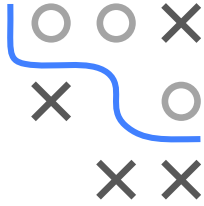
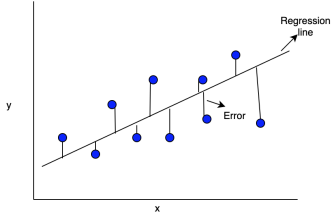
Algorithms and Data Structures



Matrix Decomposition
Overdetermined Systems & Regression
Example

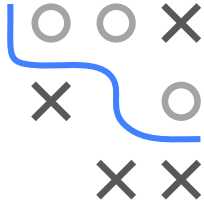


Learning goals

- Overdetermined systems
- Normal equations
- QR decomposition and ridge regression

OVERDETERMINED SYSTEMS

A system of linear equations $\boldsymbol{Ax} = \boldsymbol{b}$ with $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, $m \geq n$ with more equations than unknowns, is called **overdetermined**.

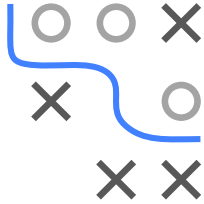


In general such a system has no (exact) solution.

A (compromise) solution using **least squares** is the vector $\boldsymbol{x}$ which minimizes the squared sum of the **residual vector** $\boldsymbol{r} = \mathbf{b} - \mathbf{A}\boldsymbol{x}$:

$$\boldsymbol{x} = \arg\min \|\mathbf{b} - \mathbf{A}\boldsymbol{x}\|_2^2$$

EXAMPLE: THE REGRESSION MODEL



Aim: Solve $\boldsymbol{X\beta} = \boldsymbol{y}$ with

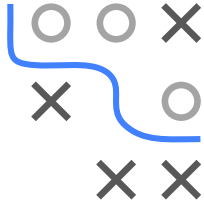
- $\mathbf{X}$: $n \times (p+1)$, Design matrix
- $\mathbf{y}$: $n \times 1$, n observations
- $\boldsymbol{\beta}$: $(p+1) \times 1$, p regressors plus intercept

Since the linear system is usually overdetermined (more observations than variables) and has no solution, we minimize the residual sum of squares:

$$\min_{\beta} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Questions: How can the problem be solved in a numerically stable way? Which algorithms are fast?

CONDITION OF NORMAL EQUATIONS



The solution of the optimization problem is (mathematically) equivalent to the solution of the **normal equation**

$$\mathbf{X}^\top \mathbf{X}\boldsymbol{\beta} = \mathbf{X}^\top \mathbf{y}$$

(Derivation: differentiate with respect to $\boldsymbol{\beta}$ and set to 0).
If the matrix $\mathbf{X}$ has full column rank, then the matrix $\mathbf{X}^\top \mathbf{X}$ is symmetric positive-definite and the following holds

$$\kappa(\mathbf{X}^T\mathbf{X}) \quad = \quad \kappa(\mathbf{X})^2$$

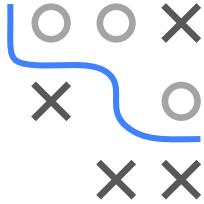
using the spectral norm.

Consequently, the error amplification is $\kappa(\mathbf{X})^2$ when using normal equations.

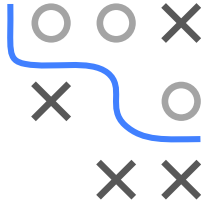
CONDITION OF NORMAL EQUATIONS / 2

Note:

- Mathematically speaking, the solution of the normal equations is equivalent to the minimization of the residual sum of squares
- However, from a numerical point of view a distinction must be made between the two of them
- A solution using the normal equations requires the calculation of $\mathbf{X}^\top\mathbf{X}$, an error in $\mathbf{X}$ is therefore amplified
- Better: Find an efficient method that operates directly on $\mathbf{X}$



SOLUTION OF THE NORMAL EQUATIONS



Model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$

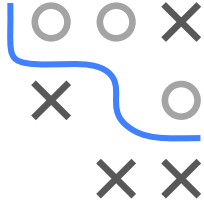
Normal equations: $\mathbf{X}^\top\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^\top\mathbf{y}$

If $\mathbf{X}$ is of full rank then $\mathbf{X}^\top\mathbf{X}$ is positive-definite and the Cholesky decomposition applicable.

1. Calculate $\mathbf{X}^\top\mathbf{X}$ and $\mathbf{X}^\top\mathbf{y}$,
2. Cholesky decomposition $\mathbf{X}^\top\mathbf{X} = \mathbf{L}\mathbf{L}^\top$,
3. Solve $\mathbf{L}\mathbf{w} = \mathbf{X}^\top\mathbf{y}$ for $\mathbf{w}$,
4. Calculate $RSS = \mathbf{y}^\top\mathbf{y} - \mathbf{w}^\top\mathbf{w}$,
5. Solve $\mathbf{L}^\top\boldsymbol{\beta} = \mathbf{w}$ for $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}$,
6. $(\mathbf{X}^\top\mathbf{X})^{-1} = \mathbf{L}^{-\top}\mathbf{L}^{-1}$.

