Machine Learning

Linear Regression

Matteo Papini

Credits to Alberto Maria Metelli and Francesco Trovò

Politecnico di Milano

Outline

1. Administrivia
2. Regression Problem
3. Practical Example

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Administrivia

Matteo Papini
Assistant Professor

- Dipartimento di Elettronica, Informazione e Bioingegneria (DEIB)
  - bulding 21
  - first floor
  - office 19
- Email: `matteo.papini@polimi.it`

Course Material

- Course materials of lectures and exercise sessions uploaded to WeBeep
  `https://webeep.polimi.it/course/view.php?id=12810`
- Material of exercise sessions
  - **Recorded exercise sessions**
  - **Slides** for lectures and exercise sessions **(some topics are only covered in exercise sessions)**
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  - **Colab notebooks (we require you to understand the code at the exam**, e.g., find and rectify mistakes).
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Suggested Literature

- Bishop, C.M., “Pattern recognition and machine learning”, 2006, Springer
  https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf
- James, G., Witten, D., Hastie, T., Tibshirani, R., “An introduction to statistical learning”, 2013, Springer
  https://www.statlearning.com/

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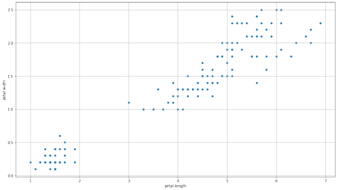
Where Everything Starts

Consider the **Iris Dataset**
(`https://en.wikipedia.org/wiki/Iris_flower_data_set`):

- Sepal length
- Sepal width
- Petal length
- Petal width
- Species (Iris setosa, Iris virginica e Iris versicolor)

$N = 150$ total samples (50 per species)



Example of Dataset

Sepal length	Sepal width	Petal length	Petal width	Class
5.1000	3.5000	1.4000	0.2000	Iris-setosa
4.9000	3.0000	1.4000	0.2000	Iris-setosa
4.7000	3.2000	1.3000	0.2000	Iris-setosa
4.6000	3.1000	1.5000	0.2000	Iris-setosa
5.0000	3.6000	1.4000	0.2000	Iris-setosa
5.4000	3.9000	1.7000	0.4000	Iris-setosa
4.6000	3.4000	1.4000	0.3000	Iris-setosa
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4.4000	2.9000	1.4000	0.2000	Iris-setosa
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Scientific Questions

- Can we extract some information from the data?
- What can we infer from them?
- Can we provide predictions on some of the quantities on newly seen data?
- Can we predict the **petal width** of a specific kind of *Iris setosa* by using the **petal length**?

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Solution: Linear Regression

We need to specify:

- Hypothesis space: **linear models**

$$\hat{t} = y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j x_j = \mathbf{w}^\top \mathbf{x}$$

where $\mathbf{w} = (w_0, w_1, \ldots, w_{M-1})^\top$ and $\mathbf{x} = (1, x_1, \ldots, x_{M-1})^\top$

- Loss function: **residual sum of squares** over the N samples $\{(\mathbf{x}_n, t_n)\}_{n=1}^N$:

$$\mathrm{RSS}(\mathbf{w}) = \sum_{n=1}^{N} (y(\mathbf{x}_n, \mathbf{w}) - t_n)^2$$

- Optimization method: closed form, gradient descent, ...

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Example of Dataset

In our Iris dataset example: $\mathbf{x} = (1, \text{Petal length})^\top$ $(M = 2)$ and $t = \text{Petal width}$

rows, instances (N)

