18.650 – Fundamentals of Statistics

6. Linear regression

Goals

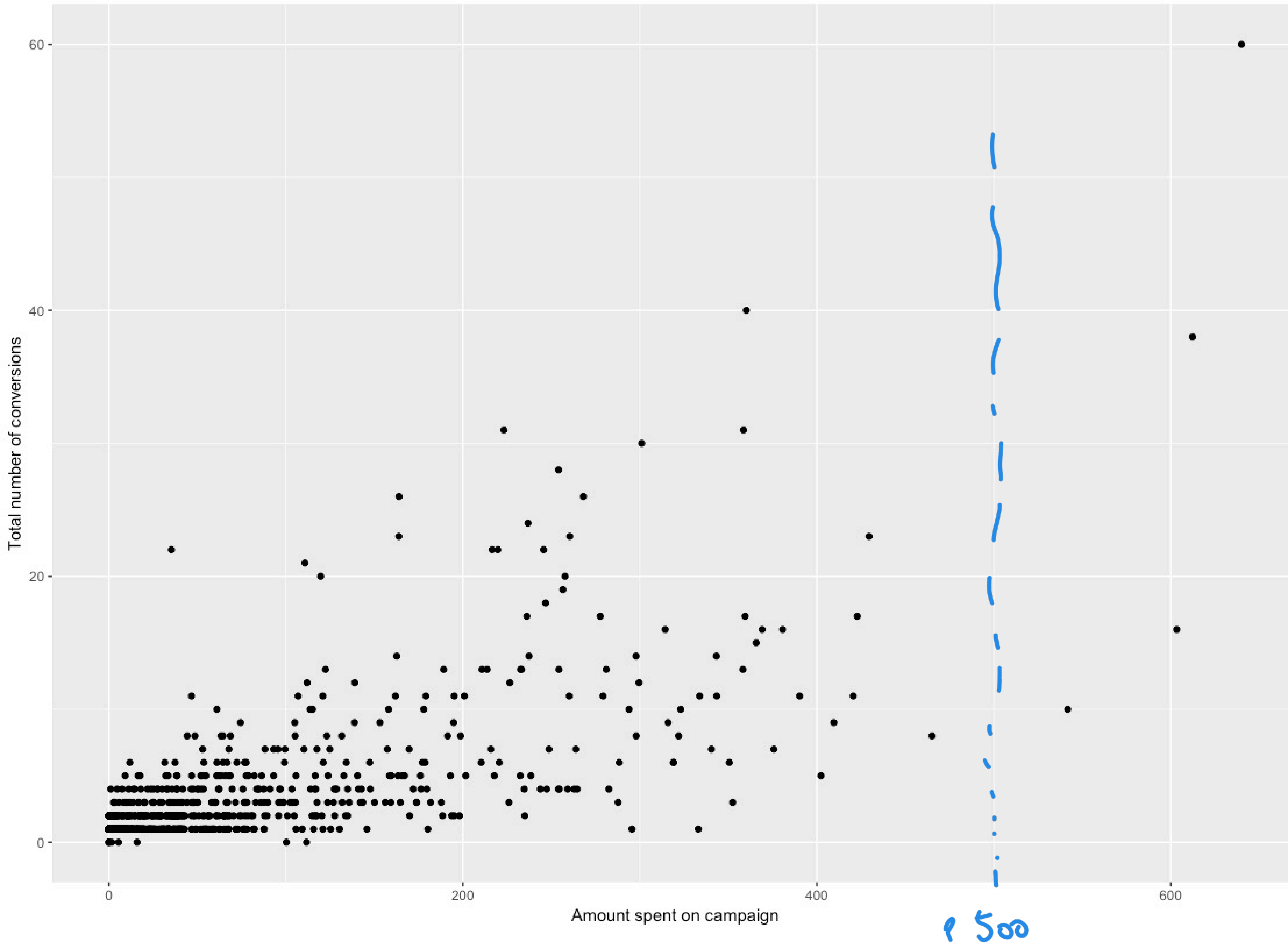
Consider two random variables X and Y. For example,

1. X is the amount of \$ spent on Facebook ads and Y is the total conversion rate
2. X is the age of the person and Y is the number of clicks

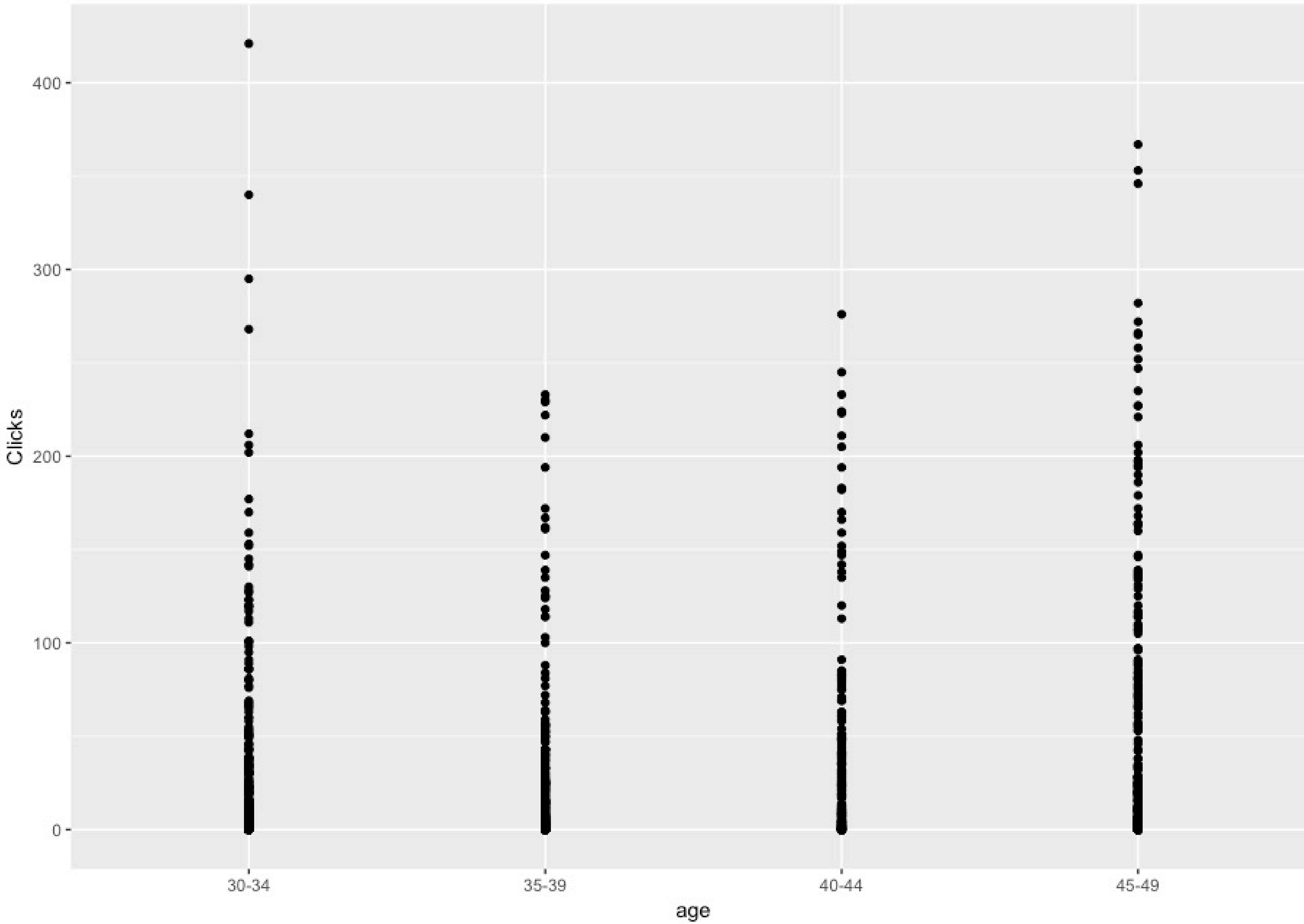
Given two random variables (X, Y), we can ask the following questions:

- How to predict Y from X?
- Error bars around this prediction?
- How much more conversions Y for an additional dollar?
- Does the number of clicks even depend on age?
- What if X is a random vector? For example, $X = (X_1, X_2)$ where X_1 is the amount of \$ spent on Facebook ads and X_2 is the duration in days of the campaign.

