Machine Learning

Regression

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Regression – Forecasting continuous values

- Supervised task
- The target variable is numeric
- Minimize the error of the prediction with respect to the target

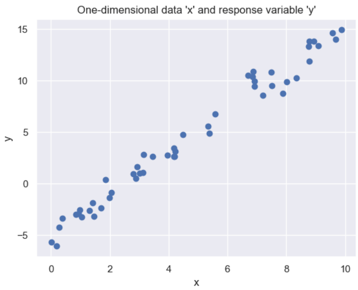
Linear Regression

- data set $\mathcal{X}$ with N rows and D columns
  - x_i is a D dimensional data element
- response vector $\bar{y}$ with N values y_i
- w is a D-dimensional vector of coefficients that needs to be learned
- we model the dependence of each response value y_i from the corresponding independent variables x_i as

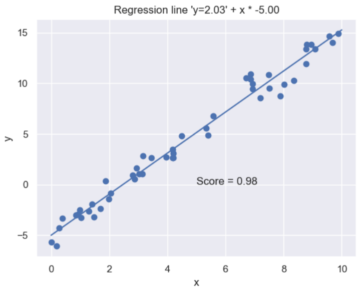
$$y_i \approx w^T \cdot x_i \quad \forall i \in [1 \dots N]$$

- such that the error of modelling is minimised
- Classical statistic method (1805)

Data and regression line



One–dimensional data and response variable



Regression and score - Score range $(-\inf : 1)$

Objective function and minimisation I

OPTIONAL

$$
\begin{aligned}
\mathcal{O} &= \sum_{i=1}^{N} (w^T \cdot x_i - y_i)^2 = ||Xw^T - y||^2 \\
&= (Xw^T - y)^T . (Xw^T - y)
\end{aligned}
$$

Gradient of $\mathcal{O}$ with respect to w

$$2X^T(Xw^T - y)$$

Constraining the gradient to 0 we obtain the optimisation condition

$$X^T X w^T = X^T y$$

Objective function and minimisation II

Optional

If the symmetric matrix $X^T X$ is invertible the solution can be derived as

$$w = (X^T X)^{-1} X^T y$$

and the forecast is given by

$$y^f = X \cdot w^T$$

Matrix calculus

Optional

- Issues related to matrix calculus if $\overline{x}^T\overline{x}$ is not invertible
- Moore–Penrose pseudoinverse
- Tikonov regularisation (also known as ridge regression)
- Lasso regularisation

Quality of the fitting - R^2

Mean of the observed data	$y^{avg} = \frac{1}{N} \sum_i y_i$
Sum of squared residuals	$SS_{res} = \sum_i (y_i - y_i^f)^2$
Total sum of squares	$SS_{tot} = \sum_i (y_i - y^{avg})^2$
Coefficient of determination	$\mathbf{R^2 = 1 - \frac{SS_{res}}{SS_{tot}}}$

Intuition about R^2

- It compares the fit of the chosen model with that of a horizontal straight line
- With perfect fitting the numerator of the second term is zero and $R^2 = 1$
- If the model does not follow the trend of the data the numerator of the second term can reach or exceed the denominator, and R^2 can also be negative
- Despite the name, R^2 isn't the square of anything

