Lecture 2 | 24.02.2025

Regression and classification

Regression ...

- Historically, an accidental word invented by Francis Galton (1822 – 1911) because the heights of sons, while following the tendency of their parents (tall parents had tall sons, small parents had small sons), tend to return – "regress" – towards the mediocrity/median/average (population stability).
- Nowadays, "regression" is understood as a technique for fitting functional relationships (not necessarily linear, nor parametric ones) to data (regardless of whether the "slope" or the direction is positive, or negative).
- Mathematically, the regression provides an explicit analytical formula for a (stochastic) relationship between one or more 'input' variable(s) $\boldsymbol{X} \in \mathbb{R}^p$ and an 'output' variable $Y \in \mathbb{R}$. It gives us an equation to predict (expected) values (or other specific characteristics) for the unknown output variable, by plugging in the observed values of the input variables.
- Generally, this functional relationship is of the form

$$Y = f(\boldsymbol{X}) + error$$

for some well-specified (but somehow still unknown) function f (model) and some unobserved random noise (errors, fluctuations, or disturbances).
$\hookrightarrow$ it is common to refer to a systematic and non-systematic part of Y...

Regression model fundaments

General/generic model formulation

$$Y = f(\boldsymbol{X}) + \varepsilon$$

- $Y \in \mathbb{R}$ is a random variable, the covariate of interest (dependent variable)
- $X \in \mathbb{R}$ (or $\boldsymbol{X} = (X_1, \ldots, X_p)^\top \in \mathbb{R}^p$) is a random variable (or a random vector respectively) which represents the set of explanatory information
- $f(\cdot)$ is a measurable regression function from the domain of X (or $\boldsymbol{X}$ respectively) to the domain of Y – the **systematic part**
- ε represents an irreducible (unobserved) error – even if we observe specific realizations of X and Y we do not know $f(\cdot)$ apriori, there is some uncertainty left due to the error term – the **non-systematic part**
- instead of "predicting" one specific value of Y using the regression (model) function $f(\cdot)$ and the observed realization "$X = x$" we would like to rather estimate some (more useful) characteristic of the whole distribution of possible values for Y when (conditionally on) "$X = x$"

Principal roles of the regression

Regression models and all kinds of data smoothing techniques (e.g., moving averages, weighted averages, splines, parametric smoothing, Whittaker-Henderson) are technically very similar but there is at least one principal and crucial difference – while the data smoothing techniques just smooth the empirical data the regression methods goes beyond as they try to learn important facts about the unknown population that is behind the data generating mechanism – the theoretical model behind the data.

- **Goal #1**
  with a good choice of the model (i.e., the regression function $f(\cdot)$) we can use the information contained in $\boldsymbol{X}$ (the explanatory variable) to say something relevant about Y (the dependent variable) **But why do we want to do so?**
- **Goal #2**
  if the set of the explanatory variables is relatively rich enough, it can be useful to say which components of $\boldsymbol{X} = (X_1, \ldots, X_p)^\top \in \mathbb{R}^p$ are relevant (play a role) in the relationship between Y and $\boldsymbol{X}$ **Why to select some if we can use all?**
- **Goal #3**
  once we know which information in $\boldsymbol{X} = (X_1, \ldots, X_p)^\top$ has an impact on the values of Y it is often of interest to quantify this effect – to evaluate how a specific component of $\boldsymbol{X}$ affects the value of Y **Why is this useful in practice?**

General regression setup

- Generic random vector $(Y, \boldsymbol{X}^\top)^\top$ with some joint distribution $F_{(Y,\boldsymbol{X})}(y, \boldsymbol{x})$
- Generic (population/theoretical) model: $Y = f(\boldsymbol{X}) + \varepsilon$

- Random sample from the population: $\{(Y_i, \boldsymbol{X}_i);\ i = 1, \ldots, n\}$ for $n \in \mathbb{N}$
- Empirical/data model: $Y_i = f(\boldsymbol{X}_i) + \varepsilon_i$ for $i = 1, \ldots, n$

- What is known: dependent observations Y_i and explanatory variable(s) $\boldsymbol{X}_i$
- What is unknown: random errors ε_i and the regression function $f(\cdot)$