Conversions vs. amount spent



Clicks vs. age



Modeling assumptions

$(X_i, Y_i), i = 1, \dots, n$ are i.i.d from some **unknown joint distribution** $\mathbb{P}$.

$\mathbb{P}$ can be described entirely by (assuming all exist)

- Either a joint PDF $h(x, y)$
- The marginal density of X $h(x) = \int h(x,y)\,dy$ **and** the conditional density

$$h(y|x) = \frac{h(x,y)}{h(x)}$$

$h(y|x)$ answers all our questions. It contains all the information about Y given X.

Partial modeling

We can also describe the distribution only partially ,e.g., using

- The expectation of Y: $\mathbb{E}[Y]$
- The conditional expectation of Y given $X = x$: $\mathbb{E}[Y|X=x]$
  The function

$$x \mapsto f(x) := \mathbb{E}[Y|X = x] = \int y\, h(y|x)\, dy$$

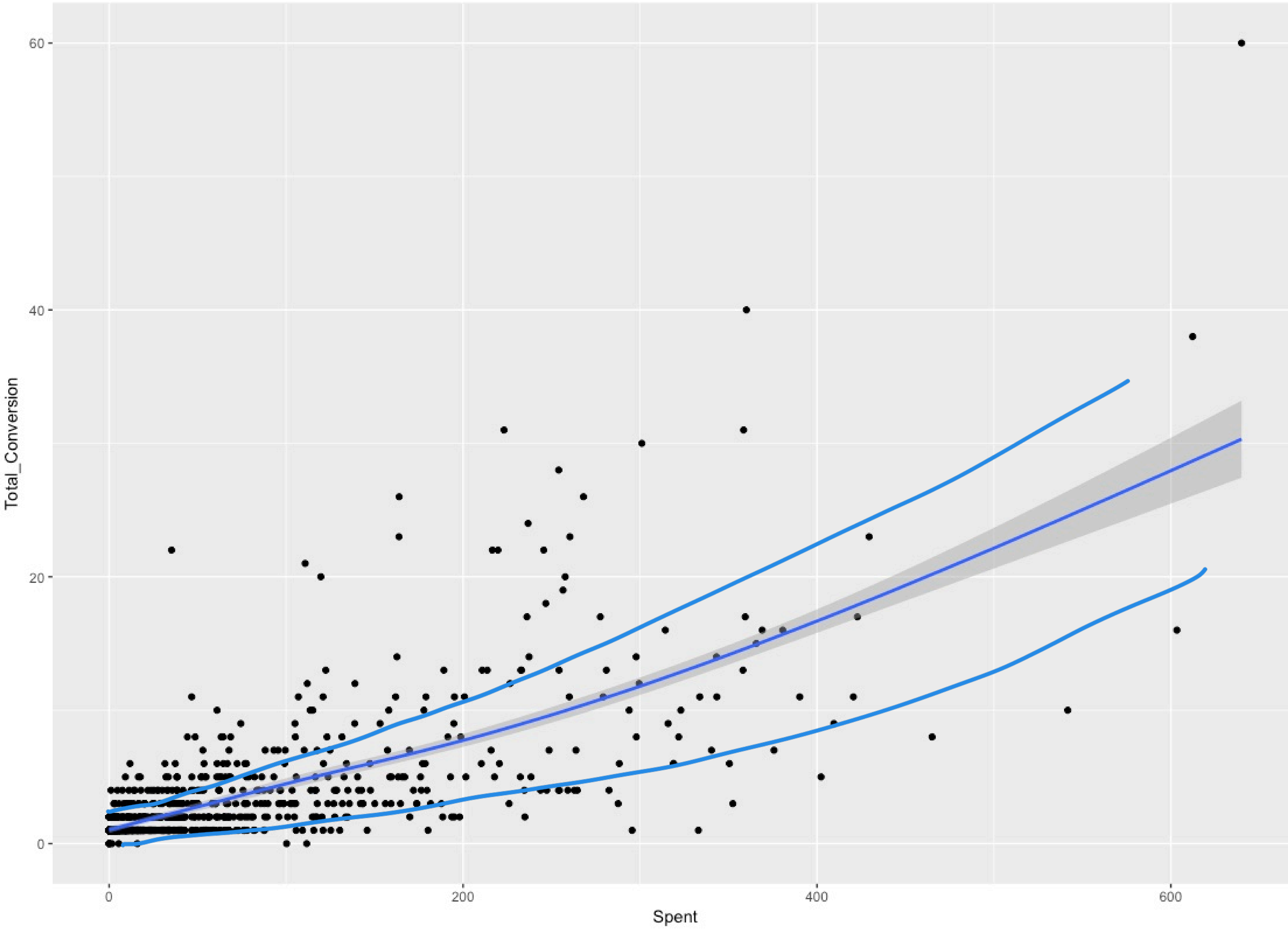
  is called regression function.

- Other possibilities:
  - The conditional median: $m(x)$ such that

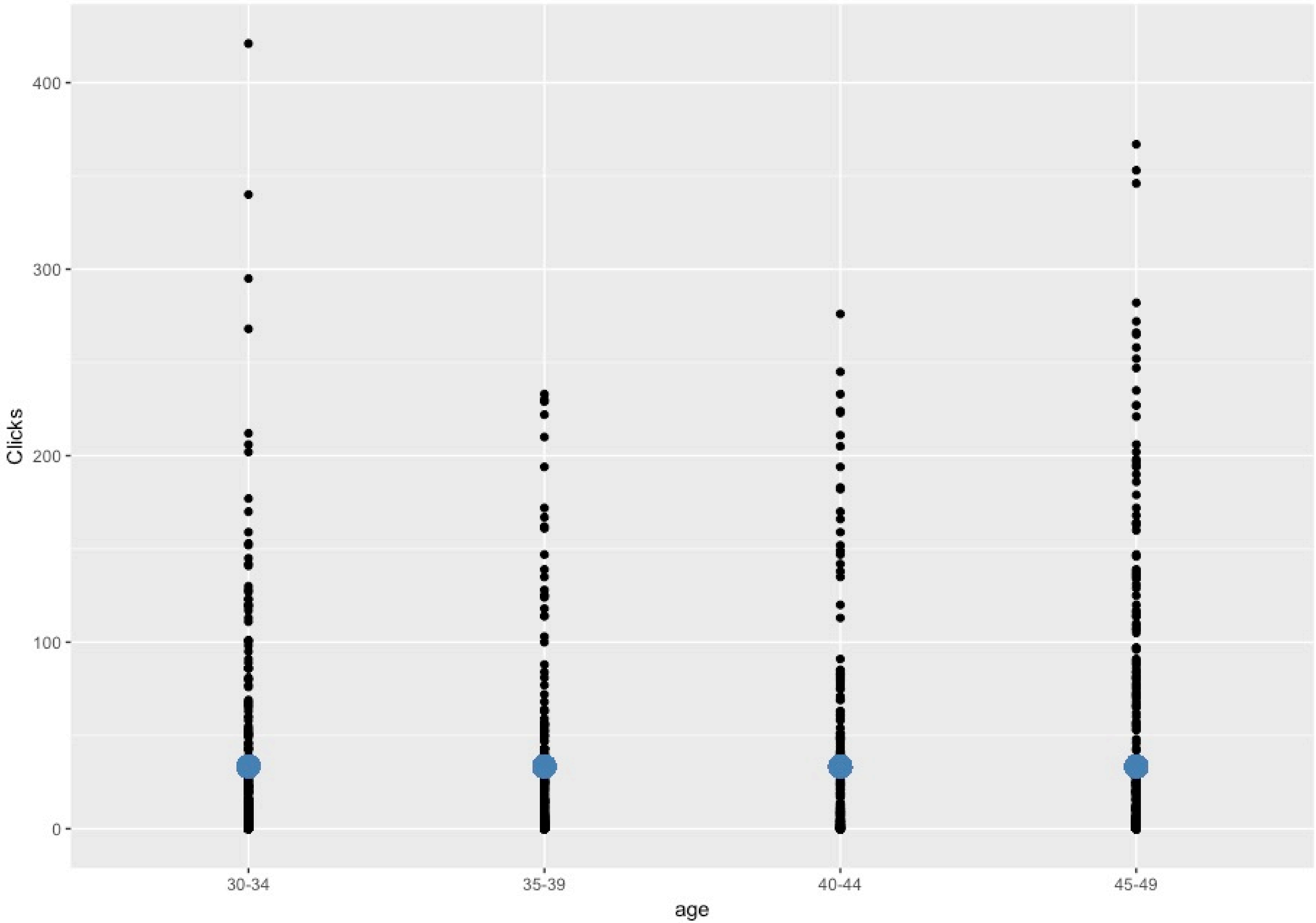
$$\int_{-\infty}^{m(x)} h(y|x)dy = \frac{1}{2}$$