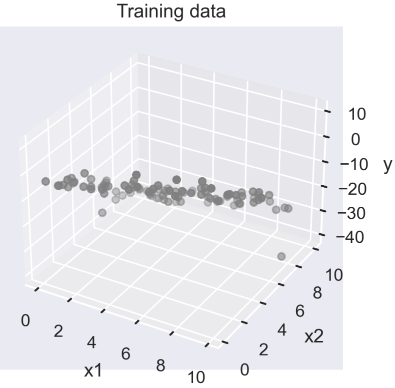
R^2 and Mean Squared Error

Optional

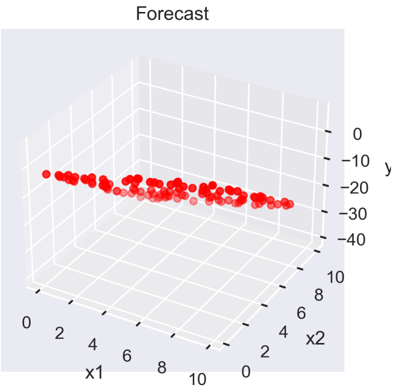
- Both refer to the error of the predictions
- R^2 is a standardised index,
- *RMSE* measures the mean error, this it is influenced by the order of magnitude of the data,
- Both *RMSE* and R^2 quantifies how well a linear regression model fits a dataset
- The RMSE tells how well a regression model can predict the value of a response variable in absolute terms
- R^2 tells how well the predictor variables can explain the variation in the response variable
- For comparing the accuracy among different linear regression models, RMSE is a better choice than R Squared
- R^2 is not meaningful for non–linear or non–algebraic regression models

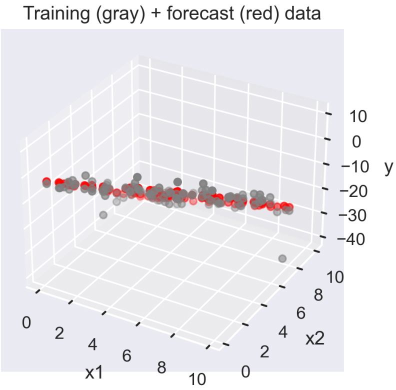
Multiple regression

- The response variable depends by two or more features
- The regression technique is quite similar to that of simple regression
- In `scikit-learn` the estimator is the same



Multiple regression - forecast



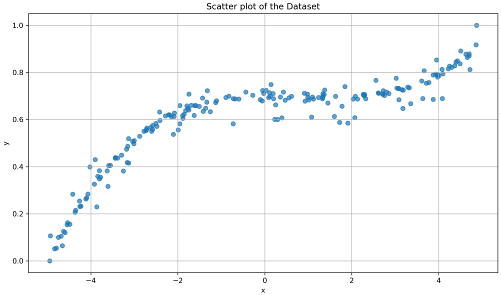


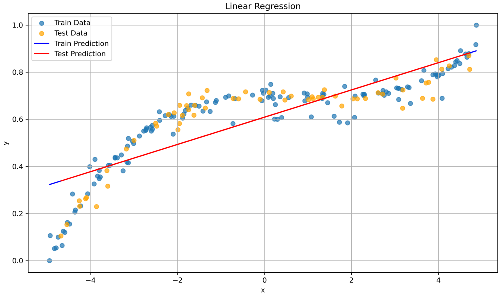
Overfitting and Regularisation

- In presence of high number of features overfitting is possible
  - performance on test data becomes much worse
- Regularisation reduces the influence of less interesting attributes and therefore reduces overfitting
  - see section 3

Polynomial regression (univariate)

What if the relationship between the independent variable and the target is not linear at all?





Univariate Polynomial Regression

- It is an extension of linear regression that models the relationship between the independent variable x and the dependent variable $y(x)$ as an n-degree polynomial.
- It fits nonlinear relationships between the input and output variables with a polynomial.
- The general equation for polynomial regression is:

$$y(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_n x^n + \epsilon$$

- Here, $\beta_0, \beta_1, \ldots, \beta_n$ are the model parameters, and ϵ represents the error term.

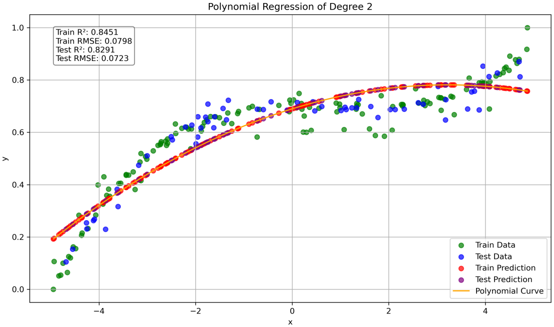
Steps in Polynomial Regression

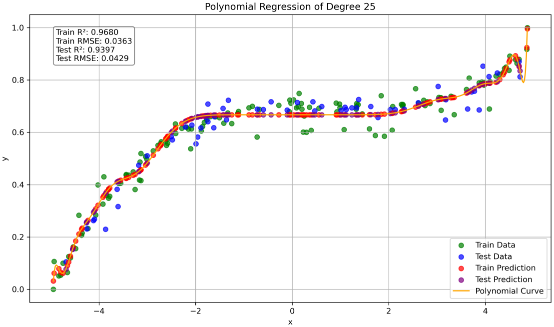
- Step 1: Generate the Polynomial Features
  - Transform the original input variable x into higher-order polynomial terms.
  - For example, if the degree $n = 2$, the polynomial features would be:

$$\mathbf{X} = [1, x, x^2]$$

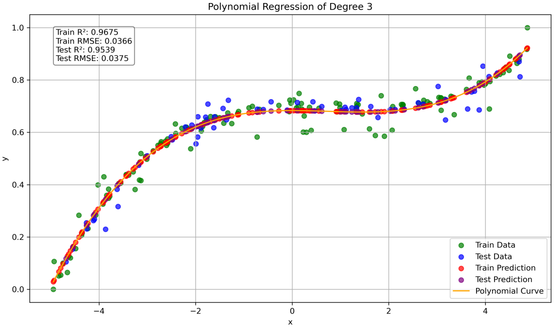
  - The transformation can be extended for higher degrees, $n = 3$, $n = 4$, etc.
- Step 2: Fit a Linear Regression Model
  - Despite being polynomial, the problem is treated as a linear regression problem in terms of the parameters $\beta_0, \beta_1, \ldots, \beta_n$.
  - The model is fit using least squares estimation to minimize the sum of squared residuals.
- Step 3: Evaluate the Model
  - Use standard regression metrics such as Root Mean Squared Error (RMSE).
  - Overfitting must be controlled using cross-validation to assess the optimal degree.

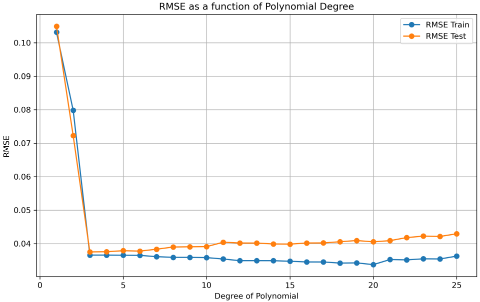
Underfitting and Overfitting





Good fitting and RMSE versus degree





Regularised regression

- The standard multivariate linear regression does not have hyperparameters for controlling the fitting quality, in particular to guarantee good performance on the test set
- A general way for controlling overfitting is to simplify the model
- How can we simplify a linear multivariate polynomial?

Regularised regression

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- A general way for controlling overfitting is to simplify the model
- How can we simplify a linear multivariate polynomial?

Adapting the loss function

Loss in Regression

- The loss function quantifies the error between the model's prediction and the actual value
- In regression, the most common loss is the Root Mean Squared Error (RMSE)

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Other loss functions:
  - Mean Absolute Error (MAE)
  - Log-loss (for probabilistic classifiers)

OLS - Ordinary Least Squares

- Cost function:

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

- OLS regression simply determines the coefficient vector **w** that minimizes the loss of predictions with respect to the ground truth

Regularisation

- Ordinary Least Squares (OLS) regression minimizes the prediction error on the training set
- Risk: overfitting, especially with many variables or noisy data
- Regularization: technique to penalize model complexity
  - a way to reduce the complexity is to reduce, in several ways, the values of the coefficients
- Goal: find a good trade-off between accuracy and model simplicity

Lasso Regression

Least Absolute Shrinkage and Selection Operator [Tibshirani(1996)]

- A linear regression method that adds $L1$-regularization to the cost function
- Encourages sparse models by shrinking some coefficients to exactly zero
- Useful for feature selection and regularization in high-dimensional data

Cost Function [1]

$$L(\mathbf{w}) = \frac{1}{2N}\sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{D} x_{ij} w_j\right)^2 + \alpha \sum_{j=1}^{D} |w_j|$$

- Components
  - Residual sum of squares: Measures prediction error
  - $L1$-norm penalization $= \sum_{j=1}^{D} |w_j| = ||\mathbf{w}||_1$
    - penalizes the sum of absolute values of coefficients