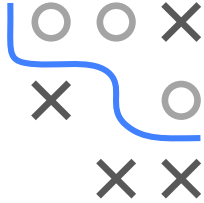
SOLUTION OF THE NORMAL EQUATIONS / 2

```
X = matrix(c(rep(1, 6), c(1.01, 1.01)), ncol = 2)
X
## [,1] [,2]
## [1,] 1 1.00
## [2,] 1 1.00
## [3,] 1 1.01
## [4,] 1 1.01
XX = t(X) %*% X
XX
## [,1] [,2]
## [1,] 4.00 4.020000000000000
## [2,] 4.02 4.040200000000000
```



SOLUTION OF THE NORMAL EQUATIONS / 3

```
XX2 = round(XX, 3)
XX2
## [,1] [,2]
## [1,] 4.00 4.02
## [2,] 4.02 4.04
```

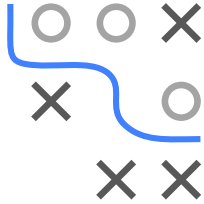


```
cholesky(XX)
## [,1] [,2]
## [1,] 2.00 0.00000000000000000
## [2,] 2.01 0.01000000000007716
```

```
cholesky(XX2)
## [,1] [,2]
## [1,] 2.00 0
## [2,] 2.01 NaN
```

$\Rightarrow$ Number of decimal digits matters, matrix no longer positive-definite!

SOLUTION OF THE NORMAL EQUATIONS / 4



In general a solution using normal equations is to be avoided

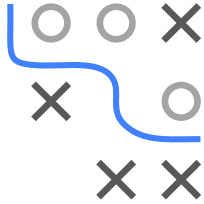
$$\mathbf{X}^\top \mathbf{X}\boldsymbol{\beta} = \mathbf{X}^\top \mathbf{y}$$

since:

- **High computational effort**: First calculation of $\boldsymbol{X}^\top \boldsymbol{X}$, then matrix decomposition of $\boldsymbol{X}^\top \boldsymbol{X}$, then forward and back substitution
- **Numeric instability**: In all these individual steps there is a risk that errors will be amplified.

  A further problem occurs if we want to solve the normal equations in case of **collinearity** in the design matrix $\mathbf{X}$. The reason for this is the singularity of the product of $\mathbf{X}^\top \mathbf{X}$ which results from collinearity.

SOLUTION OF THE NORMAL EQUATIONS / 5



It is often more suitable to operate directly on $\mathbf{X}$ by using QR decomposition $\mathbf{X} = \mathbf{QR}$:

$$\mathbf{X}^\top \mathbf{X} = (\mathbf{QR})^\top (\mathbf{QR}) = \mathbf{R}^\top \mathbf{Q}^\top \mathbf{QR} = \mathbf{R}^\top \mathbf{R}$$

The normal equations can then be written as

$$\mathbf{R}^\top \mathbf{R}\beta = \mathbf{R}^\top \mathbf{Q}\top \mathbf{y}$$

and since $\mathbf{R}^\top$ is nonsingular it follows

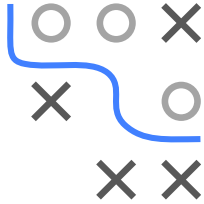
$$\mathbf{R}\beta = \mathbf{Q}^\top \mathbf{y}$$

Since $\mathbf{R}$ is an upper triangular matrix, the equation system (after multiplying $\boldsymbol{Q}^\top \boldsymbol{y}$) can be solved using back substitution in $\mathcal{O}(n^2)$.

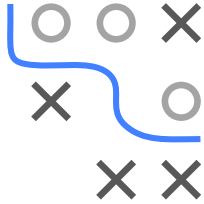
SOLUTION OF THE NORMAL EQUATIONS / 6

The steps to solve a linear regression problem using QR decomposition are therefore as follows:

1. Calculate the QR decomposition $\mathbf{X} = \mathbf{QR}$,
2. Calculate $\boldsymbol{z} = \boldsymbol{Q}^\top \boldsymbol{y}$,
3. Solve the equation system $\boldsymbol{R}\beta = \boldsymbol{z}$ using back substitution.



SOLUTION OF THE NORMAL EQUATIONS / 7



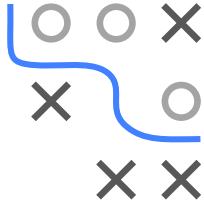
Advantage of QR decomposition: As already stated, the solution when using QR decomposition can be written as

$$\mathbf{R}\boldsymbol{\beta} = \mathbf{Q}^\top \mathbf{y}$$

- $\mathbf{X}$ (and not $\boldsymbol{X}^\top \boldsymbol{X}$) is decomposed directly.
- $\mathbf{X}^\top \mathbf{X}$ does not have to be calculated (thus avoiding numerical instability from collinearity).
- If a stable algorithm is used to calculate the QR decomposition (e.g. Householder), the method is stable.
- Extreme runtime advantages if a regression is to be performed for constant design matrix $\boldsymbol{X}$, but different $\boldsymbol{y}$.