  - Conditional quantiles
  - Conditional variance (not informative about location)

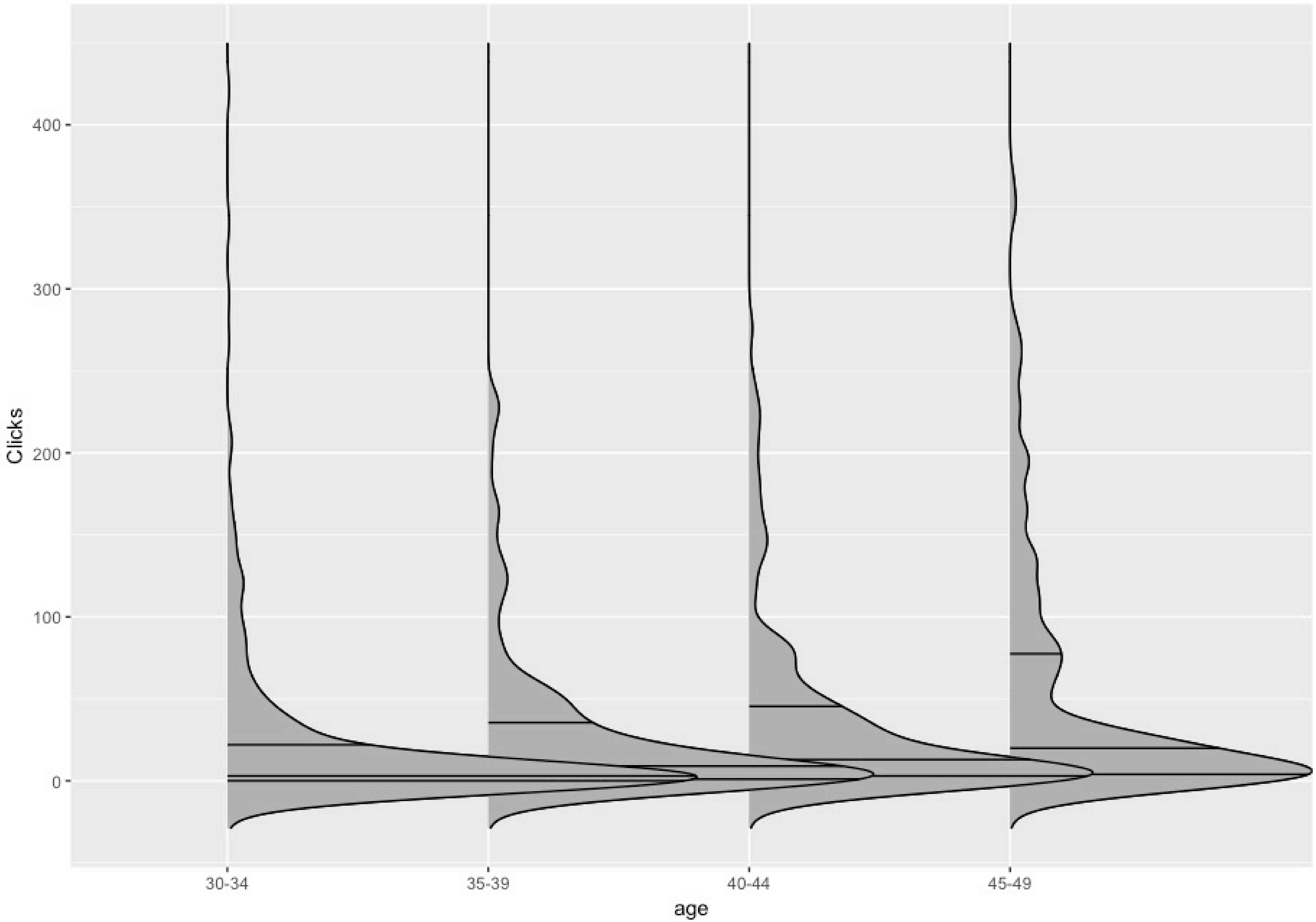
Conditional expectation and standard deviation



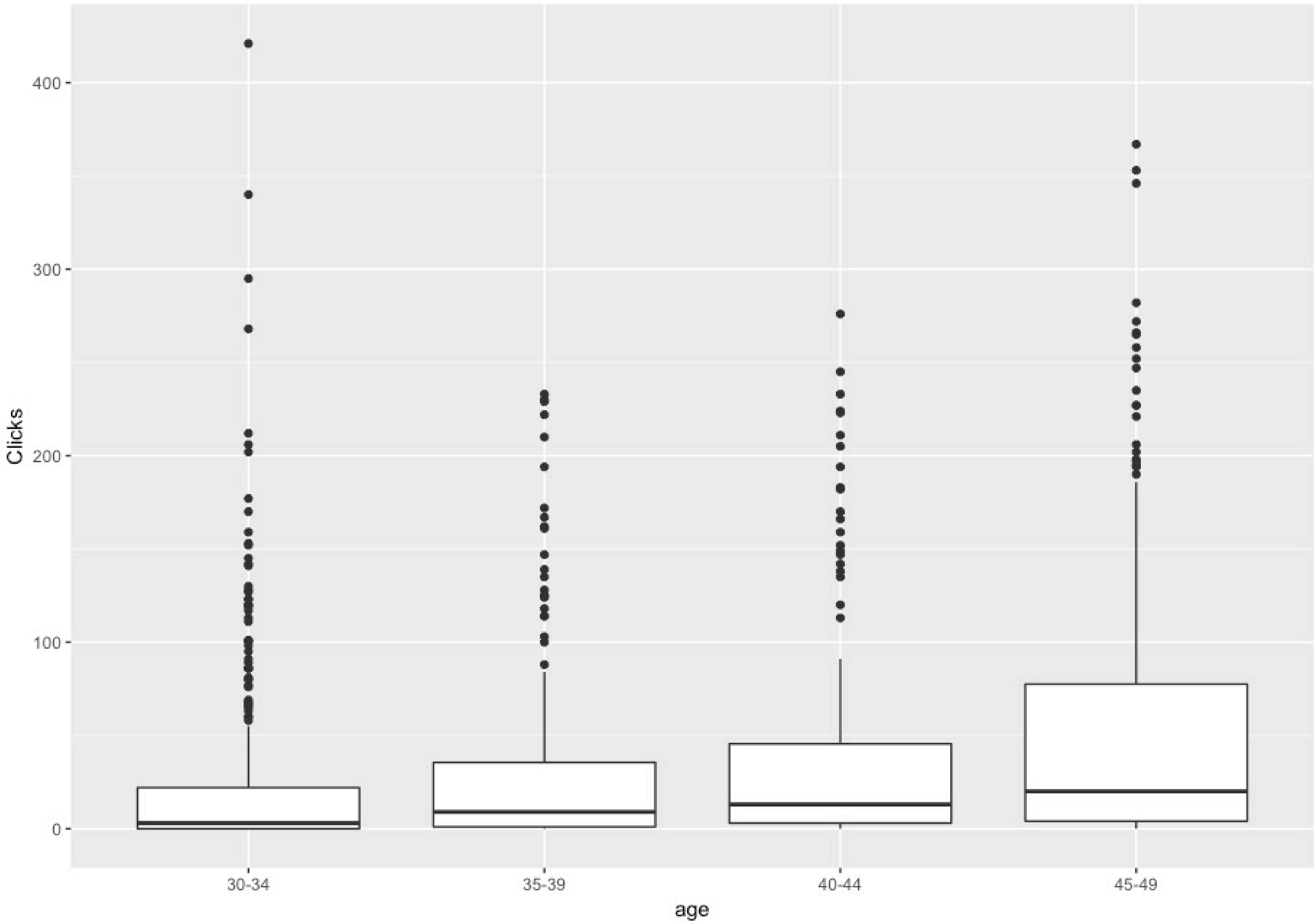
Conditional expectation



Conditional density and conditional quantiles



Conditional distribution: boxplots



Linear regression

We first focus on modeling the regression function $f(x) = \mathbb{E}[Y \mid X = x]$