- **Typical assumptions:**
  - the observations (random vectors $(Y_i, \boldsymbol{X}_i^\top)^\top$ for $i = 1, \ldots, n$) are independent and all with the same distribution as the vector $(Y, \boldsymbol{X}^\top)^\top$
  - the error terms (unobserved fluctuations or disturbances respectively) have a zero mean and some finite (typically unknown) variance $\sigma^2 > 0$
  - the unknown regression function $f(\cdot)$ is expected to belong to some well specified (reasonably defined) class of functions
  - and possibly others... (depending on the specific model formulations)

Conditional distribution of Y

- for different values of the independent variable X there are many possible values of the dependent variable Y that may theoretically occur in the data $\Longrightarrow$ conditional distribution of Y given "$X = x$"
  (in a sense an analogy to a $K \in \mathbb{N}$ sample problem, for $K \longrightarrow \infty$)
- infinitely many characteristics can be used to characterize the (conditional) distribution of Y (given X)... Which are good/ideal ones?
- the answer usually depends on the criterion we choose to measure the quality of the final model/fit – the so-called "goodness-of-fit" criterion

  - **Mean squared error** criterion (as a theoretical functional of $F_{(Y,\boldsymbol{X})(y,\boldsymbol{x})}$)

$$min_f E[Y - f(X)]^2$$

  - **Least squares** criterion (as an empirical counterpart of MSE)

$$min_f \frac{1}{n} \sum_{i=1}^{n} [Y_i - f(X_i)]^2$$

$\hookrightarrow$ where both minimization problems are taken with respect to some well-defined class of regression functions f (note the analogy between the theoretical mean and its empirical estimate – the arithmetic average)

Estimation of the regression function

- **Two sample problem**
  if X only takes two values (e.g., $X = \pm 1$), the observations (random sample) (Y_i, X_i) for $i = 1, \ldots, n$ can be split into two parts – values of Y_i for which $X_i = -1$ and the values of Y_i for which $X = 1$ and a simple average is calculated in both groups **(two-sample problem)**

- **Multiple samples**
  if X takes finitely many different values (e.g., X is a categorical variable with $K \in \mathbb{N}$ different levels), the random sample (Y_i, X_i) for $i = 1, \ldots, n$ can be split into K disjoint groups and, again, simple averages can be calculated for each of K groups **(analysis of variance – ANOVA)**

- **Continuous explanatory variable**
  if X is a continuous variable (taking infinitely/uncountable many values), the sample can not be split into all possible groups – for very many "$X = x$" there will be simply no observations of Y available
  $\Longrightarrow$ **borrowing power from the neighbors** **(regression problem)**

From local techniques to parametric ones (or vice versa?)

- **Nonparametric regression techniques**
  - the conditional distribution of Y given $X = x$ estimated locally for $x \in \mathbb{R}$
  - very flexible technique, adapts to any functional form of $f(\cdot)$
  - the number of unknown parameters to be estimated is large ($\to \infty$)
  - the amount of flexibility is an important aspect to control for

- **Parametric regression techniques**
  - a limited class of functions is used, the class depends on some parameters
  - the number of unknown parameter is relatively small (and fixed)
  - the flexibility of the model is determined by the analytical form of $f(\cdot)$
  - in many cases straightforward and relatively simple interpretation

- **Semi-parametric regression techniques**
  - a bridge between parametric and non-parametric methods
  - the idea is to select positive properties from both
  - negative properties are, however, inherited accordingly
  - still very popular in practical applications and theoretical developments

Some trade-offs to keep in mind

- **Mathematics:** parsimonious models vs. "black-box" algorithms
  (transparent models are tractable by mathematical theory)
- **Probability:** bias vs. variability of the estimate
  (small bias means better accuracy, large variance means high uncertainty)
- **Utilization:** prediction purposes vs. explanation of the relationship
  (different models are build depending on the primary purpose)
- **Computation:** computational tractability and time efficiency
  (limitations in algorithmic computations do not allow for arbitrary models)
- **Interpretation:** simple models are easy to interpret but less accurate
  (complex models are challenging (or even impossible) to be well explained)

"*All models are wrong, but some are useful!*"

George E. P. Box (1919 – 2013)

Model accuracy

Let's assume that for a (generic) model $Y = f(X) + \varepsilon$ we obtained (some) estimate $\hat{f}(\cdot)$ based on the random sample $\{(Y_i, X_i)\}_{i=1}^{n}$

How to access the quality of $\hat{f}(\cdot)$ (the model accuracy) quantitatively?