Constant	Petal length	Petal width
	variables, features, input, $\mathbf{x}$	target, response, output, t
1.0000	3.5000	0.2000
1.0000	1.4000	0.2000
1.0000	1.3000	0.2000
1.0000	1.5000	0.2000
1.0000	1.4000	0.2000
1.0000	1.7000	0.4000
1.0000	1.4000	0.3000
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1.0000	1.4000	0.2000
1.0000	1.5000	0.1000
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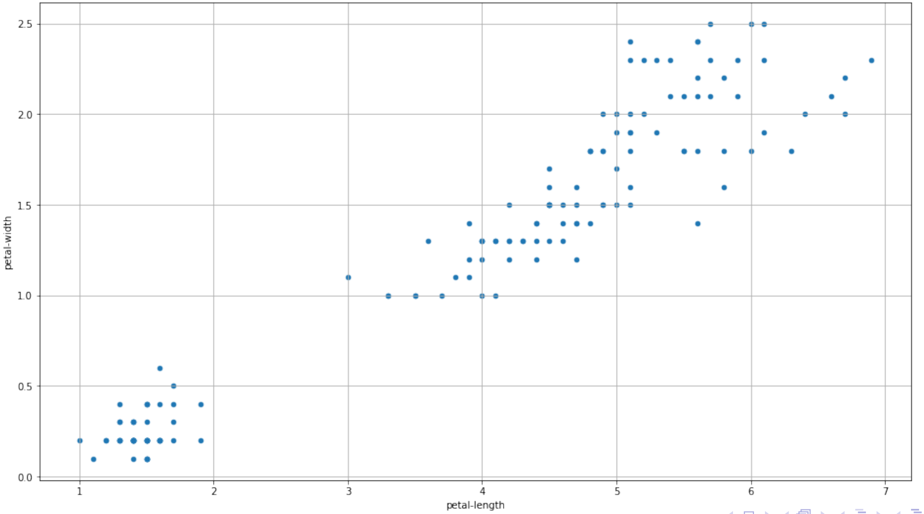

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Preliminary Operations

- Load data
- Inspect data
- Select the interesting data
- Preprocessing
  - shuffling (`shuffle()`)
  - remove inconsistent data
  - remove outliers
  - normalize or standardize data (`zscore()`)
  - fill missing data (`is_nan()`)

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Data Normalization

Samples $\{s_1, \ldots, s_N\} \rightarrow$ normalization of sample s:

- z-score

$$\frac{s - \bar{s}}{S}$$

where $\bar{s} = \frac{1}{N}\sum_{n=1}^{N} s_n$ and $S^2 = \frac{1}{N-1}\sum_{n=1}^{N}(s_n - \bar{s})^2$

- Min-max feature scaling

$$\frac{s - s_{\min}}{s_{\max} - s_{\min}}$$

where $s_{\max} = \max_{n \in \{1,\ldots,N\}} s_n$ and $s_{\min} = \min_{n \in \{1,\ldots,N\}} s_n$

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Linear Regression in Python

We have several solutions from different libraries:

- `sklearn` with `LinearRegression()`
- `statsmodels` with `OLS`
- by hand implementation $\mathbf{w}^* = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{t}$

First the `sklearn` option:

- Create a linear model (`LinearRegression()`)
- Fit the model to the data (`fit()`)
- Analyze the results

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Example

Evaluating the Results

- Residual Sum of Squares (RSS), Sum Of Squared Errors (SSE):

$$\mathrm{RSS}(\mathbf{w}) = \sum_{n=1}^{N} (\hat{t}_n - t_n)^2 \qquad \text{where} \qquad \hat{t}_n = y(\mathbf{x}_n, \mathbf{w})$$

- Mean Square Error: $\mathrm{MSE} = \frac{\mathrm{RSS}(\mathbf{w})}{N}$
- Root Mean Square Error: $\mathrm{RMSE} = \sqrt{\frac{\mathrm{RSS}(\mathbf{w})}{N}}$

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Evaluating the Results

- Coefficient of determination (R squared):

$$R^2 = 1 - \frac{\text{RSS}(\mathbf{w})}{\text{TSS}}$$

where $\text{TSS} = \sum_{n=1}^{N} (\bar{t} - t_n)^2$ is the Total Sum of Squares and $\bar{t} = \frac{1}{N} \sum_{n=1}^{N} t_n$

- Degrees of Freedom: $\text{dfe} = N - M$
- Adjusted coefficient of determination $R^2_{\text{adj}} = 1 - (1 - R^2)\frac{N-1}{\text{dfe}}$

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Statistical Tests on Coefficients

