Introduction to Statistical Machine Learning

Réda DEHAK
http://isml.dehak.org

1

Organisation

- 8 lessons : Introduction to Statistical Machine Learning Methods
  - 8 Lectures :
    - Regression - Gradient descent - Régularization Lasso and Ridge
    - Linear Classification - Logistic Regression - MultiClass Classification
    - Neural Network Methods: Backpropagation Algorithm
    - Support Vector Machine : Linear version
    - Support Vector Machine : Kernel Method
    - Decision Trees, Bagging, Boosting, Random Forest
    - Dimensionality Reduction
    - sUnsupervised Learning
  - 8 labs :
    - Python 3
    - Jupiter
    - Numpy
    - Scikit-learn
    - …
- MidTerm Exam : ? Final Exam : ?

Réda DEHAK 2

2

Why Learn?

- Machine learning is programming computers to optimize a performance criterion using example data or past experience.
- There is no need to "learn" to calculate payroll, or to sort a list of numbers
- Learning is used when:
  - Human expertise does not exist (navigating on Mars),
  - Humans are unable to explain their expertise (speech recognition)
  - Solution changes in time (routing on a computer network)
  - Solution needs to be adapted to particular cases (user biometrics)

Réda DEHAK 3

3

Machine Learning

- Study of algorithms that [T.Mitchell]:
  - Improve their **performance *P*,**
  - At some **task *T***
  - With **experience *E***
- Well defined learning task: ***<P, T, E>***

Réda DEHAK 4

4

What is Machine Learning?

- Optimize a performance criterion using example data or past experience.
- Role of Statistics: Inference from a sample
- Role of Computer science: Efficient algorithms to
  - Solve the optimization problem
  - Representing and evaluating the model for inference

Réda DEHAK 5

5

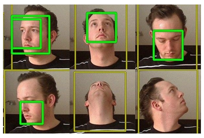
What We Talk About When We Talk About"Learning"

- Learning general models from a data of particular examples
- Data is cheap and abundant (data warehouses, data marts); knowledge is expensive and scarce.
- Example in retail: Customer transactions to consumer behavior:
  People who bought "Beer" also bought "Chips"
- Build a model that is *a good and useful approximation* to the data.

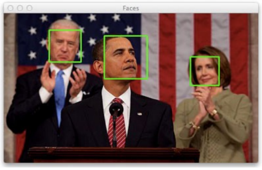
Réda DEHAK 6

6

Learning to Detect Faces in Images



Training images for different pose



7

Text Documents Classifications

Personal home page
vs.
Company home page
vs.
University home page
vs
...

8

Data Mining

- Retail: Market basket analysis, Customer relationship management (CRM)
- Finance: Credit scoring, fraud detection
- Manufacturing: Control, robotics, troubleshooting
- Medicine: Medical diagnosis
- Telecommunications: Spam filters, intrusion detection
- Bioinformatics: Motifs, alignment
- Web mining: Search engines
- ...

9

Machine Learning in Computer Science

- Machine learning already the preferred approach to
  - Speech recognition, Natural Language processing
  - Computer Vision
  - Medical outcomes analysis
  - Robot control
  - …
- This ML niche is growing (why?)

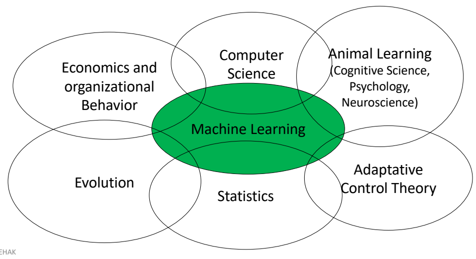
10

Machine Learning in Computer Science

- Machine learning already the preferred approach to
  - Speech recognition, Natural Language processing
  - Computer Vision
  - Medical outcomes analysis
  - Robot control
  - …
- This ML niche is growing
  - Improved machine learning algorithms
  - Increased data capture, networking, new sensors
  - Software too complex to write by hand
  - Demand for self-customization to user, environment