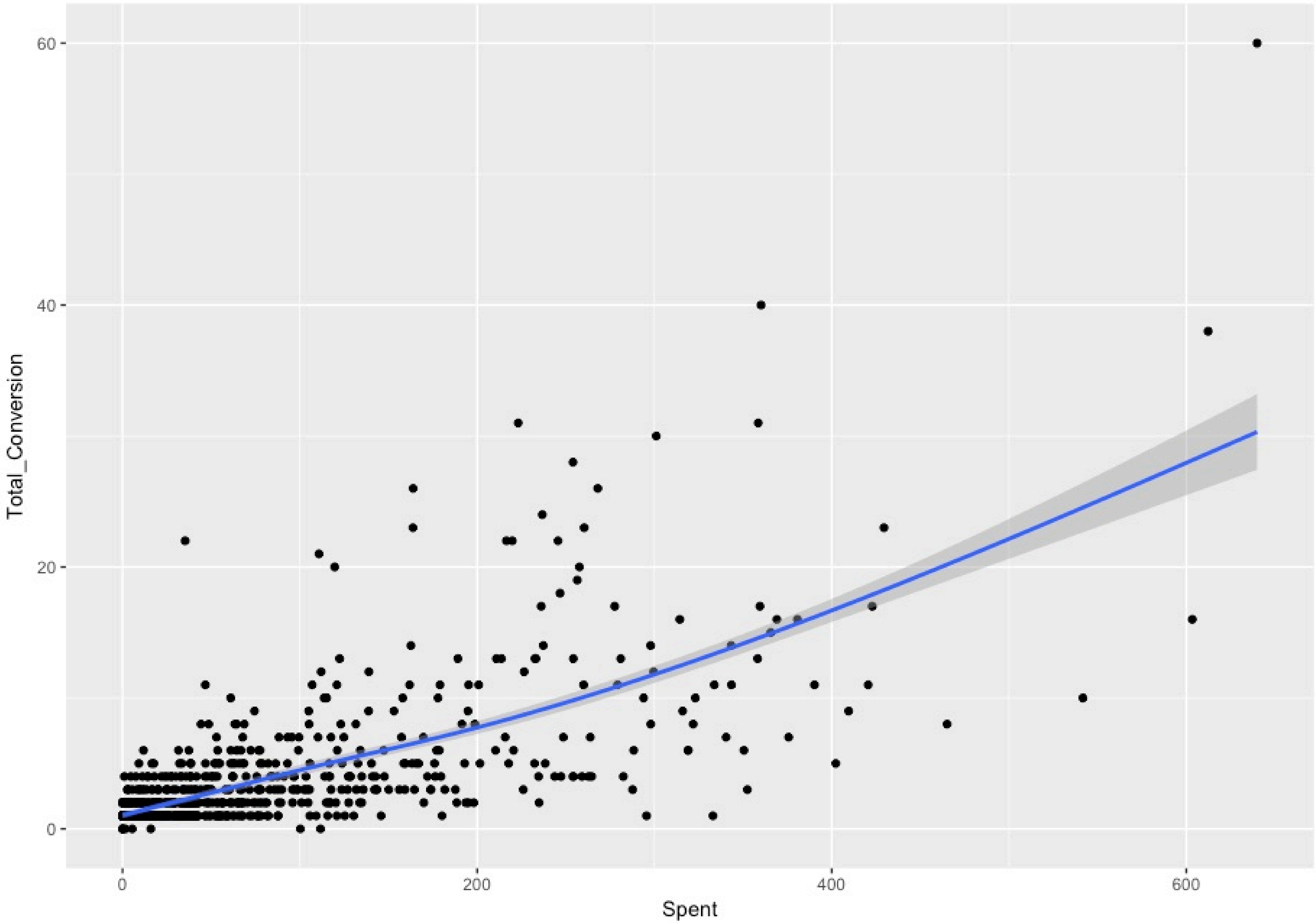
- Too many possible regression functions f (nonparametric)
- Useful to restrict to **simple** functions that are described by a few parameters
- Simplest:

$$f(x) = a + bx$$

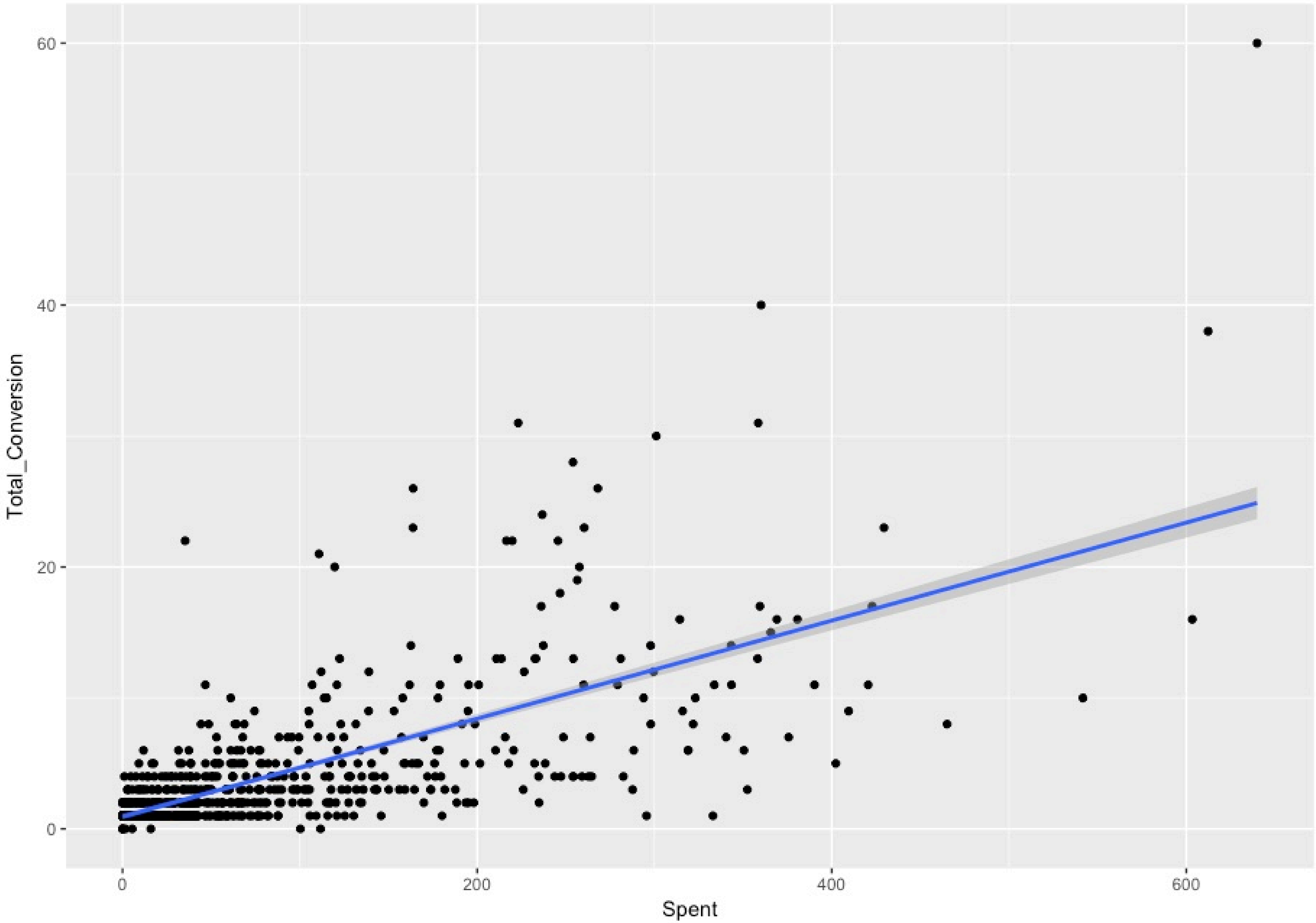
linear (or affine) function

Under this assumption, we talk about linear regression

Nonparametric regression



Linear regression



Probabilistic analysis

- Let X and Y be two real r.v. (not necessarily independent) with two moments and such that $\mathrm{var}(X) > 0$.