- Using the "training data" $\{(Y_i, X_i);\ i = 1, \ldots, n\}$
- Using a fresh "testing data" $\{(Y_i, X_i);\ i = n+1, \ldots, N\}$

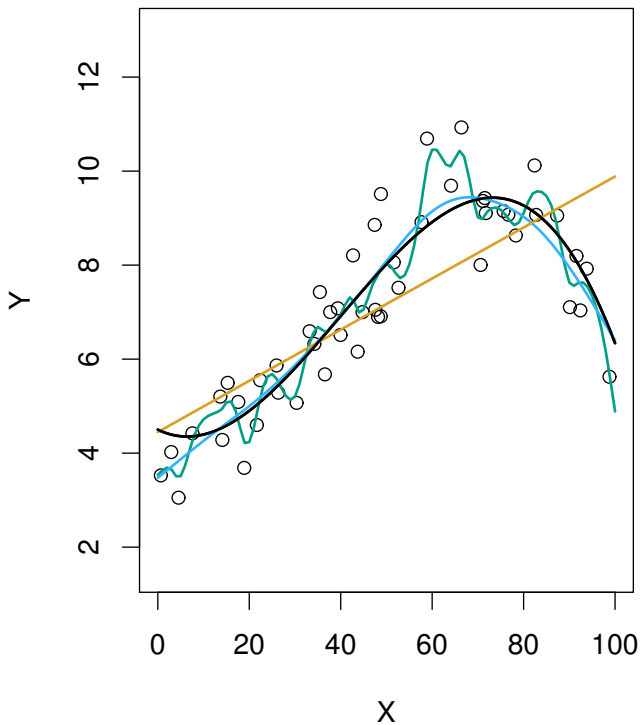
How to access the model quality (its accuracy) qualitatively?

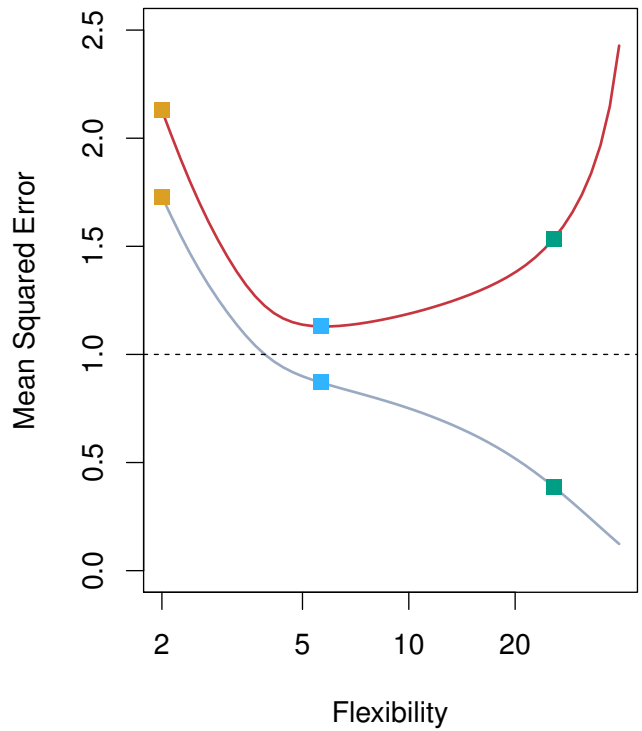
- Using mathematical/stochastic theory and various statistical tools
- Using expert knowledge, previous experience, common sense, etc.

