Machine Learning

A. Supervised Learning: Linear Models & Fundamentals
A.1. Linear Regression

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Outline

Outline

The Simple Linear Regression Problem (Review)

Given

- a set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \subseteq \mathbb{R} \times \mathbb{R}$ called **training data**,

compute the **parameters** $(\hat{\beta}_0, \hat{\beta}_1)$ of a linear **regression function**

$$\hat{y}(x) := \hat{\beta}_0 + \hat{\beta}_1 x$$

s.t. for a set $\mathcal{D}^{\text{test}} \subseteq \mathbb{R} \times \mathbb{R}$ called **test set** the **test error**

$$\text{err}(\hat{y}; \mathcal{D}^{\text{test}}) := \frac{1}{|D^{\text{test}}|} \sum_{(x,y) \in \mathcal{D}^{\text{test}}} (y - \hat{y}(x))^2$$

is minimal.

Note: $\mathcal{D}^{\text{test}}$ has (i) to be from the same data generating process and (ii) not to be available during training.

The (Multiple) Linear Regression Problem

Given

- a set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\} \subseteq \mathbb{R}^M \times \mathbb{R}$ called **training data**,

compute the **parameters** $(\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_M)$ of a linear **regression function**

$$\hat{y}(x) := \hat{\beta}_0 + \hat{\beta}_1 x_1 + \dots + \hat{\beta}_M x_M$$

s.t. for a set $\mathcal{D}^{\text{test}} \subseteq \mathbb{R}^M \times \mathbb{R}$ called **test set** the **test error**

$$\text{err}(\hat{y}; \mathcal{D}^{\text{test}}) := \frac{1}{|D^{\text{test}}|} \sum_{(x,y) \in \mathcal{D}^{\text{test}}} (y - \hat{y}(x))^2$$

is minimal.

Note: $\mathcal{D}^{\text{test}}$ has (i) to be from the same data generating process and (ii) not to be available during training.

Several predictors

Several predictor variables $x_{n,1}, x_{n,2}, \ldots, x_{n,M}$:

$$\begin{aligned}\hat{y}_n =& \hat{\beta}_0 + \hat{\beta}_1 x_{n,1} + \hat{\beta}_2 x_{n,2} + \cdots \hat{\beta}_M x_{n,M} \\ =& \hat{\beta}_0 + \sum_{m=1}^{M} \hat{\beta}_m x_{n,m}\end{aligned}$$

with $M+1$ parameters $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_M$.

Note: $n \in 1{:}N$ denotes the sample/example/instance/case.

Linear form

Several predictor variables $x_{n,1}, x_{n,2}, \ldots, x_{n,M}$:

$$\begin{aligned}\hat{y}_n =& \hat{\beta}_0 + \sum_{m=1}^{M} \hat{\beta}_m x_{n,m}\\ =& \langle \hat{\beta}, x_n \rangle = \hat{\beta}^T x_n\end{aligned}$$

where

$$\hat{\beta} := \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_M \end{pmatrix}, \quad x_n := \begin{pmatrix} 1 \\ x_{n,1} \\ \vdots \\ x_{n,M} \end{pmatrix},$$

Thus, the intercept is handled like any other parameter, for the artificial constant predictor $x_{n,0} \equiv 1$.

Simultaneous equations for the whole dataset

For the whole dataset $\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}$:

$$y \approx \hat{y} := X\hat{\beta}$$

where

$$y := \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}, \hat{y} := \begin{pmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_N \end{pmatrix}, \quad X := \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & \ldots & x_{1,M} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N,1} & x_{N,2} & \ldots & x_{N,M} \end{pmatrix}$$

Least squares estimates

Least squares estimates $\hat{\beta}$ minimize

$$\text{err}(\hat{y}, \mathcal{D}^{\text{train}}) := \text{RSS}(\hat{\beta}, \mathcal{D}^{\text{train}}) := \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 = ||y - \hat{y}||^2 = ||y - X\hat{\beta}||^2$$

$$\hat{\beta} := \arg\min_{\hat{\beta} \in \mathbb{R}^M} ||y - X\hat{\beta}||^2$$