- The **theoretical linear regression** of Y on X is the line $x \mapsto a^* + b^* x$ where

$$(a^*, b^*) = \underset{(a,b)\in\mathbb{R}^2}{\mathrm{argmin}}\, \mathbb{E}\left[(Y - a - bX)^2\right]$$

- Setting partial derivatives to zero gives
  - $b^* = \dfrac{\mathrm{cov}(X,Y)}{\mathrm{var}(X)}$,
  - $a^* = \mathbb{E}[Y] - b^*\mathbb{E}[X] = \mathbb{E}[Y] - \dfrac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}\mathbb{E}[X]$.

Noise

Clearly the points are not exactly on the line $x \mapsto a^* + b^* x$ if Var $(Y|X = x) > 0$. The random variable $\varepsilon = Y - (a^* + b^* X)$ is

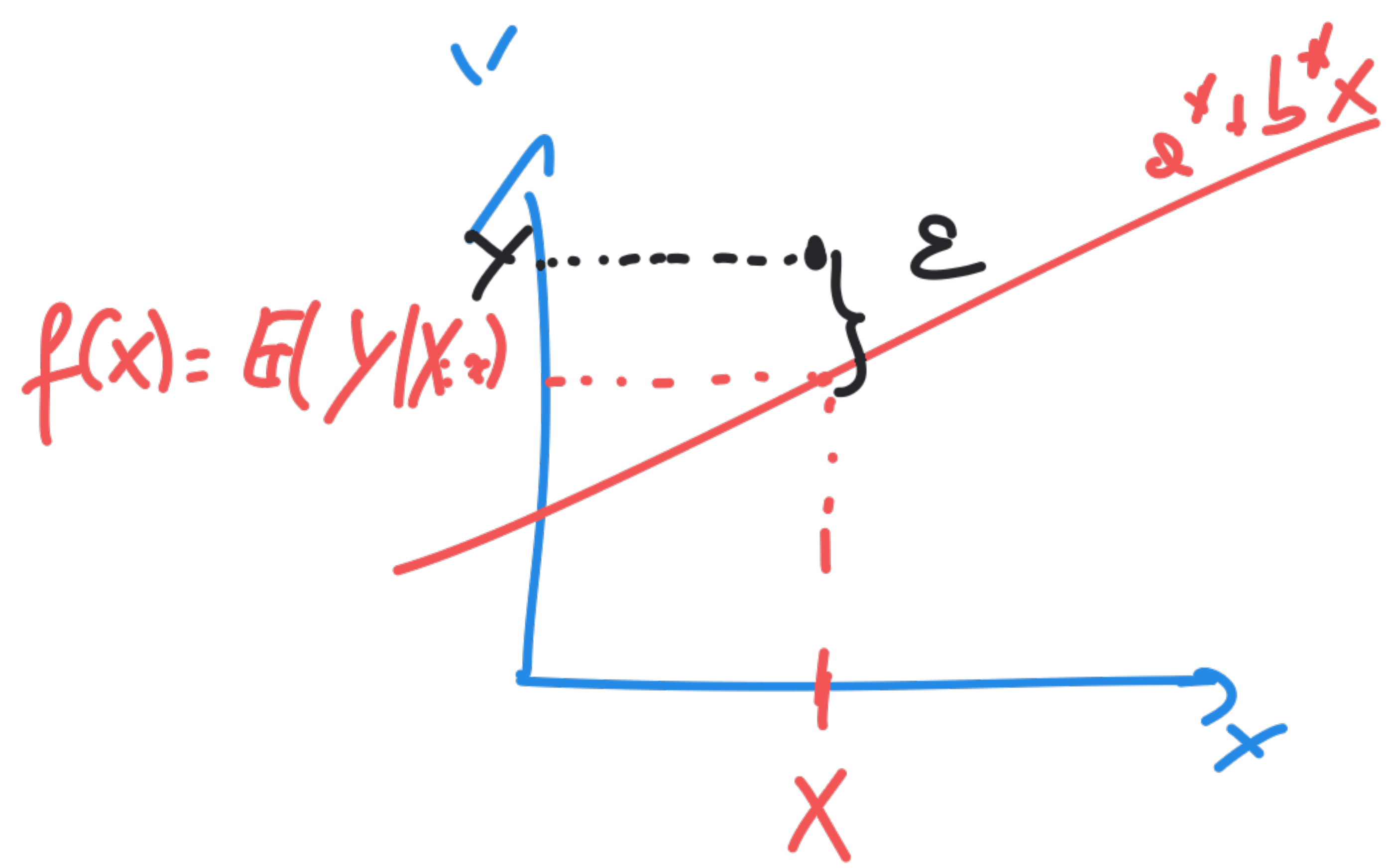
called *noise* and satisfies

$$Y = a^* + b^* X + \varepsilon,$$

with

- $\mathbb{E}[\varepsilon] = 0$ and
- $\text{cov}(X, \varepsilon) = 0$. (exercise)

$$\mathbb{E}[\varepsilon] = \mathbb{E}[Y] - a^* - b^* \mathbb{E}[X] = 0$$



Statistical problem

In practice a^*, b^* need to be estimated from data.

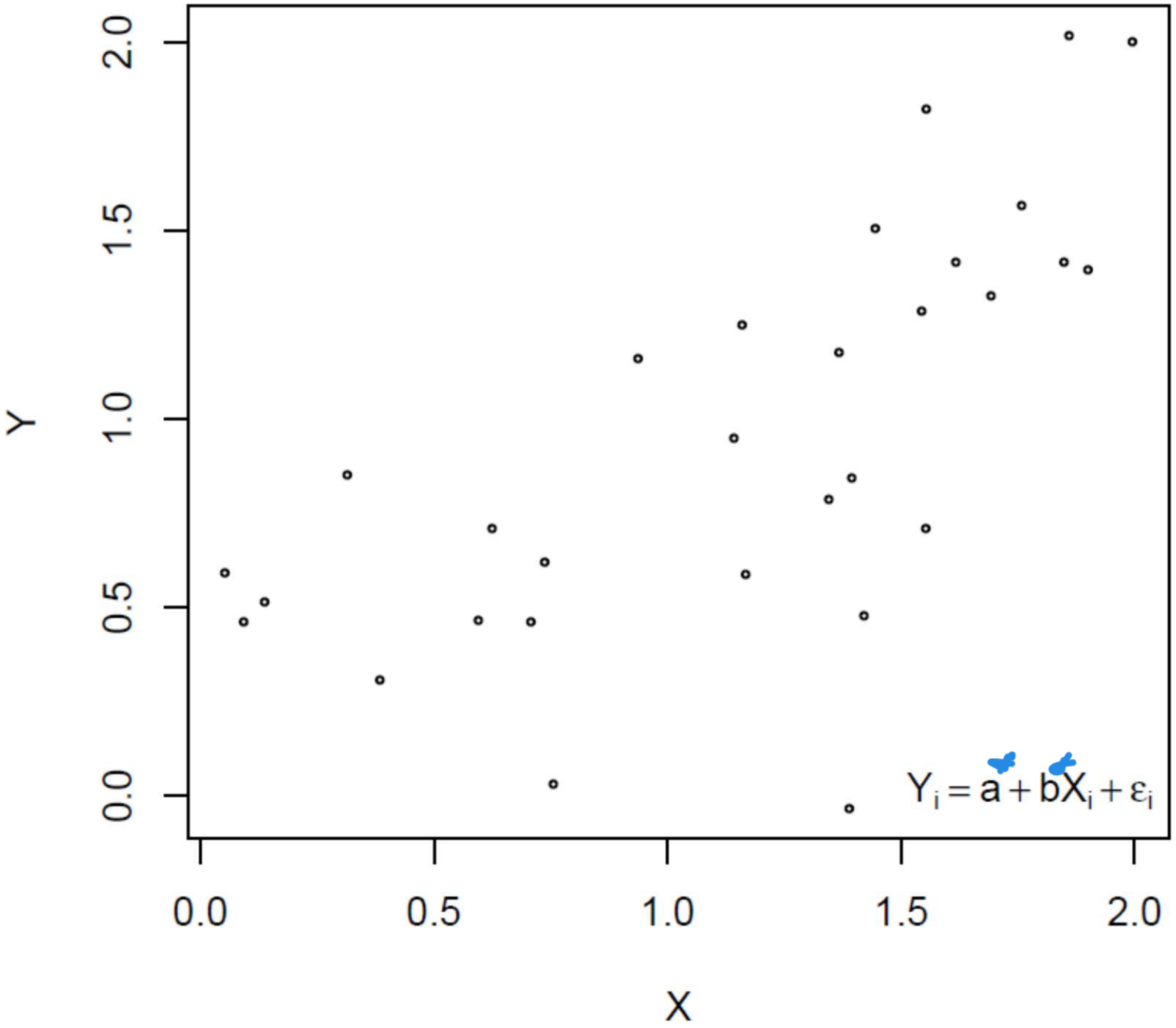
- Assume that we observe n i.i.d. random pairs $(X_1, Y_1), \dots, (X_n, Y_n)$ with same distribution as (X, Y):

$$Y_i = a^* + b^* X_i + \varepsilon_i$$

- We want to estimate a^* and b^*.

