Machine Learning

Linear Regression and its variants. ML and MAP principles. Regression Quality Metrics.

Aleksandr Petiushko

ML Research

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SOFIA UNIVERSITY

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1. Linear Regression formulation
2. ML and MAP principles
3. Least Squares method

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1. Linear Regression formulation
2. ML and MAP principles
3. Least Squares method
4. Polynomial Regression
5. Ridge Regression, LASSO and Elastic Net
6. Quality metrics for Regression

Main math concepts: a reminder

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- L_1-norm of a vector $w = (w_1, \ldots, w_n)$: $|w| = \sum_{i=1}^{n} |w_i|$

Problem Statement: Linear Regression

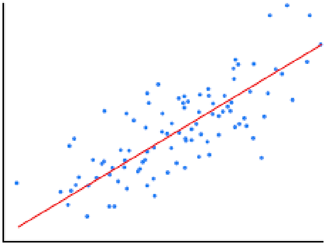
Given

$$y_i = w^T x_i + \varepsilon_i \Rightarrow y_i \sim N(w^T x_i, \sigma^2),$$

for $i = 1, \ldots, m$, where $w \in \mathbf{R}^{n+1}$, $\varepsilon_i \sim N(0, \sigma^2)$, $X^m = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ — the training dataset.

Task

Find w



Two kinds of parameter estimation

Maximum Likelihood (**ML**) Principle

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Principle of Maximum A Posterior (**MAP**) Probability

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Problem statement and assumptions

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Analytical solution

Theorem

The solution to the problem $\arg\min_w (\sum_{i=1}^{m} (w^T \cdot x_i - y_i)^2)$ is $\hat{w} = (X^T X)^{-1} \cdot X^T \cdot y$, where $X_{i,j} = x_i^j$, $y = (y_1, \ldots, y_m)^T$.

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Proof idea

Let's write the problem in vector form $||Xw - y||^2 \to \min_w$. The necessary condition for a minimum in matrix form is:

$$\frac{\partial}{\partial w}||Xw - y||^2 = 0$$

Polynomial Regression

Idea

It is possible to generate new features based on existing ones by applying non-linear functions

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Transformation examples

- Exponentiation
- Pairwise products
- Square root

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- Simple algorithm, not computationally complex
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- Despite its simplicity, it can describe quite complex dependencies (for example, polynomials)

Disadvantages

- The algorithm assumes that all features are numeric
- The algorithm assumes that the data is normally distributed, which is not always the case
- The algorithm is highly sensitive to outliers

Maximum A Posterior Probability Method

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An additional term appeared in the minimization problem, which depends only on the prior distribution on the weights w

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Ridge Regression

L_2 regularization

- $L(w, X_{train}) = MSE(w, X_{train}) + \frac{\alpha}{2}\sum_{i=0}^{n} w_i^2 = \frac{1}{m}\sum_i (w^T \cdot x_i - y_i)^2 + \frac{\alpha}{2}\sum_{i=0}^{n} w_i^2$ — loss function

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Note: L_2 regularization and MAP with the normally distributed weights are the same!

Ridge regression: solution

Theorem

The solution of the problem $\arg\min_w (\sum_{i=1}^{m} (w^T \cdot x^{(i)} - y_i)^2 + \alpha \sum_{i=0}^{n} w_i^2)$ is $\hat{w} = (X^T X + \alpha I_{n+1})^{-1} \cdot X^T \cdot y$, where $X_{i,j} = x_i^j$, $y = (y_1, \ldots, y_m)^T$, I_{n+1} is the identity matrix.