Least squares estimates

Least squares estimates $\hat{\beta}$ minimize

$$\text{err}(\hat{y}, \mathcal{D}^{\text{train}}) := \text{RSS}(\hat{\beta}, \mathcal{D}^{\text{train}}) := \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 = ||y - \hat{y}||^2 = ||y - X\hat{\beta}||^2$$

$$\hat{\beta} := \arg\min_{\hat{\beta} \in \mathbb{R}^M} ||y - X\hat{\beta}||^2$$

The least squares estimates $\hat{\beta}$ can be computed analytically via **normal equations**

$$X^T X \hat{\beta} = X^T y$$

Proof:
$$||y - X\hat{\beta}||^2 = \langle y - X\hat{\beta}, y - X\hat{\beta} \rangle$$

$$\frac{\partial(\ldots)}{\partial \hat{\beta}} = 2\langle -X, y - X\hat{\beta} \rangle = -2(X^T y - X^T X \hat{\beta}) \overset{!}{=} 0$$

How to compute least squares estimates $\hat{\beta}$

Solve the $M \times M$ system of linear equations

$$X^T X \hat{\beta} = X^T y$$

i.e., $Ax = b$ (with $A := X^T X, b = X^T y, x = \hat{\beta}$).

There are several numerical methods available:

1. Gaussian elimination
2. Cholesky decomposition
3. QR decomposition

Learn Linear Regression via Normal Equations

```
learn-linreg-NormEq($\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}$):
    $X := (x_1, x_2, \ldots, x_N)^T$
    $y := (y_1, y_2, \ldots, y_N)^T$
    $A := X^T X$
    $b := X^T y$
    $\hat{\beta} :=$ solve-SLE($A, b$)
    return $\hat{\beta}$
```

Example

Given is the following data:

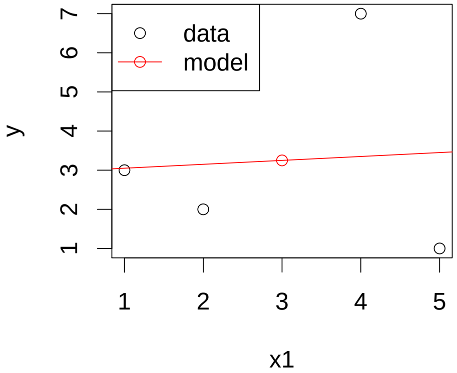
x_1	x_2	y
1	2	3
2	3	2
4	1	7
5	5	1

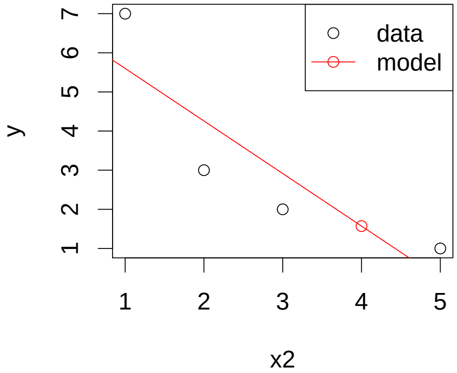
Predict a y value for $x_1 = 3, x_2 = 4$.

Example / Simple Regression Models for Comparison

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 \\ = 2.95 + 0.1 x_1$$

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_2 x_2 \\ = 6.943 - 1.343 x_2$$





$$\hat{y}(x_1 = 3) = 3.25$$
$$\text{RSS} = 20.65, \quad \text{RMSE} = 4.02$$

$$\hat{y}(x_2 = 4) = 1.571$$
$$\text{RSS} = 4.97, \quad \text{RMSE} = 2.13$$

Example

Now fit

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2$$

to the data:

x_1	x_2	y
1	2	3
2	3	2
4	1	7
5	5	1

$$X = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 3 \\ 1 & 4 & 1 \\ 1 & 5 & 5 \end{pmatrix}, \quad y = \begin{pmatrix} 3 \\ 2 \\ 7 \\ 1 \end{pmatrix}$$

$$X^T X = \begin{pmatrix} 4 & 12 & 11 \\ 12 & 46 & 37 \\ 11 & 37 & 39 \end{pmatrix}, \quad X^T y = \begin{pmatrix} 13 \\ 40 \\ 24 \end{pmatrix}$$