Model prediction error – Example I

- unknown theoretical model $f(\cdot)$
- linear model estimate $\hat{f}_1(\cdot)$
- cubic model estimate $\hat{f}_2(\cdot)$
- polynomial model estimate $\hat{f}_3(\cdot)$

- least squares on training data
- least squares on **testing data**

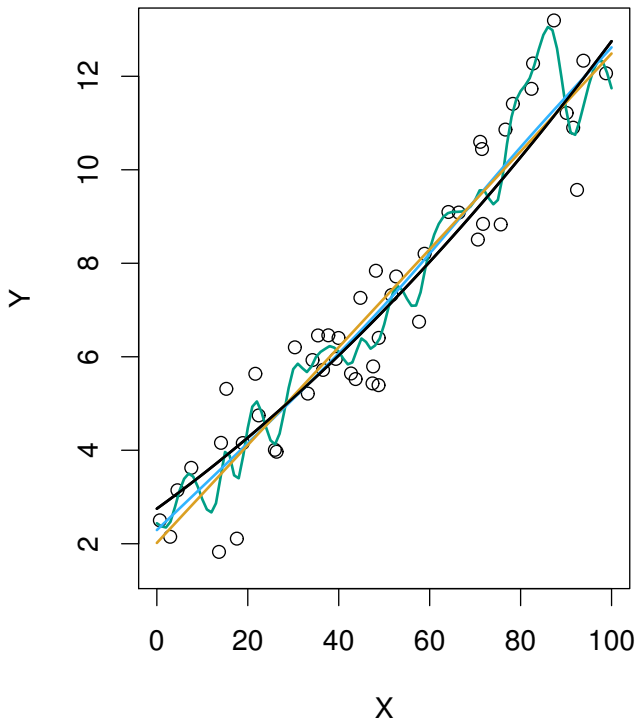


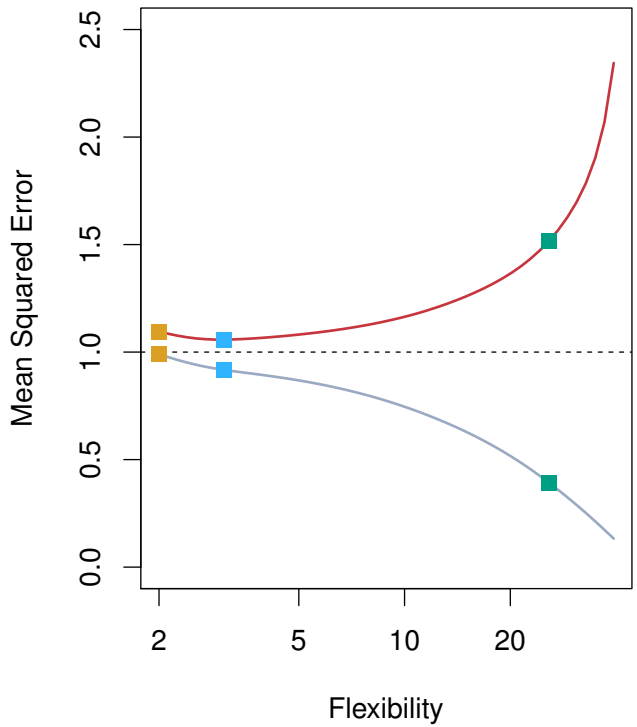


Model prediction error – Example II

- unknown theoretical model $f(\cdot)$
- linear model estimate $\hat{f}_1(\cdot)$
- cubic model estimate $\hat{f}_2(\cdot)$
- polynomial model estimate $\hat{f}_3(\cdot)$