1 For simplicity, here we do not consider the intercept

L1 Regularization: Penalizes Coefficients with an Absolute Value Constraint

- The Lasso penalty, $\alpha \sum_{j=1}^{D} |w_j|$, grows linearly with the magnitude of the coefficients
- This penalty creates a strong incentive to make some coefficients exactly zero due to:
  - Equal contribution to the penalty:
    - Small changes in the magnitude of a coefficient contribute equally to the penalty, whether the coefficient is large or small
  - Efficient penalty reduction:
    - When coefficients are near zero, shrinking them to zero entirely results in a significant penalty reduction with minimal cost to the residual sum of squares (RSS)

Lasso Regression: Compact Coordinate Descent

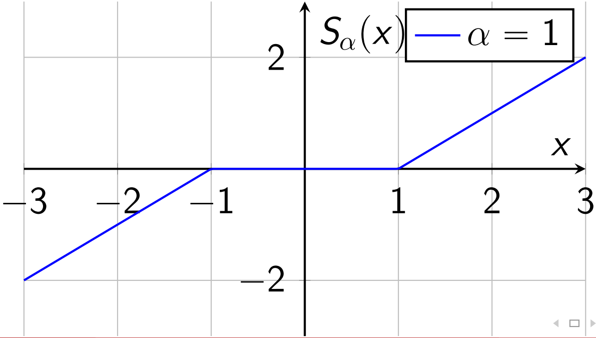
Input : $\mathbf{X} \in \mathbb{R}^{N \times D}$, $\mathbf{y} \in \mathbb{R}^{N}$, α, ϵ
Output: $\mathbf{w} \in \mathbb{R}^{D}$
Initialize $w \leftarrow \mathbf{0}$;
repeat
  for $j = 1$ **to** D **do**
    $r \leftarrow \mathbf{y} - \mathbf{X}\mathbf{w} + X_j w_j$;
    $\rho \leftarrow \frac{1}{N} \sum_i X_{ij} r_i$;
    $z \leftarrow \frac{1}{N} \sum_i X_{ij}^2$;
    $w_j \leftarrow \mathrm{sign}(\rho) \cdot \max(|\rho| - \alpha, 0)/z$;
until $\|\Delta\mathbf{w}\|_\infty < \epsilon$;

Soft-Thresholding Function in Lasso

- Lasso updates coefficients using the **soft-thresholding function**:

$$S_\alpha(x) = \mathrm{sign}(x) \cdot \max(|x| - \alpha, 0)$$

- Promotes sparsity by shrinking small values to zero.



Computational Complexity

- Training Complexity
  - Depends on the number of features D, samples N, and iterations T
  - for coordinate descent:
$$\mathcal{O}(TND)$$
  - for large datasets, this is linear in N and D
- Convergence
  - Faster convergence if many coefficients are sparse
  - Slower for high-dimensional dense datasets
- Prediction Complexity
  - Linear in $\bar{D}$ (number of nonzero coefficients):

Understanding **w** in Lasso Regression

- w represents the coefficients (or weights) of the linear regression model
- Structure of **w**:
  - $\mathbf{w} = [w_0, w_1, \ldots, w_p]$
    - w_0: The intercept term of the model
    - w_j: The weight for the j-th feature, where $j = 1, \ldots, D$
- Predicted value $\hat{y}_i$ for a sample x_i:

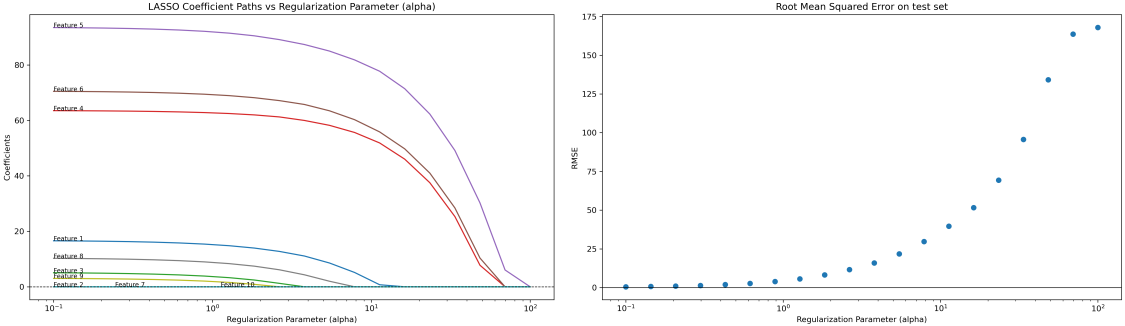
$$\hat{y}_i = w_0 + \sum_{j=1}^{D} w_j x_{ij}$$