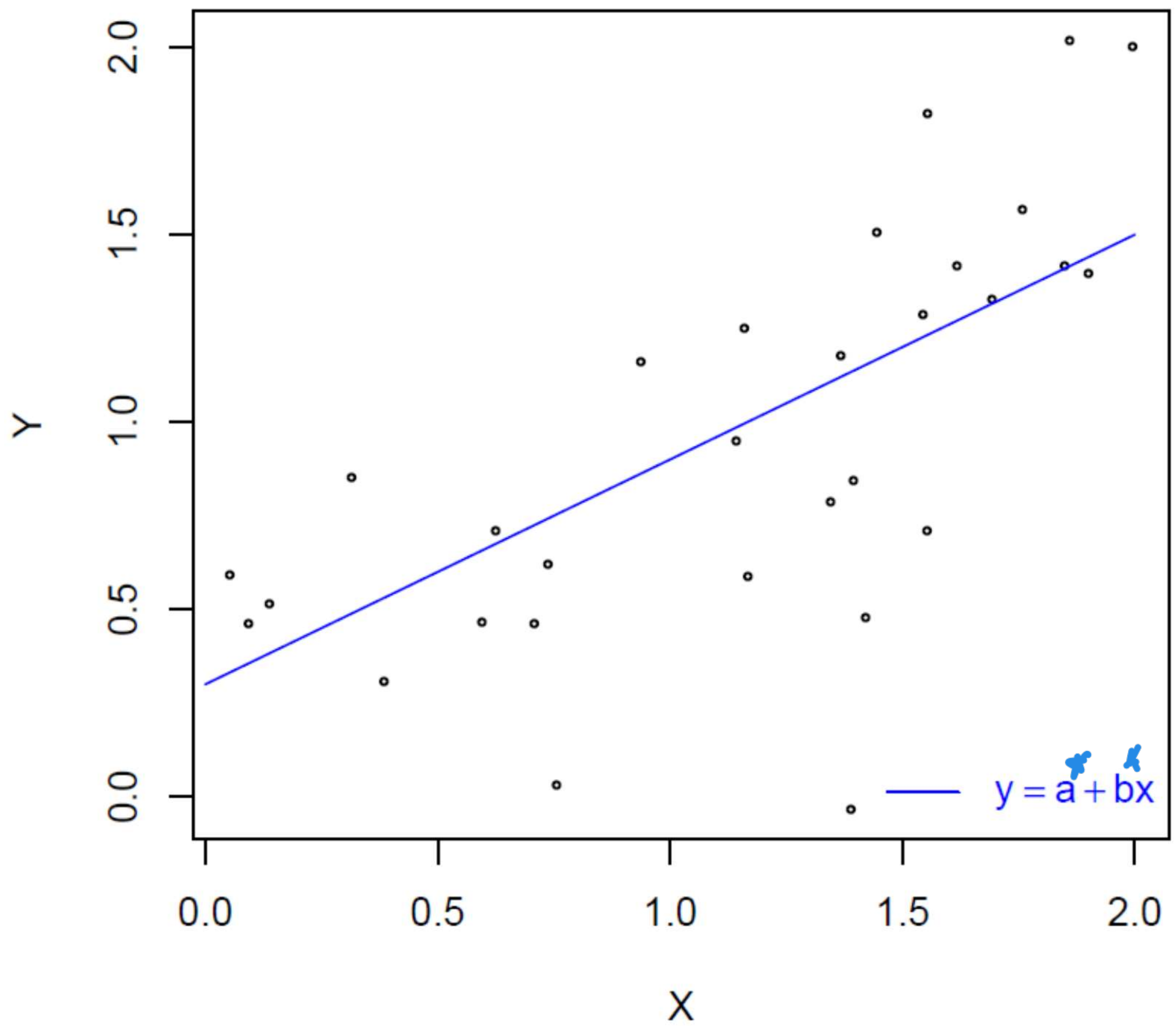
Statistical problem

$$Y_i = a^* + b^* X_i + \varepsilon_i$$



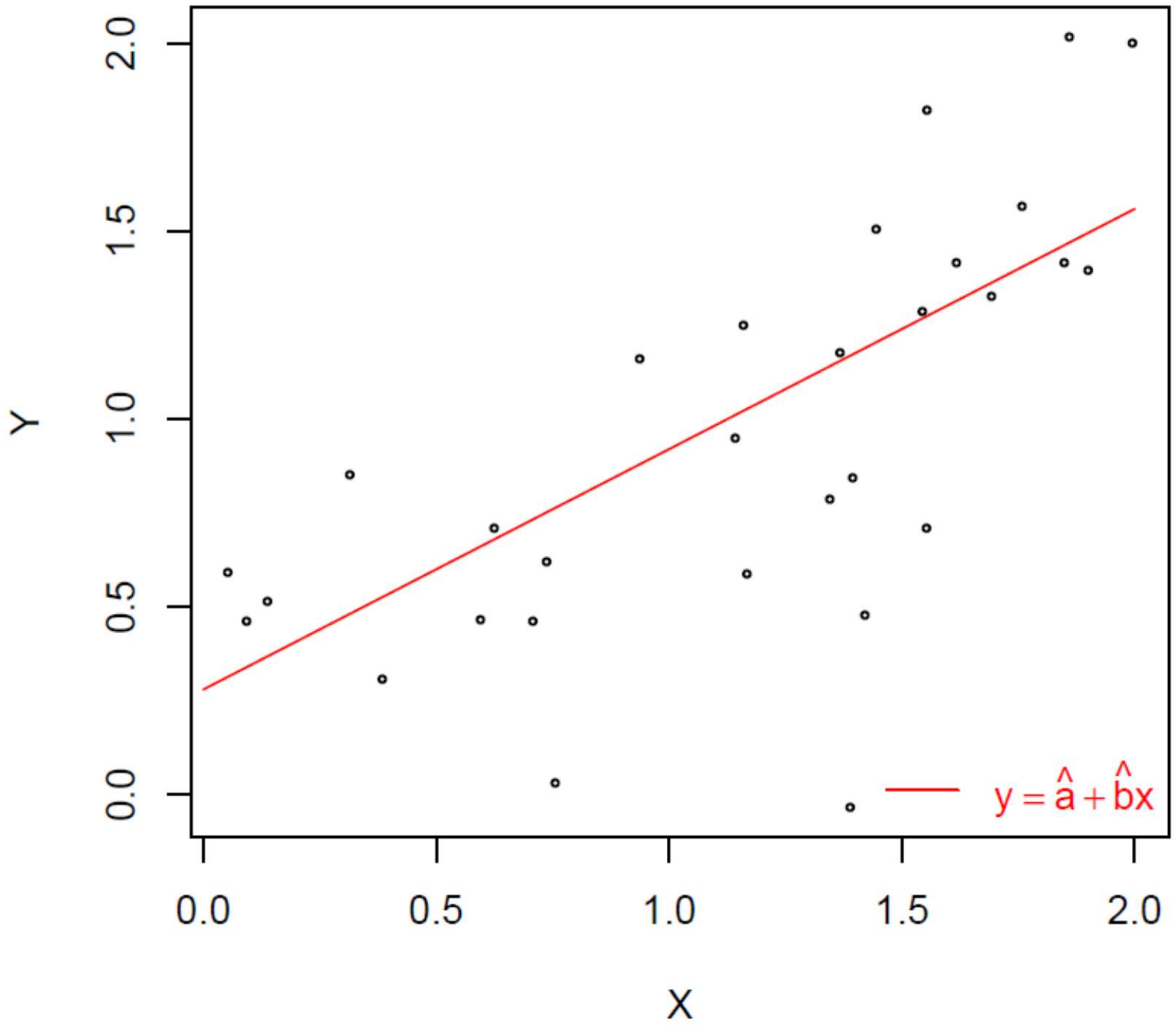
Statistical problem

$$Y_i = a^* + b^* X_i + \varepsilon_i$$



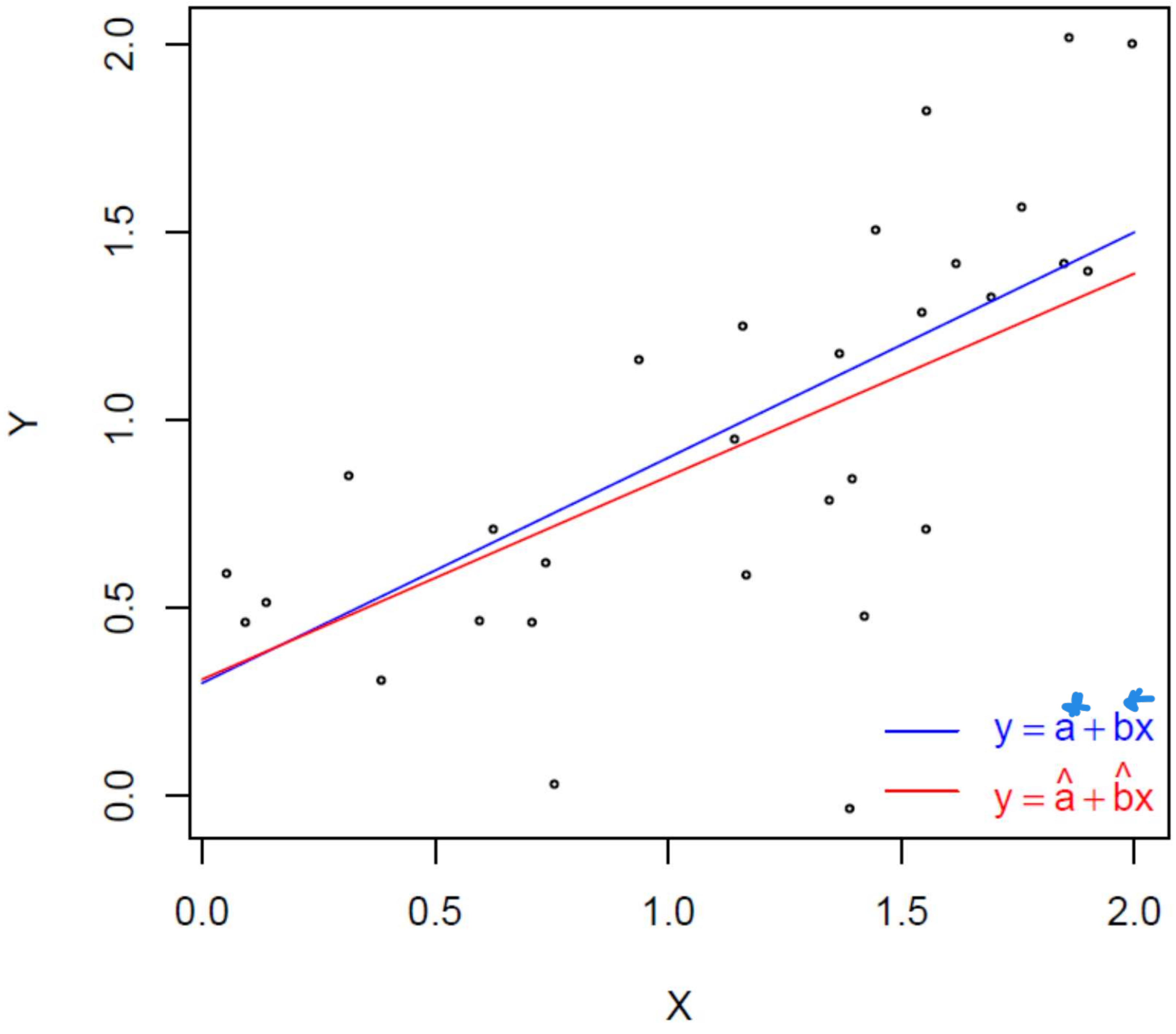
Statistical problem

$$Y_i = a^* + b^* X_i + \varepsilon_i$$



Statistical problem

$$Y_i = a^* + b^* X_i + \varepsilon_i$$