Example

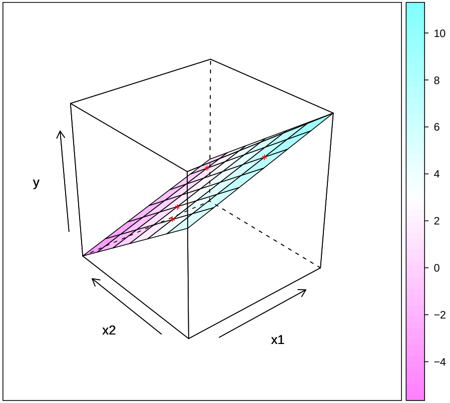
$$\left(\begin{array}{rrr|r} 4 & 12 & 11 & 13 \\ 12 & 46 & 37 & 40 \\ 11 & 37 & 39 & 24 \end{array}\right) \sim \left(\begin{array}{rrr|r} 4 & 12 & 11 & 13 \\ 0 & 10 & 4 & 1 \\ 0 & 16 & 35 & -47 \end{array}\right) \sim \left(\begin{array}{rrr|r} 4 & 12 & 11 & 13 \\ 0 & 10 & 4 & 1 \\ 0 & 0 & 143 & -243 \end{array}\right)$$

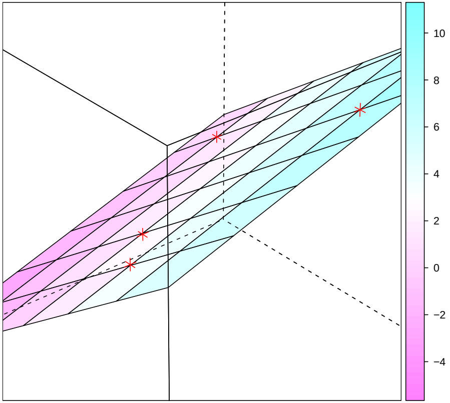
$$\sim \left(\begin{array}{rrr|r} 4 & 12 & 11 & 13 \\ 0 & 1430 & 0 & 1115 \\ 0 & 0 & 143 & -243 \end{array}\right) \sim \left(\begin{array}{rrr|r} 286 & 0 & 0 & 1597 \\ 0 & 1430 & 0 & 1115 \\ 0 & 0 & 143 & -243 \end{array}\right)$$

i.e.,

$$\hat{\beta} = \begin{pmatrix} 1597/286 \\ 1115/1430 \\ -243/143 \end{pmatrix} \approx \begin{pmatrix} 5.583 \\ 0.779 \\ -1.699 \end{pmatrix}$$

Example





$$\hat{y}(x_1 = 3, x_2 = 4) = 1.126$$

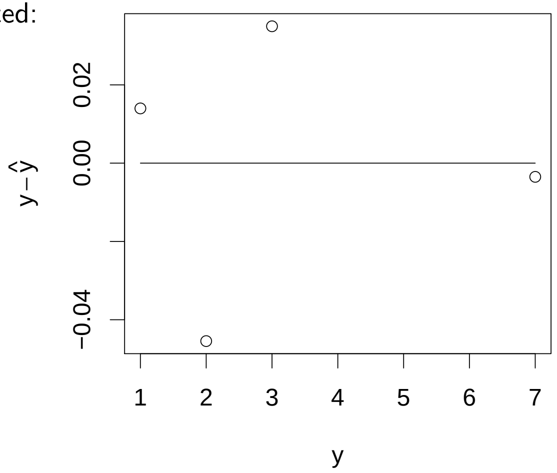
$$\text{RSS} = 0.0035, \quad \text{RMSE} = 0.58$$