  - $\hat{y}_i$: Predicted output for the i-th sample
  - x_{ij}: Value of the j-th feature for the i-th sample

Role of $\mathbf{w}$ in Lasso Regression

- The optimization process adjusts $\mathbf{w}$ to:
  - Minimize residual error: $\frac{1}{2N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$
  - Penalize large values of w_j using $L1$-norm regularization: $\alpha \sum_{j=1}^{D} |w_j|$
    - α is a multiplying factor: a hyper parameter allowing to calibrate the penalty
    - try several values for α together with cross–validation
- Effect of $L1$-regularization:
  - Encourages sparsity in $\mathbf{w}$
    - Many coefficients w_j are set to exactly zero
- $\mathbf{w}$ embodies the importance of each feature in the regression model, while ensuring simplicity and robustness

LASSO effect and RMSE



Lasso: Summary

- Advantages
  - Produces sparse models for feature selection
  - Scales linearly with the size of the dataset
- Limitations
  - Struggles with collinearity among features
  - Computationally expensive for very large Ddue to iterative updates
- Applications
  - High-dimensional datasets where feature selection is essential

Ridge Regression[2]

- Ridge Regression is a type of linear regression
  - It adds a penalty term to the cost function to prevent overfitting
- Key Features:
  - Reduces model complexity
  - Improves generalization performance

2 The name derives from the matrix representation of the solution, where the α value adds a ridge to the main diagonal

The Ridge Regression Cost Function

- Ridge Regression modifies OLS by adding a penalty:

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \alpha \|\mathbf{w}\|$$

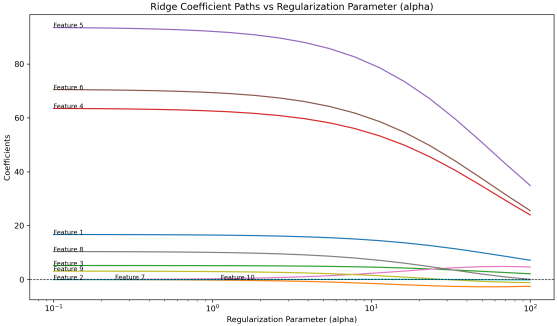
  - α: Regularization parameter controlling penalty strength
  - $\|\mathbf{w}\|$: $L2$ norm of the weight vector

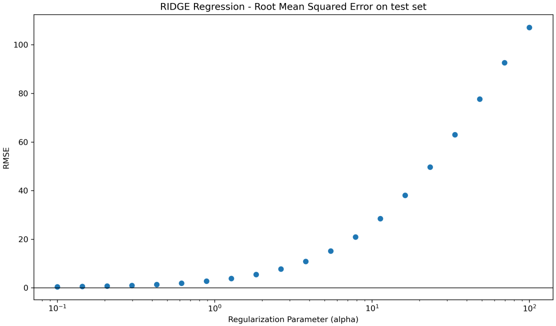
$$\beta_j \leftarrow \frac{1}{1+\alpha} \cdot \left(\frac{1}{N} \sum_{i=1}^{N} X_{ij} \left(y_i - \sum_{k \neq j} X_{ik} \beta_k \right) \right)$$

Effects of Regularization

- High α:
  - More penalty, leading to smaller weights
  - Reduces variance but increases bias
- Low α:
  - Less penalty, resembling OLS regression
  - Retains variance but may overfit the data
- Choosing α:
  - Cross-validation is commonly used to find the optimal α

RIDGE effect and RMSE





Ridge Regression: Coordinate Descent[3]