Least squares

Definition

The *least square~~d~~* s estimator *~~error~~ (LSE)* ~~estimator~~ of (a, b) is the minimizer of the sum of squared errors:

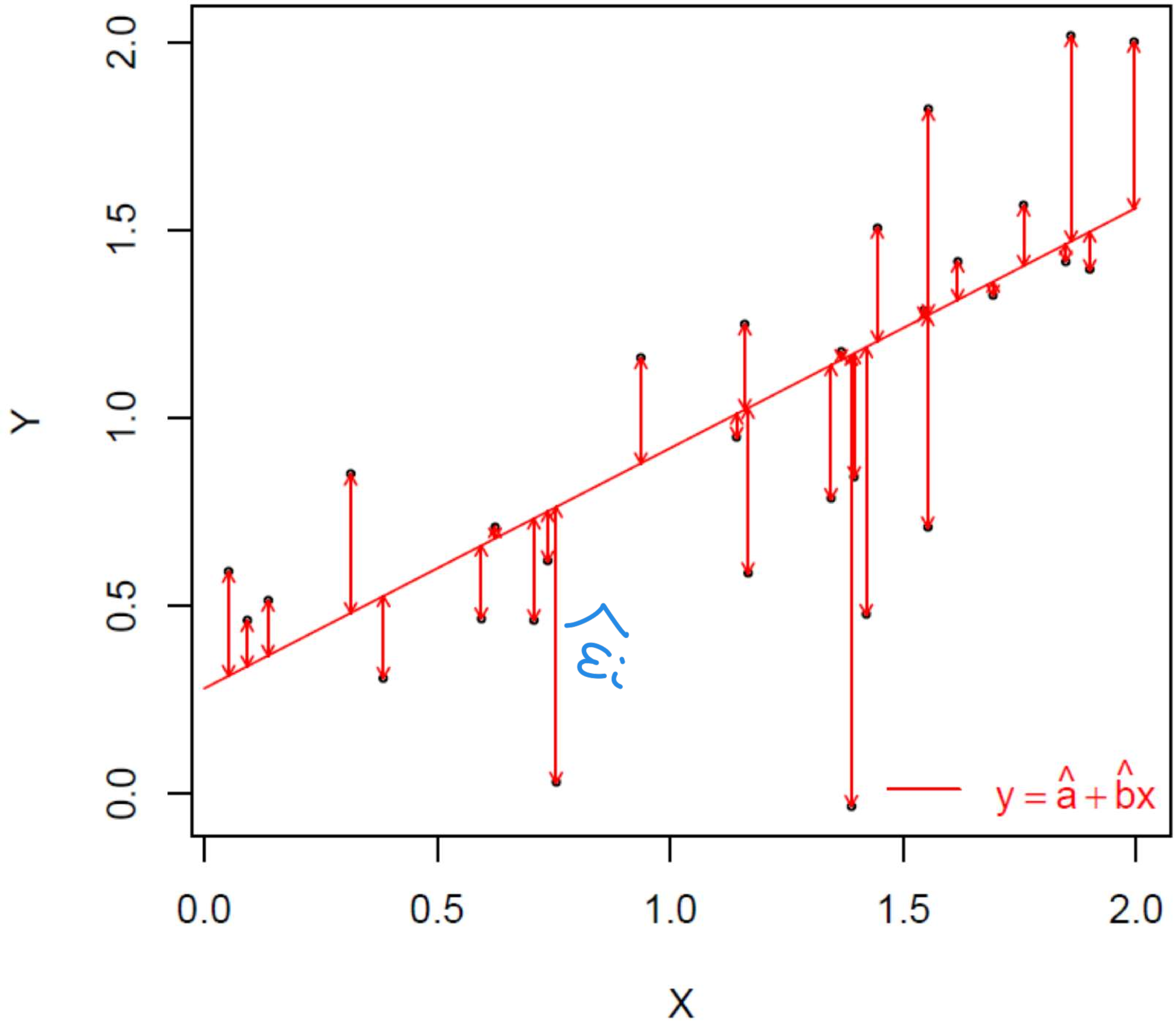
$$\sum_{i=1}^{n} (Y_i - a - bX_i)^2.$$

$(\hat{a}, \hat{b})$ is given by

$$\hat{b} = \frac{\overline{XY} - \bar{X}\bar{Y}}{\overline{X^2} - \bar{X}^2} \qquad \text{(exercise)}$$