Note: For linear models `lm()` in `R` the QR decomposition is applied when calculating $\boldsymbol{\beta}$.

QR DECOMPOSITION AND RIDGE REGRESSION



In order to avoid a high variance, large parameters are often penalized by a penalty term. We minimize a penalized version of the residual sum of squares

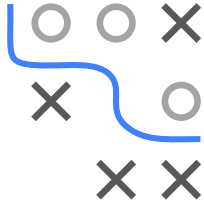
$$\min_{\beta} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_2^2$$

with regularization parameter $\lambda > 0$. If the L_2 norm is selected for the penalty, the procedure is known as **ridge regression**.

We obtain a general version of the normal equations by setting the first derivative to 0

$$\left(\mathbf{X}^\top \mathbf{X} + \lambda I\right) \boldsymbol{\beta} = \mathbf{X}^\top \mathbf{y}$$

QR DECOMPOSITION AND RIDGE REGRESSION / 2



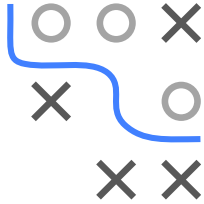
With $\boldsymbol{A}oneqq\left(\begin{smallmatrix}\boldsymbol{X}\\ \sqrt{\lambda}\boldsymbol{I}\end{smallmatrix}\right) \in \mathbb{R}^{n+p,p}$ the normal equations for ridge regression can be rewritten as

$$\begin{aligned}\left(\mathbf{X}^\top\mathbf{X} + \lambda I\right)\beta &= \mathbf{X}^\top\mathbf{y} \\ \mathbf{A}^\top\mathbf{A}\beta &= \mathbf{A}^\top\begin{pmatrix}\mathbf{y}\\ \mathbf{0}\end{pmatrix}\end{aligned}$$

We use the QR decomposition of $\boldsymbol{A} = \boldsymbol{Q}_\lambda\boldsymbol{R}_\lambda$ depending on λ:

$$\begin{aligned}\mathbf{A}^\top\mathbf{A}\beta &= \mathbf{A}^\top\begin{pmatrix}\mathbf{y}\\ \mathbf{0}\end{pmatrix} \\ \mathbf{R}_\lambda^\top\mathbf{Q}_\lambda^\top\mathbf{Q}_\lambda\mathbf{R}_\lambda\beta &= \mathbf{R}_\lambda^\top\mathbf{Q}_\lambda^\top\begin{pmatrix}\mathbf{y}\\ \mathbf{0}\end{pmatrix} \\ \mathbf{R}_\lambda^\top\mathbf{R}_\lambda\beta &= \mathbf{R}_\lambda^\top\mathbf{Q}_\lambda^\top\begin{pmatrix}\mathbf{y}\\ \mathbf{0}\end{pmatrix}\end{aligned}$$

QR DECOMPOSITION AND RIDGE REGRESSION / 3



- If $\boldsymbol{R}_\lambda$ is singular, we have to solve two LES in echelon form
- If $\boldsymbol{R}_\lambda$ is nonsingular and thus invertible, the equation simplifies to one linear system in echelon form

The regularization parameter λ is a hyperparameter that must be selected by the user. Often the linear system has to be solved several times for different λ to find a sensible degree of regularization.

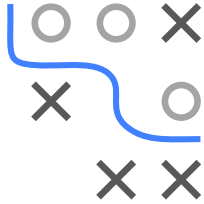
In such situations the QR decomposition

$$\mathbf{R}_\lambda^\top \mathbf{R}_\lambda \beta \quad = \quad \mathbf{R}_\lambda^\top \mathbf{Q}_\lambda^\top \begin{pmatrix} \mathbf{y} \\ \mathbf{0} \end{pmatrix}$$

has to be calculated anew for each λ. The QR decomposition of the matrix $\boldsymbol{A}$ is calculated in $\mathcal{O}(n^3)$. Forward and back substitution are operations of $\mathcal{O}(n^2)$, so in total the runtime is given by $\mathcal{O}(n^3)$.

COMPARISON OF METHODS FOR REGRESSION

Method	Runtime	General Numerical Stability	Stability in Collinearity
Naive approach	- -	no	no
LU	+ +	yes, with pivotisation	no
QR (Householder)	-	yes	yes



$\Rightarrow$ **Note:** QR decomposition is not the fastest method regarding runtime, but it is always numerically stable in a regression context.

COMPARISON OF METHODS FOR REGRESSION / 2