Example / Visualization of Model Fit

To visually assess the model fit, a **scatter plot**

$$\text{residuals } \hat{\epsilon} := y - \hat{y} \text{ vs. true values } y$$

can be plotted:



Computational Complexity

- overall complexity of learning a linear regression model via normal equations:

$$O(NM^2 + M^3)$$

  - $M \times N, N \times M$ matrix multiplication $X^T X$: $O(NM^2)$
  - solve system of M equations: $O(M^3)$

- example runtimes:

  (Intel i5-760 2.8 MHz, 2010, Python numpy)

M	runtime [s]
100	0.002
200	0.004
400	0.022
800	0.086
1600	0.555
3200	6.275
6400	27.902

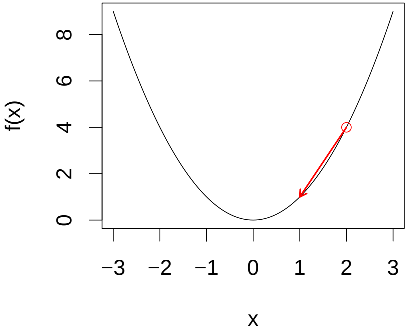
Outline

Gradient Descent

Given a function $f : \mathbb{R}^N \rightarrow \mathbb{R}$, find x with minimal $f(x)$.

Idea: start from a random x_0 and then improve step by step, i.e., choose x_{i+1} with

$$f(x_{i+1}) \leq f(x_i)$$



Choose the negative gradient $-\nabla f(x_i) := -\frac{\partial f}{\partial x}(x_i)$ as direction for descent, i.e.,

$$x_{i+1} - x_i = -\mu_i \cdot \nabla f(x_i)$$

with a suitable step size $\mu_i > 0$.

Gradient Descent

```
minimize-GD-fss($f : \mathbb{R}^N \rightarrow \mathbb{R}, x_0 \in \mathbb{R}^N, \mu \in \mathbb{R}^+, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+$):
    for $i = 1, \ldots, i_{\max}$:
        $x_i := x_{i-1} - \mu \cdot \nabla f(x_{i-1})$
        if $f(x_{i-1}) - f(x_i) < \epsilon$:
            return $x_i$
    raise exception ``not converged in $i_{\max}$ iterations''
```

x_0	start value
μ	(fixed) step size (aka step length, learning rate)
$i_{\max}$	maximal number of iterations
ϵ	minimum stepwise improvement

Example

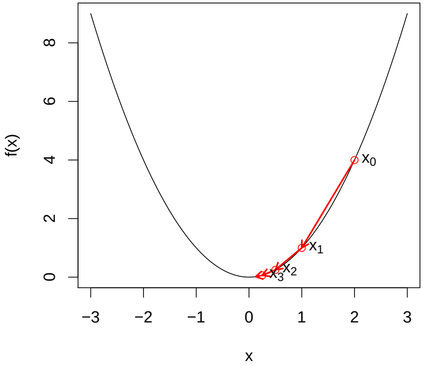
$$f(x) := x^2, \quad \nabla f(x) = \frac{\partial f}{\partial x}(x) = 2x, \quad x_0 := 2, \quad \mu := 0.25$$

Then we compute iteratively:

i	x_i	$\frac{\partial f}{\partial x}(x_i)$	x_{i+1}
0	2	4	1
1	1	2	0.5
2	0.5	1	0.25
3	0.25	$\vdots$	$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

using

$$x_{i+1} = x_i - \mu \cdot \nabla f(x_i)$$

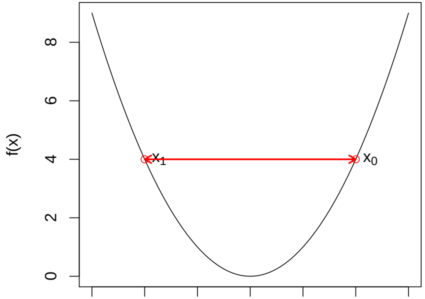


Step Size

Why do we need a step size? Can we set $\mu := 1$?