11

Machine Learning



12

Machine Learning Methods

1. Supervised Methods:
   a) Regression
   b) Classification
2. Unsupervised Methods
3. Reinforcement Learning

Réda DEHAK 13

13

Supervised Learning

- learning a function that maps an input (features) to an output (target or labels) based on examples input-output pairs.
- Discrete Output Values → Classification
- Continuous Output Values → Regression
- Examples:
  - Face recognition, Character recognition, Speech and Language recognition
  - Predicting age, nationality and weight of a person, Predicting whether stock price of a company will increase tomorrow

Réda DEHAK 14

14

Unsupervised Learning

- Learning “what normally happens”
- No output
- Clustering: Grouping similar instances
- Example applications
  - Customer segmentation in CRM
  - Image compression: Color quantization
  - Bioinformatics: Learning motifs

Réda DEHAK 15

15

Reinforcement Learning

- Learning a policy: A sequence of outputs
- No supervised output but delayed reward
- Examples:
  - Credit assignment problem
  - Game playing
  - Robot in a maze
  - Multiple agents, partial observability, ...

Réda DEHAK 16

16

The four "aspects" of Machine Learning

- **Representation**: How best to represent data for best processing
- **Modeling**: How to *model* the systematic and statistical characteristics of the data
- **Classification**: How do we assign a class to the data?
- **Prediction**: How do we predict new or unseen values or attributes of the data

Réda DEHAK 17

17

What we will cover

1. Regression - Gradient descent - Régularization Lasso and Ridge
2. Linear Classification - Logistic Regression - MultiClass Classification
3. Backpropagation Algorithm, Neural Networks
4. Support Vector Machine : Linear version
5. Support Vector Machine : Kernel Method
6. Decision Trees, Bagging, Boosting, Random Forest
7. Dimensionality Reduction
8. Unsupervised Learning

Réda DEHAK 18

18

Recommended Background

- Linear Algebra
  - Definitions, vectors, matrices, operations, properties
- Probability
  - Basics: what is a random variable, probability distributions, functions of a random variable
- Machine learning
  - Learning, modelling and classification techniques

19

Data

Structured Data

Area	estate type	Distance to center	Energy class	Age	Number bedrooms	Price
100	Apartement	1,1	A	20	3	130000
150	House	5,6	A	21	5	180000
247	House	2,2	C	20	7	250000
987	House	0,5	D	1	10	1250000

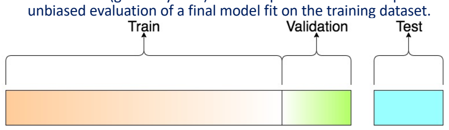
features

targets/labels

20

Training, Validation and Testing Datasets

- The available dataset is subdivided into 3 datasets:
  1. Training Dataset (generally 60%): sample data used to fit the model.
  2. Validation Dataset(generally 20%): used to provide an unbiased evaluation of the model fit when you tune the model's parameters (avoid overffiting).
  3. Test Dataset (generally 20%): The sample of data used to provide an unbiased evaluation of a final model fit on the training dataset.



21

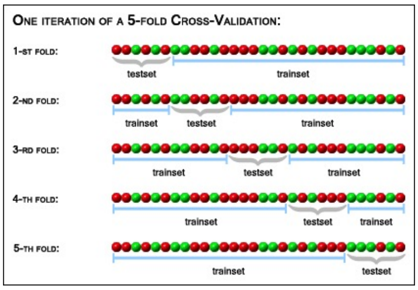
Resampling and K-Fold Cross-Validation

- The need for multiple training/validation sets $\{X_i, V_i\}_i$: Training/validation sets of fold i
- K-fold cross-validation: Divide X into k, X_i, $i=1,\dots,K$

$$\begin{aligned}
\mathcal{V}_1 &= \mathcal{X}_1 & \mathcal{T}_1 &= \mathcal{X}_2 \cup \mathcal{X}_3 \cup \cdots \cup \mathcal{X}_K \\
\mathcal{V}_2 &= \mathcal{X}_2 & \mathcal{T}_2 &= \mathcal{X}_1 \cup \mathcal{X}_3 \cup \cdots \cup \mathcal{X}_K \\
&\vdots \\
\mathcal{V}_K &= \mathcal{X}_K & \mathcal{T}_K &= \mathcal{X}_1 \cup \mathcal{X}_2 \cup \cdots \cup \mathcal{X}_{K-1}
\end{aligned}$$