$$\hat{a} = \bar{Y} - \hat{b}\bar{X}.$$

Residuals



Multivariate regression

$a^* + b^* X_i$

$$X_i = \begin{pmatrix} X_i^{(1)} \\ X_i^{(2)} \\ \vdots \\ X_i^{(p)} \end{pmatrix}$$

$$Y_i = \mathbf{X}_i^\top \boldsymbol{\beta}^* + \varepsilon_i, \quad i = 1, \dots, n.$$

$$X_i^T \beta^* = \sum_{j=1}^{p} X_i^{(j)} \beta_j^*$$

- Vector of **explanatory variables** or **covariates**: $\mathbf{X}_i \in \mathbb{R}^p$ (wlog, assume its first coordinate is 1).
- **Response / Dependent variable**: Y_i.
- $\boldsymbol{\beta}^* = (a^*, \mathbf{b}^{*\top})^\top$; $\beta_1^* (= a^*)$ is called the **intercept**.
- $\{\varepsilon_i\}_{i=1,\dots,n}$: noise terms satisfying $\mathrm{cov}(\mathbf{X}_i, \varepsilon_i) = \mathbf{0}$.

Definition

The **least squares estimator (LSE)** of $\boldsymbol{\beta}^*$ is the minimizer of the sum of square errors:

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{i=1}^{n} (Y_i - X_i^T \beta)^2$$

LSE in matrix form

- Let $\mathbf{Y} = (Y_1, \ldots, Y_n)^\top \in \mathbb{R}^n$.
- Let $\mathbb{X}$ be the $n \times p$ matrix whose rows are $\mathbf{X}_1^\top, \ldots, \mathbf{X}_n^\top$ ($\mathbb{X}$ is called the **design matrix**). $\mathbb{X}$ has size $n \times p$
- Let $\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_n)^\top \in \mathbb{R}^n$ (unobserved noise)
- $\mathbf{Y} = \mathbb{X}\beta^* + \varepsilon$, $\boldsymbol{\beta}^*$ unknwon.

$$\underset{\mathbf{Y}}{\begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}} = \underset{\mathbb{X}}{\begin{bmatrix} X_1^T \\ \vdots \\ X_n^T \end{bmatrix}} \underset{\beta^*}{\begin{bmatrix} \; \end{bmatrix}} + \underset{\boldsymbol{\varepsilon}}{\begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}}$$

- The LSE $\hat{\boldsymbol{\beta}}$ satisfies:

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{Y} - \mathbb{X}\boldsymbol{\beta}\|_2^2.$$

$$\sum_{i=1}^n (Y_i - X_i^T \beta)^2$$

$$\|w\|_2^2 = \sum_{i=1}^n w_i^2$$

$w \in \mathbb{R}^n$

Closed form solution

- Assume that $\operatorname{rank}(\mathbb{X}) = p$.
- Analytic computation of the LSE:

$$\hat{\boldsymbol{\beta}} = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top \mathbf{Y}.$$

- Geometric interpretation of the LSE: $\mathbb{X}\hat{\boldsymbol{\beta}}$ is the orthogonal projection of $\mathbf{Y}$ onto the subspace spanned by the columns of $\mathbb{X}$:

$$\mathbb{X}\hat{\boldsymbol{\beta}} = P\mathbf{Y},$$

where $P = \mathbb{X}(\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top$.

Statistical inference

$$Y = \mathbb{X}\beta^* + \varepsilon$$

To make inference (confidence regions, tests) we need more assumptions.

Assumptions:

- The design matrix $\mathbb{X}$ is deterministic and $\mathrm{rank}(\mathbb{X}) = p$.
- The model is **homoscedastic**: $\varepsilon_1, \ldots, \varepsilon_n$ are i.i.d.
- The noise vector $\boldsymbol{\varepsilon}$ is Gaussian:

$$\boldsymbol{\varepsilon} \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

for some known or unknown $\sigma^2 > 0$. $\Rightarrow Y \sim \mathcal{N}_n(\mathbb{X}\beta^*, \sigma^2 I)$

Properties of LSE

- LSE = MLE
- Distribution of $\hat{\boldsymbol{\beta}}$: $\hat{\boldsymbol{\beta}} \sim \mathcal{N}_p\left(\beta^*, \sigma^2 (\mathbb{X}^\top \mathbb{X})^{-1}\right)$.
- Quadratic risk of $\hat{\boldsymbol{\beta}}$: $\mathbb{E}\left[\|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\|_2^2\right] = \sigma^2 \mathrm{tr}\left((\mathbb{X}^\top \mathbb{X})^{-1}\right)$.
- Prediction error: $\mathbb{E}\left[\|\mathbf{Y} - \mathbb{X}\hat{\boldsymbol{\beta}}\|_2^2\right] = \sigma^2 (n-p)$.
- Unbiased estimator of σ^2: $\hat{\sigma}^2 = \dfrac{\|Y - \mathbb{X}\hat{\beta}\|_2^2}{n-p} = \dfrac{1}{n-p}\sum_{i=1}^{n} \hat{\varepsilon}_i^2$

Theorem

- $(n-p)\dfrac{\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p}$.
- $\hat{\boldsymbol{\beta}} \perp\!\!\!\perp \hat{\sigma}^2$. (Cochran's theorem)

Significance tests

- Test whether the j-th explanatory variable is significant in the linear regression ($1 \leq j \leq p$).

- $H_0 : \beta_j = 0$ v.s. $H_1 : \beta_j \neq 0$.

- If γ_j is the j-th diagonal coefficient of $(\mathbb{X}^\top \mathbb{X})^{-1}$ ($\gamma_j > 0$):

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 \gamma_j}} \sim t_{n-p}$$

- Let $T_n^{(j)} = \dfrac{\hat{\beta}_j}{\sqrt{\hat{\sigma}^2 \gamma_j}}$.

- Test with non asymptotic level $\alpha \in (0, 1)$:

$$R_{j,\alpha} = \left\{ |T_n^{(j)}| > q_{\frac{\alpha}{2}}(t_{n-p}) \right\}$$

where $q_{\frac{\alpha}{2}}(t_{n-p})$ is the $(1 - \alpha/2)$-quantile of t_{n-p}.

- We can also compute p-values.

Bonferroni's test

- Test whether a **group** of explanatory variables is significant in the linear regression.

- $H_0 : \beta_j = 0, \forall j \in S$ v.s. $H_1 : \exists j \in S, \beta_j \neq 0$, where $S \subseteq \{1, \ldots, p\}$.

- *Bonferroni's test*: $R_{S,\alpha} = \bigcup_{j \in S} R_{j,\frac{\alpha}{k}}$, where $k = |S|$.

- This test has nonasymptotic level at most α.

Type I is $\mathbb{P}_{H_0}[R_{S,\alpha}] \leq \sum_{j \in S} \underbrace{\mathbb{P}_{H_0}[R_{j,\frac{\alpha}{k}}]}_{=\alpha/k} = \alpha$

Remarks

- Linear regression exhibits correlations, **NOT** causality
- Normality of the noise: One can use goodness of fit tests to test whether the residuals $\hat{\varepsilon}_i = Y_i - \mathbb{X}_i^\top \hat{\boldsymbol{\beta}}$ are Gaussian.
- Deterministic design: If $\mathbb{X}$ is not deterministic, all the above can be understood conditionally on $\mathbb{X}$, if the noise is assumed to be Gaussian, conditionally on X.