The negative gradient gives a direction of descent only in an infinitesimal neighborhood of x_n.

Thus, the step size may be too large, and the function value of the next point does not decrease.



Step Size

There are many different strategies to adapt the step size s.t.

1. the function value actually decreases and
2. the step size becomes not too small
   (and thus convergence slow)

Backtracking linesearch:

$$\mu_i := \max\{\mu \in \{\beta^j \mid j \in \mathbb{N}_0\} \mid f(x_i - \mu \nabla f(x_i)) \leq f(x_i) - \mu\,\alpha\,\nabla f(x_i)^T \nabla f(x_i) \}$$

with $\alpha \in (0, \frac{1}{2})$

Backtracking Line Search

```
stepsize-backtracking($f, x, \alpha \in (0, 0.5), \beta \in (0, 1)$):
  $\mu := 1$
  while $f(x - \mu \nabla f(x)) > f(x) - \alpha\mu \nabla f(x)^T \nabla f(x)$:
    $\mu := \beta\mu$
  return $\mu$
```

x	last position
α	steepness
β	stepsize reduction factor

Loop eventually terminates as for sufficient small μ:

$$f(x - \mu \nabla f(x)) \approx f(x) - \mu \nabla f(x)^T \nabla f(x) < f(x) - \alpha\mu \underbrace{\nabla f(x)^T \nabla f(x)}_{\geq 0}$$

Gradient Descent

```
**minimize-GD**$(f : \mathbb{R}^N \rightarrow \mathbb{R}, x_0 \in \mathbb{R}^N, \mu, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:
  for $i = 1, \ldots, i_{\max}$:
    $\mu_i := \mu(f, x_{i-1})$
    $x_i := x_{i-1} - \mu_i \cdot \nabla f(x_{i-1})$
    if $f(x_{i-1}) - f(x_i) < \epsilon$:
      return $x_i$
  raise exception ''not converged in $i_{\max}$ iterations''
```

x_0	start value
μ	step size function, e.g., **steplength-backtracking** (with fixed α, β).
$i_{\max}$	maximal number of iterations
ϵ	minimum stepwise improvement

Bold Driver Step Size [Battiti, 1989]

A variant of backtracking with memory:

```
**steplength-bolddriver**($f : \mathbb{R}^N \rightarrow \mathbb{R}, x \in \mathbb{R}^N, d \in \mathbb{R}^N, \mu^{\text{old}}, \mu^+, \mu^- \in (0,1)$):
    $\mu := \mu^{\text{old}}\mu^+$
    while $f(x) - f(x + \mu d) \leq 0\}$:
        $\mu = \mu\mu^-$
    return $\mu$
```

μ^{old}	last step size
μ^+	step size increase factor, e.g., 1.1.
μ^-	step size decrease factor, e.g., 0.5.
d	descent direction, e.g., $d := -\nabla f(x)$

Simple Step Size Control in Machine Learning

- Backtracking and Bold Driver step sizes evaluate the objective function (including the loss) several times, and thus often are too costly and not used.
  - But useful for debugging as they guarantee decrease in f.
- Constant step sizes $\mu \in (0, 1)$ are frequently used.
  - If chosen (too) small, the learning algorithm becomes slow, but usually still converges.
  - The step size becomes a hyperparameter that has to be searched.
- Regimes of shrinking step sizes are used:

$$\mu_i := \mu_{i-1}\gamma, \quad \gamma \in (0, 1) \text{ not too far from } 1$$

  - If the initial step size μ_0 is too large, later iterations will fix it.
  - If γ is too small, GD may get stuck before convergence.

How Many Minima can a Function have?

- In general, a function f can have several different **local minima** i.e., points x with $\frac{\partial f}{\partial x}(x) = 0$.
- GD will find a random one
  (with small step sizes, usually one close to the starting point; **local optimization method**).