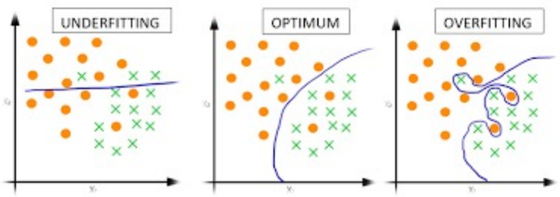
- T_i share K-2 parts

22



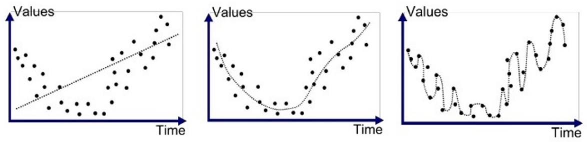
23

Under – Over Fitting



24

Under – Over fitting



Underfitted | Good Fit/Robust | Overfitted

Réda DEHAK 25

25

Under – Over fitting

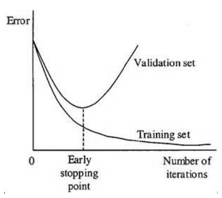
- Overfitting:
  - Model too complex (flexible)
  - Fits « noise » in the training data
  - Don't perform well on new data (bad generalization)
- Underfitting:
  - Model too simplistic (too rigid)
  - Not powerful enough to capture salient patterns in data

Réda DEHAK 26

26

Avoid Overfitting

- Train with more data
- Early stopping



- Regularization
- Reduce model complexity

Réda DEHAK 27

27

Regression - Gradient descent - Regularization Lasso and Ridge

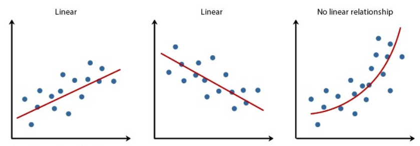
28

What is a regression

- Analyzing relationship between variables
- Expressed in many forms
- Wikipedia
  - Linear regression, Simple regression, Ordinary least squares, Polynomial regression, General linear model, Generalized linear model, Discrete choice, Logistic regression, Multinomial logit, Mixed logit, Probit, Multinomial probit, ….
- Generally a tool to ***predict*** variables

29

Regressions for prediction

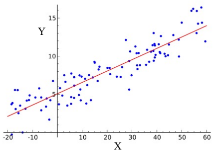


$$y = f(x;\theta) + \epsilon$$

- x is a scalar or a vector
- $f(.)$ is a linear or affine function → Linear Regression
- $f(.)$ is a non-linear function → Non Linear Regression
- θ is the model's (f) parameters

30

A *linear* regression



- Assumption: relationship between variables is linear
  - A linear *trend* may be found relating x and y
  - y = *dependent* variable
  - x = *explanatory* variable
  - Given x, y can be predicted as an affine function of x

Réda DEHAK 31

31

Linear Regressions

$$y = ax + b + \varepsilon$$

ε : prediction error

- Given a "training" set of $\{x, y\}$ values: estimate a and b
  - $y_1 = ax_1 + b + \varepsilon_1$
  - $y_2 = ax_2 + b + \varepsilon_2$
  - $y_3 = ax_3 + b + \varepsilon_3$
  - …
- If a and b are well estimated, prediction error will be small

Réda DEHAK 32

32

Matrix representation of Linear Regression

- $y_1 = ax_1 + b + \varepsilon_1$
- $y_2 = ax_2 + b + \varepsilon_2$
- $y_3 = ax_3 + b + \varepsilon_3$
- …

- **Define:**

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix} \qquad X = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots \\ 1 & 1 & 1 & \cdots \end{bmatrix}$$

$$e = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \end{bmatrix} \qquad A = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$Y = X^T A + e$$