Input : $\mathbf{X} \in \mathbb{R}^{N \times D}$, $\mathbf{y} \in \mathbb{R}^{N}$, α, ϵ
Output: $\mathbf{w} \in \mathbb{R}^{D}$
Initialize $\mathbf{w} \leftarrow \mathbf{0}$;
$z \leftarrow 1 + \alpha$;
repeat
  for $j = 1$ **to** D **do**
    $r \leftarrow \mathbf{y} - \mathbf{X}\mathbf{w} + X_j w_j$;
    $\rho \leftarrow \frac{1}{N} \sum_i X_{ij} r_i$;
    $w_j \leftarrow \rho / z$;
until $\|\Delta\mathbf{w}\|_\infty < \epsilon$;

Coefficient update

$$w_j \leftarrow \frac{1}{1+\alpha} \cdot \left(\frac{1}{N} \sum_{i=1}^{N} X_{ij} \left(y_i - \sum_{k \neq j} X_{ik} w_k \right) \right)$$

3 Assumes that $\mathbf{X}$ is normalised and $\mathbf{y}$ is centered

Ridge - Applications and Summary

- Applications:
  - Multicollinear data where features are highly correlated
  - Scenarios requiring reduced overfitting
- Summary:
  - Ridge Regression introduces a regularization term
  - Balances bias and variance for better generalization
  - Cross-validation helps in optimal parameter selection

Elastic Net Regression

- Elastic Net Regression is a linear regression method
  - Combines penalties from Ridge Regression and Lasso Regression
- Why Elastic Net?
  - Addresses limitations of Ridge and Lasso:
    - Ridge cannot perform feature selection
    - Lasso struggles when features are highly correlated
  - Offers a balance between these methods

The Elastic Net Cost Function

- Ordinary Least Squares (OLS) cost function:

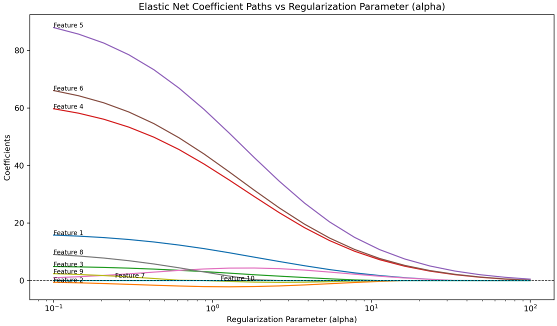
$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

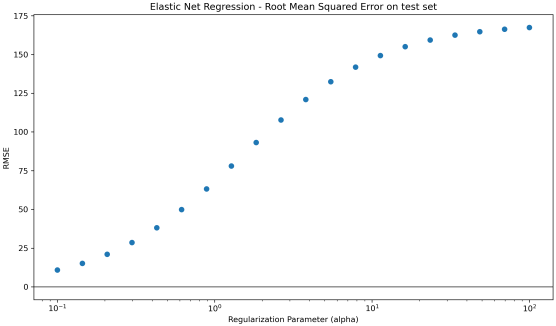
- Elastic Net modifies OLS with two penalties:

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \alpha_1 \|\mathbf{w}\|_1 + \alpha_2 \|\mathbf{w}\|^2$$

  - α_1: Controls the Lasso penalty (L1 norm)
  - α_2: Controls the Ridge penalty (L2 norm)

Elastic Net effect and RMSE





Elastic Net: Coordinate Descent

Input : $\mathbf{X} \in \mathbb{R}^{N \times D}$, $\mathbf{y} \in \mathbb{R}^{N}$, α, η, ϵ
Output: $w \in \mathbb{R}^{D}$
Initialize $w \leftarrow \mathbf{0}$;
repeat
  for $j = 1$ **to** D **do**
    $r \leftarrow \mathbf{y} - \mathbf{X}w + X_j w_j$;
    $\rho \leftarrow \frac{1}{N} \sum_i X_{ij} r_i$;
    $z \leftarrow \frac{1}{N} \sum_i X_{ij}^2 + \alpha(1 - \eta)$;
    $w_j \leftarrow \mathrm{sign}(\rho) \cdot \max(|\rho| - \alpha\eta, 0)/z$;
until $\|\Delta w\|_\infty < \epsilon$;