- **Assumption**: t_n satisfy $t_n = \mathbf{w}^T \mathbf{x}_n + \epsilon_n$, where ϵ_n is i.i.d. Gaussian white zero-mean noise and variance σ^2
- Exact distribution of the statistic:

$$\frac{\hat{w}_j - w_j}{\hat{\sigma}\sqrt{v_j}} \sim t_{N-M},$$

where w_j is the true parameter, $\hat{w}_j$ the estimated parameter with N samples, v_j is the j-th diagonal element of the matrix $(\mathbf{X}^\top \mathbf{X})^{-1}$, t_{N-M} is the T-student distribution with $\mathrm{dfe} = N - M$ degrees of freedom, and $\hat{\sigma}^2$ is is the unbiased estimated for the target variance:

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Statistical Tests on Coefficients

- **Test on single coefficients** $j \in \{0, \dots, M-1\}$:

$$H_0 : w_j = 0 \qquad \text{vs.} \qquad H_1 : w_j \neq 0$$

$$t_{\text{stat}} = \frac{\hat{w}_j - w_j}{\hat{\sigma}\sqrt{v_j}} \sim t_{N-M}$$

where t_{N-M} is the T-Student distribution with $N - M$ degrees of freedom

Statistical Tests on Coefficients

- **Test on the overall significance of the model**:

$$H_0 : w_1 = \dots = w_{M-1} = 0 \qquad \text{vs.} \qquad H_1 : \exists j \in \{1, \dots, M-1\} \text{ s.t. } w_j \neq 0$$

$$F_{\text{stat}} = \frac{N-M}{M-1} \cdot \frac{\text{TSS} - \text{RSS}(\hat{\mathbf{w}})}{\text{RSS}(\hat{\mathbf{w}})} \sim F_{M-1,N-M}$$

where $F_{M-1,N-M}$ is the Fisher-Snedecor distribution with parameters $M-1$ and $N-M$

  - We are comparing the full linear model $y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j x_j$ (with $N-M$ d.o.f.) against the constant model $y(\mathbf{x}, w_0) = w_0$ (with $N-1$ d.o.f.).

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Example of `OLS(x, t).fit()` Output

```
Dep. Variable:                  y   R-squared (uncentered):          0.927
Model:                        OLS   Adj. R-squared (uncentered):     0.926
Method:             Least Squares   F-statistic:                     1889.
Date:            Wed, 10 Mar 2021   Prob (F-statistic):           1.56e-86
Time:                    12:28:24   Log-Likelihood:                -16.645
No. Observations:             150   AIC:                             35.29
Df Residuals:                 149   BIC:                             38.30
Df Model:                       1
Covariance Type:        nonrobust
==========================================================================
        coef      std err         t       P>|t|       [0.025      0.975]
--------------------------------------------------------------------------
x1     0.9628      0.022     43.467      0.000        0.919       1.007
==========================================================================
Omnibus:                    2.326   Durbin-Watson:                   1.437
Prob(Omnibus):              0.313   Jarque-Bera (JB):                1.852
Skew:                       0.210   Prob(JB):                        0.396
Kurtosis:                   3.347   Cond. No.                         1.00
```

Different Implementations

`fit()`

- Slow in the execution
- Many checks for consistency
- Recap

By-hand solution

- Very fast
- No checks for consistency
- No tests on the coefficients

Code Exercise

```
x = zscore(dataset['petal-length'].values).reshape(-1, 1)
y = zscore(dataset['petal-width'].values)
Phi = np.ones((len(x), 2))
Phi[:, 1] = x.flatten()
model = inv(Phi.T @ Phi) @ (Phi.T.dot(y))
r_model = linear_model.Ridge(alpha=10)
r_model.fit(x, y)
l_model = linear_model.Lasso(alpha=10)
l_model.fit(x, y)
```

1. Which problem is the snippet above solving?
2. Which algorithms are implemented by the snippet above?
3. Which model would you choose to provide an interpretable solution, e.g., a model whose parameters influence are easy to explain?
4. Which are the pros and the cons of using the algorithm in lines 3-5?