- least squares on training data
- least squares on **testing data**

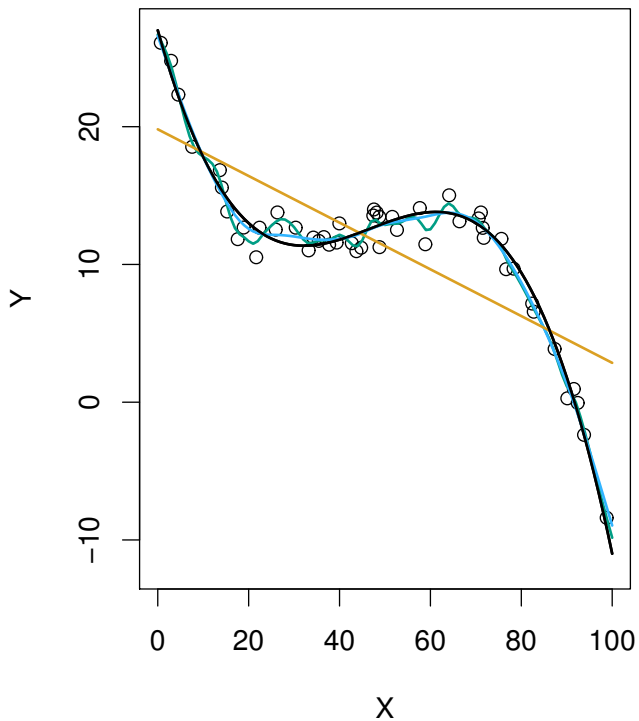


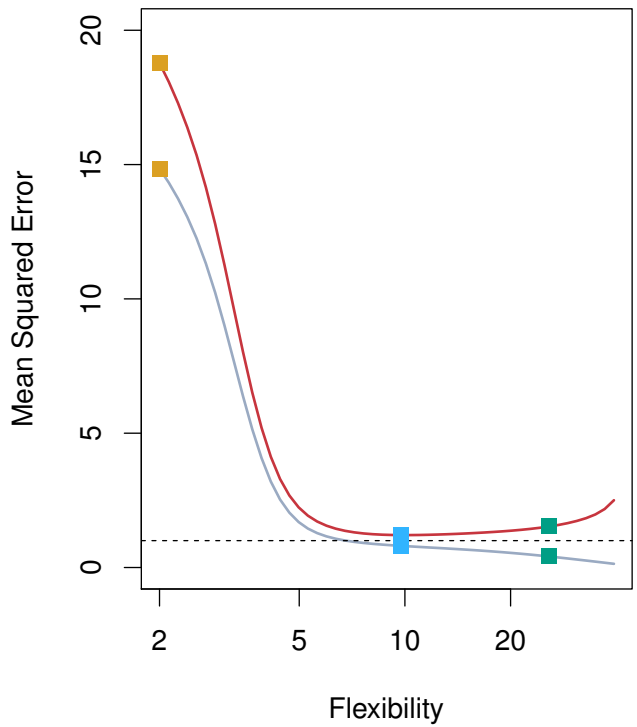


Model prediction error – Example III

- unknown theoretical model $f(\cdot)$
- linear model estimate $\hat{f}_1(\cdot)$
- cubic model estimate $\hat{f}_2(\cdot)$
- polynomial model estimate $\hat{f}_3(\cdot)$