Convexity

- A function $f : \mathbb{R}^N \rightarrow \mathbb{R}$ is called **convex** if

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2), \quad \forall x_1, x_2 \in \mathbb{R}^N, t \in [0,1]$$

- for a convex function, all local minima have the same function value (**global minimum**)

- **2nd-order criterion for convexity**: A two-times differentiable function is convex if its Hessian is positive semidefinite, i.e.,

$$x^T \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)_{i=1,\ldots,N, j=1,\ldots,N} x \geq 0 \quad \forall x \in \mathbb{R}^N$$

- For any matrix $A \in \mathbb{R}^{N \times M}$, the matrix $A^T A$ is positive semidefinite.

- Thus linear regression with RSS/L2/quadratic loss is convex and GD will find a global minimum.

Outline

Sparse Predictors

Many problems have predictors $x \in R^M$ that are

- **high-dimensional**: M is large, and
- **sparse**: most x_m are zero.

For example, **text regression**:

- task: predict the rating of a customer review.
- predictors: a text about a product — a sequence of words.
  - can be represented as vector via **bag of words**:
    x_m encodes the frequency of word m in a given text.
  - dimensions 30,000-60,000 for English texts
  - in short texts as reviews with a couple of hundred words, maximally a couple of hundred dimensions are non-zero.
- target: the customers rating of the product — a (real) number.

Sparse Predictors — Dense Normal Equations

- Recall, the normal equations

  $$X^T X \hat{\beta} = X^T y$$

  have dimensions $M \times M$.

- Even if X is sparse, generally $X^T X$ will be rather dense.

  $$(X^T X)_{m,l} = X_{.,m}^T X_{.,l}$$

  - For text regression, $(X^T X)_{m,l}$ will be non-zero for every pair of words m, l that co-occurs in any text.

- Even worse, even if $A := X^T X$ is sparse, standard methods to solve linear systems (such as Gaussian elimination, LR decomposition etc.) do not take advantage.

Learn Linear Regression via Loss Minimization

Alternatively to learning a linear regression model via solving the linear normal equation system one can minimize the loss directly:

$$\begin{aligned} f(\hat{\beta}) &:= \hat{\beta}^T X^T X \hat{\beta} - 2y^T X \hat{\beta} + y^T y \\ &= (y - X\hat{\beta})^T (y - X\hat{\beta}) \\ \frac{\partial f}{\partial \hat{\beta}}(\hat{\beta}) &= -2(X^T y - X^T X \hat{\beta}) \\ &= -2X^T (y - X\hat{\beta}) \end{aligned}$$

When computing f and $\frac{\partial f}{\partial \hat{\beta}}$,

- avoid computing (dense) $X^T X$.
- always compute (sparse) X times a (dense) vector.

Objective Function and Gradient as Sums over Instances

$$
\begin{aligned}
f(\hat{\beta}) &:= (y - X\hat{\beta})^T (y - X\hat{\beta})^T \\
&= \sum_{n=1}^{N} (y_n - x_n^T \hat{\beta})^2 \\
&= \sum_{n=1}^{N} \epsilon_n^2, \qquad\qquad \epsilon_n := y_n - x_n^T \hat{\beta} \\
\frac{\partial f}{\partial \hat{\beta}}(\hat{\beta}) &= -2X^T(y - X\hat{\beta}) \\
&= -2 \sum_{n=1}^{N} (y_n - x_n^T \hat{\beta}) x_n \\
&= -2 \sum_{n=1}^{N} \epsilon_n x_n
\end{aligned}
$$

Learn Linear Regression via Loss Minimization: GD

```
learn-linreg-GD($\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \mu, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+$):
    $X := (x_1, x_2, \ldots, x_N)^T$
    $y := (y_1, y_2, \ldots, y_N)^T$
    $\hat{\beta}_0 := (0, \ldots, 0)$
    $\hat{\beta} :=$ minimize-GD( $f(\hat{\beta}) := (y - X\hat{\beta})^T(y - X\hat{\beta})$,
                              $\hat{\beta}_0, \mu, i_{\max}, \epsilon$)
    return $\hat{\beta}$
```

