputs, curvilinear and non-linear regressions

- Multiple output regression $Y = X\,B + E$, $Y\ in \mathrm{M}(n, K)$ and $X \in \mathrm{M}(n,p)$ so $RSS(B) = \mathrm{Tr}\left(^\top(Y - XB)(Y - XB)\right)$ (column-wise) or $\sum_i {}^\top(y_i - x_{i,.}B)\Sigma^{-1}(y_i - x_{i,.}B)$, with $\Sigma = \mathrm{Cov}(\epsilon)$ (correlated errors).



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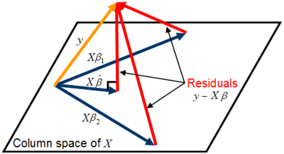

- Curvilinear models are of the form

$$Y = \beta_0 + \sum_j \beta_j x^j + \sum_{k,l} \beta_{k,l} x^k x^l + \epsilon.$$

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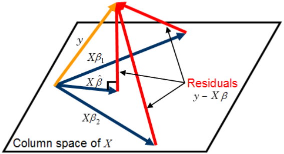

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- Non-linear (parametric) regression has the form $Y = f(x; \theta) + \epsilon$. Examples include exponential or logistic models.

Today's session is over

Next time: A practical R session to be studied by you !