- least squares on training data
- least squares on **testing data**

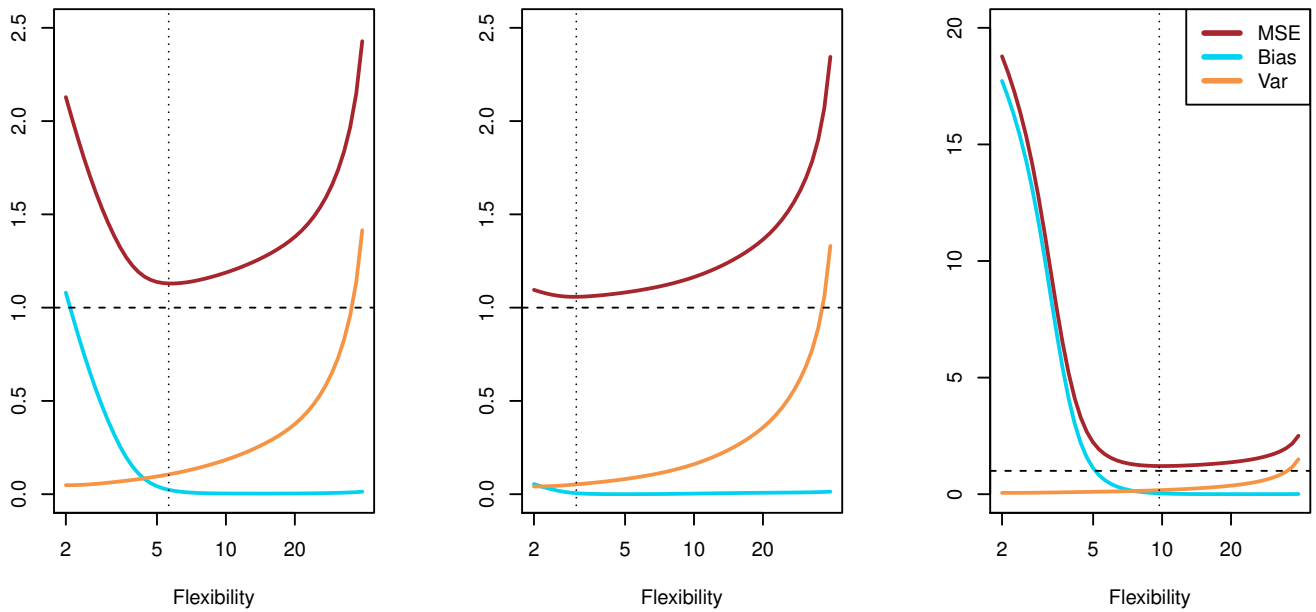




Bias-variance Trade-Off

Mean Squared Error (MSE):

$$
\begin{aligned}
E[Y - \hat{f}(X)]^2 &= E[(f(X) + \varepsilon - E\hat{f}(X)) - (\hat{f}(X) - f(X))]^2 \\
&= E[\hat{f}(X) - E\hat{f}(X)]^2 + \left(E\hat{f}(X) - f(X)\right)^2 + E\varepsilon^2 \\
&= Var\ \hat{f}(X) + \left(Bias\ \hat{f}(X)\right)^2 + Var\ \varepsilon
\end{aligned}
$$



Optimal model

- again, there are many different approaches to say which model is a good one (optimal one, useful or practical one, ...)
- in terms of the bias-variance trade-off the optimal model is the one that minimizes the mean squared error criterion
- the minimization of the mean squared criterion results in the minimization of the expected square of the error term
- in applications, instead of the theoretical (generic) error term ε we work with the empirical residual terms (residuals respectively)
- instead of minimizing the MSE criterion, we minimize the sum of the squared residuals (i.e., empirical counterpart for MSE)

More general: Regression vs. Classification

- what is the nature of the input variable(s) $\boldsymbol{X} \in \mathbb{R}^p$?
- what is the nature of the output variable $Y \in \mathbb{R}$?

- ordinary linear regression model
- analysis of variance
- classification
- contingency table

Vague motivation of the classification problem

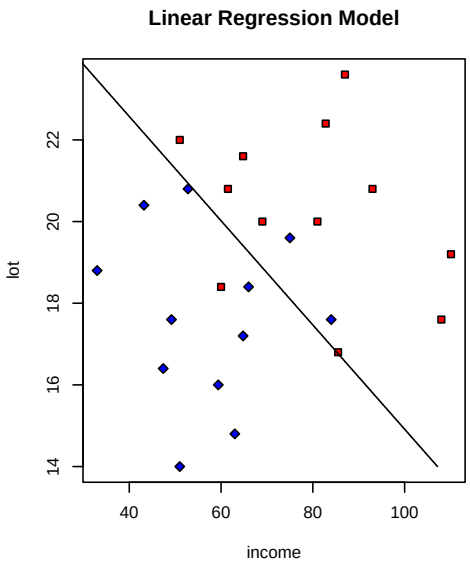
- in linear **regression problems** we typically deal with the situation where the response Y is continuous and the explanatory variables $\boldsymbol{X} = (X_1, \ldots, X_p)^\top$ are continuous/discrete/mixed
- if the response variable Y is qualitative (i.e., various labels) and the explanatory variables $\boldsymbol{X} = (X_1, \ldots, X_p)^\top$ are continuous/discrete/mixed we are (typically) referring to **classification problems**