Outline

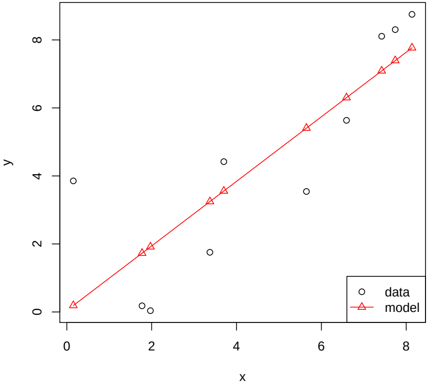
Cases of Different Importance

Sometimes different cases are of different importance, e.g., if their measurements are of different accurracy or reliability.

Example: assume the left most point is known to be measured with lower reliability.

Thus, the model does not need to fit to this point equally as well as it needs to do to the other points.

I.e., residuals of this point should get lower weight than the others.



Case Weights

In such situations, each case (x_n, y_n) is assigned a **case weight** $w_n \geq 0$:

- the higher the weight, the more important the case.
- cases with weight 0 should be treated as if they have been discarded from the data set.

Case weights can be managed as an additional pseudo-variable w in implementations.

Weighted Least Squares Estimates

Formally, one tries to minimize the **weighted residual sum of squares**

$$\sum_{n=1}^{N} w_n(y_n - \hat{y}_n)^2 = ||W^{\frac{1}{2}}(y - \hat{y})||^2$$

with

$$W := \begin{pmatrix} w_1 & & & 0 \\ & w_2 & & \\ & & \ddots & \\ 0 & & & w_n \end{pmatrix}$$

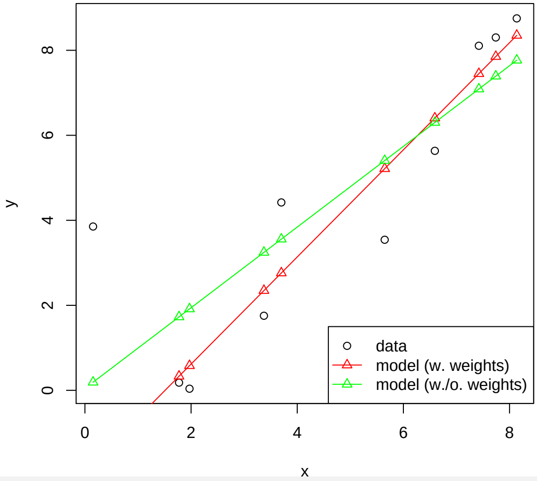
The same argument as for the unweighted case yields the **weighted least squares estimates**

$$X^T W X \hat{\beta} = X^T W y$$

Weighted Least Squares Estimates / Example

To downweight the left most point, we assign case weights as follows:

w	x	y
1	5.65	3.54
1	3.37	1.75
1	1.97	0.04
1	3.70	4.42
0.1	0.15	3.85
1	8.14	8.75
1	7.42	8.11
1	6.59	5.64
1	1.77	0.18
1	7.74	8.30



Summary

- For regression, **linear models** of type $\hat{y} = x^T \hat{\beta}$ can be used to predict a quantitative y based on several (quantitative) x.
  - A **bias term** can be modeled as additional predictor that is constant 1.
- The **ordinary least squares estimates (OLS)** are the parameters with minimal **residual sum of squares** (RSS).
- OLS estimates can be computed by solving the **normal equations** $X^T X \hat{\beta} = X^T y$ as any system of linear equations via **Gaussian elimination**.
- Alternatively, OLS estimates can be computed iteratively via **Gradient Descent**.
  - Especially for **high-dimensional, sparse predictors** GD is advantageous as it never has to compute the large, dense $X^T X$.

Further Readings

- [James et al., 2013, chapter 3], [Murphy, 2012, chapter 7], [Hastie et al., 2005, chapter 3].

References

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