Réda DEHAK 33

33

Learning the Parameters

- $Y = X^T A + e$
- Learning the parameters → minimize cost function

$$E = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_i^2 = \frac{\|e\|^2}{N} = \frac{e^T e}{N}$$

- $e = Y - X^T A$
- $E = \frac{\|e\|^2}{N} = \frac{1}{N}(Y - X^T A)^T (Y - X^T A)$
- E= $\frac{1}{N}(Y^T Y - 2\, A^T XY + A^T XX^T A)$
- $\frac{dE}{dA} = \frac{1}{N}(-2XY + 2XX^T A)$
- $\frac{dE}{dA} = 0 \Rightarrow A = (XX^T)^{-1} XY$

Réda DEHAK 34

34

Learning Parameters

- Linear Regression :

$$A = (XX^T)^{-1} XY$$

- If the dimension of (XX^T) is important, we can use numeric solution rather than analytic one
- Gradient Descent on the Error formula :
  - $\underset{A}{\text{Argmin}}\, \frac{1}{N}(Y^T Y - 2\, A^T XY + A^T XX^T A) = \text{Argmin}_A\, \frac{1}{N}(A^T XX^T A - 2\, A^T XY)$

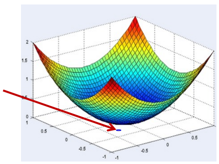
Cost function = $\frac{1}{N}(A^T XX^T A - 2\, A^T XY)$

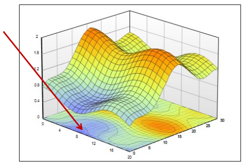
Réda DEHAK 35

35

Examples of Optimization : Multivariate functions

- Find the optimal point in these functions





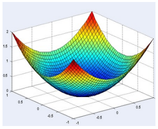
Réda DEHAK 36

36

Gradients of scalar functions with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \dots, x_n)$

$$\nabla f(X) = \begin{bmatrix} \frac{\partial f(X)}{\partial x_1} \\ \frac{\partial f(X)}{\partial x_2} \\ \vdots \\ \frac{\partial f(X)}{\partial x_n} \end{bmatrix}$$

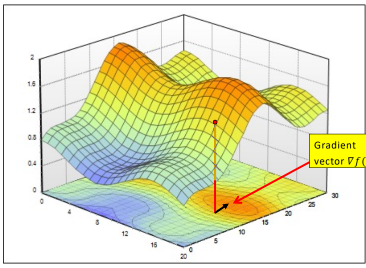


- The function $f(X)$ increases most rapidly if the input increment ΔX is perfectly aligned to $\nabla f(X)$
- **The gradient is the direction of fastest increase in f(X)**

Réda DEHAK 37

37

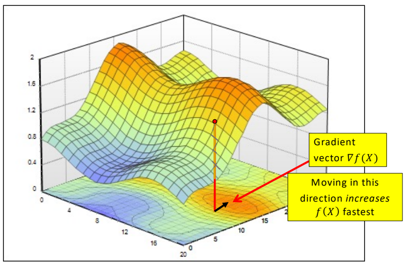
Gradient



Réda DEHAK 38

38

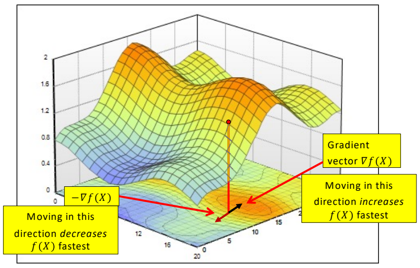
Gradient



Réda DEHAK 39

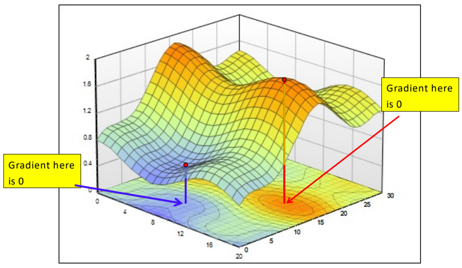
39

Gradient



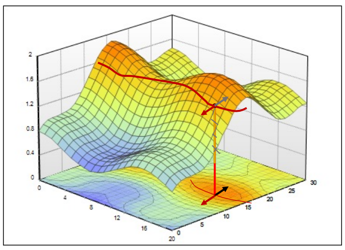
40

Gradient



41

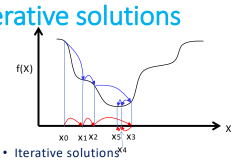
Properties of Gradient:

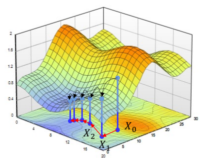


- The gradient vector $\nabla f(X)$ is perpendicular to the level curve

42

Iterative solutions





- Iterative solutions
  - Start from an initial guess X_0 for the optimal X
  - Update the guess towards a (hopefully) "better" value of $f(X)$
  - Stop when $f(X)$ no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

Réda DEHAK 43

43

Descent methods

- Iterative solutions that attempt to "descend" the function in steps to arrive at the minimum
- Based on the first order derivatives (gradient) and in some cases the second order derivatives (Hessian).
  - **Gradient descent** is based only on the first derivative
  - **Newton's method** is based on both first and second derivatives

For Gradient Descent

Réda DEHAK 44

44

Gradient descent/ascent

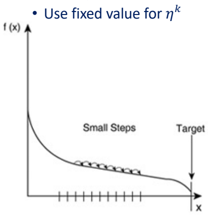
- The gradient descent/ascent method to find the minimum or maximum of a function f iteratively
  - To find a *maximum* move *in the direction of the gradient*
    $$x^{k+1} = x^k + \eta^k \nabla f(x^k)$$
  - To find a *minimum* move *exactly opposite the direction of the gradient*
    $$x^{k+1} = x^k - \eta^k \nabla f(x^k)$$
- What is the step size η^k (Learning rate)

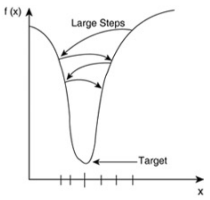
Réda DEHAK 45

45

Fixed step size

- Fixed step size
  - Use fixed value for η^k



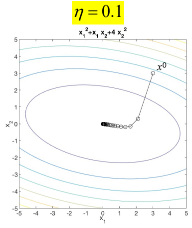


46

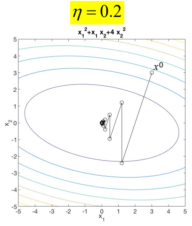
Influence of step size example (constant step size)

$$f(x_1,x_2)=(x_1)^2+x_1x_2+4(x_2)^2 \qquad x^{initial}=\begin{bmatrix}3\\3\end{bmatrix}$$

$\eta=0.1$



$\eta=0.2$



47

Newton's method for multivariate functions

1. Select an initial starting point X^0
2. Evaluate the gradient $\nabla f(X^k)$ and Hessian $\nabla^2 f(X^k)$ at X^k
3. Calculate the new X^{k+1} using the following

$$X^{k+1}=X^k-\left[\nabla^2 f(X^k)\right]^{-1}.\nabla f(X^k)$$

4. Repeat Steps 2 and 3 until convergence

48

Gradient Descent for linear Regression

$$E = \frac{1}{N}(Y^TY - 2\,A^TXY + A^TXX^TA)$$

$$\nabla E = \frac{2}{N}(XX^TA - XY)$$

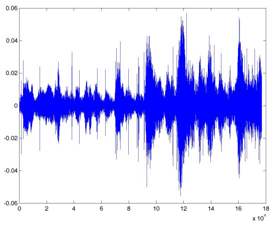
$$\nabla^2 E = \frac{2}{N}XX^T$$

Réda DEHAK 49

49

A Common Problem

- Can you spot the glitches?

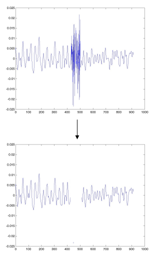


Réda DEHAK 50

50

How to fix this problem?