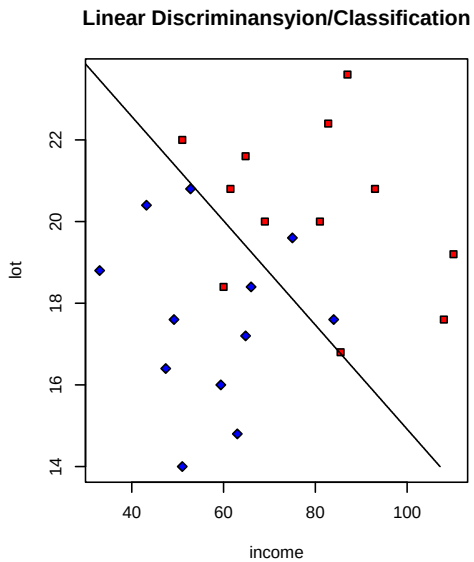
- However, vaguely speaking, the goal (in both) is to use the information in $\boldsymbol{X}$ to assign a value/classification label for Y (in other words, to decide into which "category" specified by "$\boldsymbol{X} = \boldsymbol{x}$" it belongs)
- the "goodness-of-fit" in classification problems is (commonly) measured by a missclassification error rate $\sum_{i=1}^{n} \mathbb{I}_{\{Y_i \neq \widehat{C}(\boldsymbol{X}_i)\}}$ where $\widehat{C}(\cdot)$ can be seen (for simplicity) as a classification version of the regression function $\hat{f}(\cdot)$
- the value $\widehat{C}(\boldsymbol{X}_i) \in \{1, \ldots K\}$ is the assigned classification label (a group assignment) which typically maximizes the posterior probability
  $\hookrightarrow$ so called the Bayes classification rule

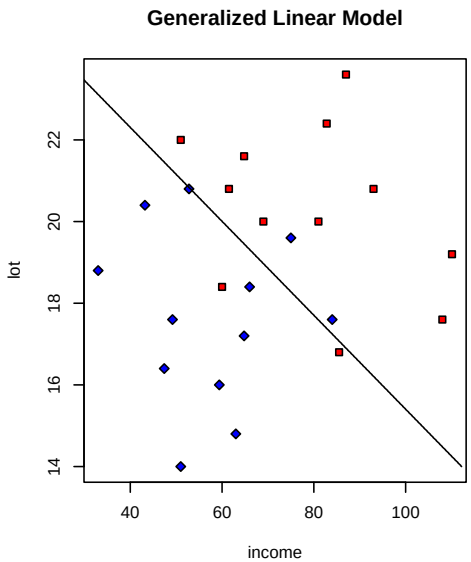
$\hookrightarrow$ **there are, in some sense, equivalent problems...**

Classification vs. regression problem

- Mowers data: $\{(Y_i, X_{i1}, X_{i2})^\top;\ i = 1, \ldots, 24\}$ Model: $Y_i \sim X_{i1} + X_{i2}$







Model 1

Model 2

Model 3

$$E[Y|X_1, X_2] = \alpha + \beta_1 X_1 + \beta_2 X_2$$

$$C(X_1, X_2) = \begin{cases} +1 & \text{if } \beta_1 X_1 + \beta_2 X_2 > \frac{\mu_1 + \mu_2}{2} \\ -1 & \text{if } \beta_1 X_1 + \beta_2 X_2 < \frac{\mu_1 + \mu_2}{2} \end{cases}$$

$$\log \frac{P[Y=1|X_1,X_2]}{1-P[Y=1|X_1,X_2]} = \alpha + \beta_1 X_1 + \beta_2 X_2$$

An outlook: Generalized regression models

- considering the model $Y = f(X) + \varepsilon$ and the support of the dependent variable Y which is limited/bounded/finite, it is not reasonable to assume, for instance, linear/unbounded/continuous function $f(\cdot)$ in the model...
- on the other hand, recall that model expressed as $Y = f(X) + \varepsilon$ and $E[Y|X = x] = f(x)$ are, actually (under some mild assumptions), two equivalent (linear regression) model formulations
- even discrete distribution of Y can be well-specified by some continuous characteristic – e.g., some probability parameter $p \in (0, 1)$
- how to mathematically formalize a regression model in such situations? $\hookrightarrow$ generalized (linear) regression models $g(E[Y = 1|X = x]) = f(x)$
- what are the analogies with the regression model $Y = f(X) + \varepsilon$?