Proof idea

Let's write the problem in vector form $||Xw - y||^2 + \alpha ||w||^2 \to \min_w$. The necessary condition for a minimum in matrix form is:

$$\frac{\partial}{\partial w} \left((Xw - y)^T \cdot (Xw - y) + \alpha w^T w \right) = 0$$

Ridge Regression: Properties

- Regularization prevents model parameters from being too large
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- More resistant to outliers
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The probabilistic meaning of the α parameter

$\alpha = \frac{1}{\tau^2}$, where τ is the standard deviation of the prior distribution on w

LASSO

L_1-regularization

- $L(w, X_{train}) = MSE(w, X_{train}) + \alpha \sum_{i=0}^{n} |w_i| = \sum_i (w^T \cdot x_i - y_i)^2 + \alpha \sum_{i=0}^{n} |w_i|$ — loss function

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Properties

- This regularization provides feature selection
- No analytical solution

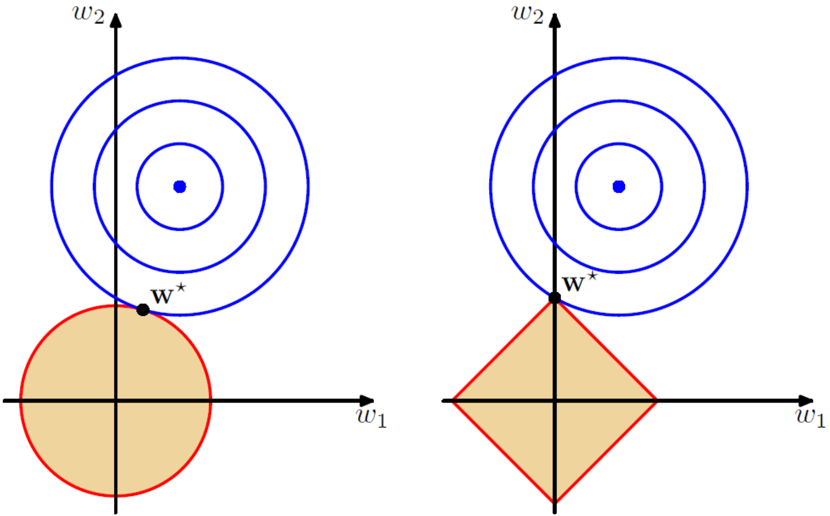
Probabilistic interpretation of LASSO

The probabilistic meaning of the α parameter

The parameter α — is inversely proportional to the standard deviation of the prior distribution by w. In this case, this is the *Laplace* distribution

$$p(w) = \frac{1}{\tau} exp\left(-\frac{||w||}{2\tau}\right)$$

Intuition of feature selection under L_1-regularization



Elastic Net

L_1-regularization and L_2-regularization

- $L(w, X_{train}) = MSE(w, X_{train}) + r\alpha \sum_{i=0}^{n} |w_i| + (1-r)\frac{\alpha}{2} \sum_{i=0}^{n} w_i^2 = \sum_i (w^T \cdot x_i - y_i)^2 + r\alpha \sum_{i=0}^{n} |w_i| + (1-r)\frac{\alpha}{2} \sum_{i=0}^{n} w_i^2$ — loss function

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Properties

- No analytical solution
- Combines the positive properties of Ridge regression and LASSO.

Quality Metrics for the Regression Problem

Motivation

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- As a rule, the customer does not think in terms of metrics and can only explain the problem he wants to solve in business language
- Understanding the impact of the choice of a particular metric on the customer's business is the key to successful problem setting

Quality Metrics for the Regression Problem[1]

Mean Square Error

$$MSE = \frac{1}{m}\sum_{i}(y_i - a(x_i))^2$$

[1]**Note**: unless otherwise specified, metrics are applied on top of the test dataset.

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Mean Absolute Error

$$MAE = \frac{1}{m}\sum_i |y_i - a(x_i)|$$

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Mean Squared Logarithmic Error

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Mean Squared Logarithmic Error

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R^2 score (also known as Coefficient of Determination)

$$R^2 = 1 - \frac{\sum_i (y_i - a(x_i))^2}{\sum_i (y_i - \bar{y})^2},$$

where $\bar{y} = \frac{1}{m}\sum_i y_i$.

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- Regularization is a great way to deal with the overfitting and data noise
- Ridge Regression == L_2-regularization == adding weighted square (L_2) norm of w to MSE of linear regression
- LASSO == L_1-regularization == adding weighted L_1 norm of w to MSE of linear regression
- Elastic Net == $L_1 + L_2$-regularization == adding weighted L_1 and squared L_2 norm of w to MSE of linear regression

Thank you!