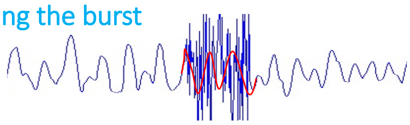
- "Glitches" in audio
  - Must be detected
  - How?
- Then what?
- Glitches must be "fixed"
  - Delete the glitch
    - Results in a "hole"
  - Fill in the hole
  - How?



Réda DEHAK 51

51

Finding the burst

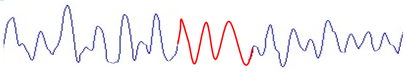


- At each time
  - Learn a "forward" predictor $\mathbf{a}_t$
  - At each time, predict next sample $x_t^{est} = \Sigma_i\, a_{t,k}\, x_{t-k}$
  - Compute error: $ferr_t = |x_t - x_t^{est}|^2$
  - Learn a "backward" predict and compute backward error
    - $berr_t$
  - Compute average prediction error over window, threshold
- If the error exceeds a threshold, identify burst

Réda DEHAK 52

52

Filling the hole

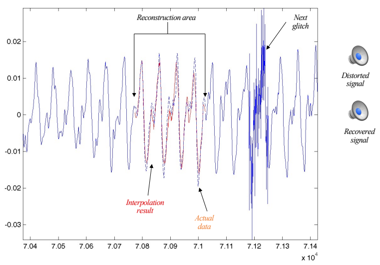


- Learn "forward" predictor at left edge of "hole"
  - For each missing sample
  - At each time, predict next sample $x_t^{est} = \Sigma_i\, a_{t,k} x_{t-k}$
    - Use estimated samples if real samples are not available
- Learn "backward" predictor at left edge of "hole"
  - For each missing sample
  - At each time, predict next sample $x_t^{est} = \Sigma_i\, b_{t,k} x_{t+k}$
    - Use estimated samples if real samples are not available
- Average forward and backward predictions

Réda DEHAK 53

53

Reconstruction zoom in



Réda DEHAK 54

54

Linear Regression

- **Goal :** find a linear relationship between the dependent target variable y and the regression value x

$$y = ax + b + \varepsilon = \hat{x}^T A + \varepsilon$$

Where $A = \begin{bmatrix} a \\ b \end{bmatrix}$ and $\hat{x} = \begin{bmatrix} x \\ 1 \end{bmatrix}$

- **Solution:** Find the optimal value of the cost function MSE(Mean Squared Error)

$$E = MSE = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_i^2 = \frac{1}{N}(Y^T Y - 2\,A^T XY + A^T X X^T A)$$

Where $Y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix}$ $\quad X = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots \\ 1 & 1 & 1 & \cdots \end{bmatrix}$

$$A = (XX^T)^{-1} XY$$

55

Multiple Linear Regression

- **Goal:** find a linear relationship between the dependent target variable y and the regression d vector x

$$y = a_1 x_{(1)} + a_2 x_{(2)} + \cdots + a_d x_{(d)} + b + \varepsilon = \hat{x}^T A + \varepsilon$$

Where $A = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_d \\ b \end{bmatrix}$ and $\hat{x} = \begin{bmatrix} x_{(1)} \\ x_{(2)} \\ \vdots \\ x_{(d)} \\ 1 \end{bmatrix}$

- **Solution:** Find the optimal value of the cost function MSE(Mean Squared Error)

$$E = MSE = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_i^2 = \frac{1}{N}(Y^T Y - 2\,A^T XY + A^T X X^T A)$$

Where $Y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix}$ $\quad X = \begin{bmatrix} x_{1(1)} & x_{2(1)} & x_{3(1)} & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ x_{1(d)} & x_{2(d)} & x_{3(d)} & \cdots \\ 1 & 1 & 1 & \cdots \end{bmatrix}$

$$A = (XX^T)^{-1} XY$$

56

Regularization

- **Goal:** Avoid Overfitting
- Add penalty to the optimization process of the cost function

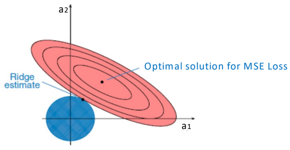
57

Regularization: Ridge Regression

- The **Ridge Regression** is a **regularization** technique that uses L_2 regularization to impose a penalty on the size of coefficients.

$$E_{\text{Ridge}} = \underset{A}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N} \|\hat{x}^T A - y_i\|^2 \qquad \textbf{MSE Loss}$$

$$\|A\|^2 = \sum_{i=1}^{d} a_i^2 \leq \boldsymbol{\tau} \qquad \textbf{Penalty}$$



Réda DEHAK 58

58

Regularization: Ridge Regression

- The **Ridge Regression** is a **regularization** technique that uses L_2 regularization to impose a penalty on the size of coefficients.

$$E_{\text{Ridge}} = \underset{A}{\operatorname{argmin}} \underbrace{\frac{1}{N}\sum_{i=1}^{N} \|\hat{x}^T A - y_i\|^2}_{\text{MSE Loss}} + \underbrace{\boldsymbol{\lambda}\|A\|^2}_{\text{Penalty}} \qquad \|A\|^2 = \sum_{i=1}^{d} a_i^2$$

- Here $\lambda \geq 0$ is a tuning parameter, which controls the strength of the penalty term. Note that:
  - When $\lambda = 0$ ($\tau = +\infty$), we get the linear regression estimate
  - When $\lambda = +\infty$ ($\tau = 0$)we get $A_{\text{Ridge}} = 0$
  - For λ in between, we are balancing two ideas: fitting a linear model of y on x, and shrinking the coefficients

Réda DEHAK 59

59

Regularization: Ridge Regression

- The x **vectors must be centered and normalized** to prevent influence of high variance features
- The target variable y **must be centered to remove** the constant of the regression
- **Solution:**

$$A = (XX^T + \lambda I_d)^{-1} XY$$

Where I_d is the identity matrix

sklearn.linear_model.Ridge

Réda DEHAK 60

60

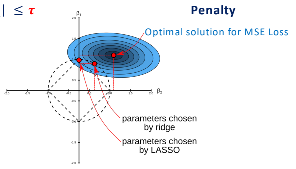
Regularization: Lasso Regression

Least Absolute Shrinkage and Selection Operator

- The **Lasso Regression** is a **regularization** technique that uses L_1 regularization to impose a penalty on the size of coefficients.

$$A_{\text{Lasso}} = \underset{w}{\text{argmin}} \frac{1}{N}\sum_{i=1}^{N}\|\hat{x}^T A - y_i\|^2 \quad \textbf{MSE LOSS}$$

$$\|A\|_1 = \sum_{i=1}^{d}|a_i| \le \boldsymbol{\tau} \quad \textbf{Penalty}$$



61

Regularization: Lasso Regression

Least Absolute Shrinkage and Selection Operator

- The **Lasso Regression** is a **regularization** technique that uses L_1 regularization to impose a penalty on the size of coefficients.

$$A_{\text{Lasso}} = \underset{w}{\text{argmin}} \underbrace{\frac{1}{N}\sum_{i=1}^{N}\|\hat{x}^T A - y_i\|^2}_{\text{MSE Loss}} + \underbrace{\boldsymbol{\lambda}\|A\|_{\mathbf{1}}}_{\text{Penalty}} \qquad \|A\|_1 = \sum_{i=1}^{d}|a_i|$$

- Here $\lambda \ge 0$ is a tuning parameter, which controls the strength of the penalty term. Note that:
  - When $\lambda = 0$ $(\tau = +\infty)$, we get the linear regression estimate
  - When $\lambda = +\infty$ $(\tau = 0)$, we get $W_{\text{Lasso}} = 0$
  - For λ in between, we are balancing two ideas: fitting a linear model of y on X, and shrinking the coefficients

62

Regularization: Lasso Regression

- The lasso regression performs a **feature selection**
- No analytic formula: Gradient descent

  Sklearn.linear_model.Lasso

63

Conclusions:

- Linear Regression is simple and useful method
- Two training algorithms:
  - Analytic solution
  - Numeric solution: Gradient descent
- Question: Relationships are not always linear, so how do we model these cases?

Réda DEHAK 64

64