Properties and Advantages

- Properties:
  - Encourages sparsity in coefficients (like Lasso)
  - Groups correlated features (like Ridge)
- Advantages:
  - Handles multicollinear data effectively
  - Can select relevant features while maintaining stability
  - Useful in high-dimensional data scenarios

Applications and Summary

- Applications:
  - Genomics (e.g., selecting gene expressions)
  - Financial modeling with highly correlated features
  - High-dimensional datasets with potential multicollinearity
- Summary:
  - Elastic Net combines Lasso and Ridge penalties
  - Effective in handling multicollinear data and sparse solutions
  - Requires hyperparameter tuning (α_1, α_2)

Comparison of regularized regression techniques

- Lasso, Ridge, and Elastic Net are regularization techniques used in regression
- They address overfitting and multicollinearity by introducing penalties in the cost function
- This presentation compares their real-world use cases, strengths, and limitations

Lasso Regression

- Strengths:
  - Performs feature selection, producing sparse models by setting some coefficients to zero
  - Useful for high-dimensional datasets with many irrelevant features
- Limitations:
  - Struggles with datasets where predictors are highly correlated
- Use Cases:
  - Genomics: Identifying relevant genes influencing a disease
  - Text Processing: Selecting keywords or n-grams in sentiment analysis
  - Sparse Sensor Networks: Identifying critical sensors in IoT or environmental monitoring

Ridge Regression

- Strengths:
  - Handles multicollinearity by shrinking coefficients
  - Retains all predictors, avoiding the elimination of variables
- Limitations:
  - Does not perform feature selection
- Use Cases:
  - Finance: Predicting stock prices using correlated economic indicators
  - Marketing: Modeling customer demand influenced by correlated factors
  - Engineering: Calibration of multivariate systems like chemical processes
  - Medical Imaging: Predicting outcomes from high-dimensional MRI or CT data

Elastic Net Regression

- Strengths:
  - Combines Lasso and Ridge penalties, balancing sparsity and multicollinearity handling
  - Selects groups of correlated features, unlike Lasso alone
- Limitations:
  - Requires careful tuning of two parameters (α_1 and α_2)
- Use Cases:
  - Genomics: Selecting groups of genes associated with traits
  - Healthcare Analytics: Modeling patient outcomes from clinical predictors
  - Customer Segmentation: Identifying clusters of customer behaviors in retail
  - Climate Science: Modeling climate variables with correlated predictors
  - Social Media Analysis: Predicting trends from sparse and correlated features

Comments

- Lasso, Ridge, and Elastic Net offer distinct strengths tailored to different data characteristics
- Choosing the right method depends on:
  - Presence of multicollinearity
  - Sparsity of the solution required
  - Dimensionality of the dataset
- Elastic Net is often a robust choice when both sparsity and correlation must be addressed

Comparison of Lasso, Ridge, and Elastic Net Regression

Feature	**Lasso**	**Ridge**	**Elastic Net**
Feature Selection	Yes	No	Yes groups correlated features
Handles Multicollinearity	Weak	Strong	Strong
Model Interpretability	High (sparse coefficients)	Moderate	Moderate (sparse, but groups features)
Dataset Characteristics	High-dimensional, sparse predictors	Correlated predictors	Sparse and correlated predictors

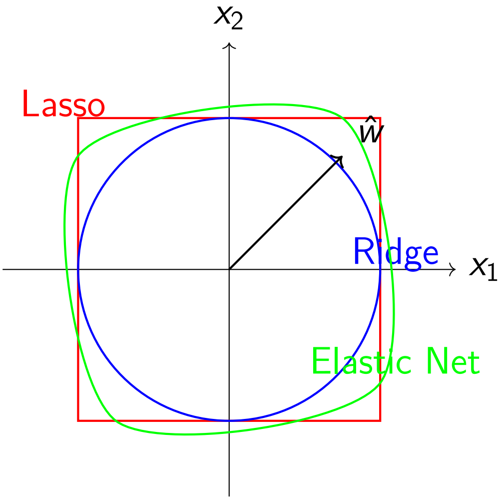
Explanation

- Sparsity:
    - Elastic Net can set some coefficients to zero, removing irrelevant predictors
    - This results in a simpler and more interpretable model, similar to Lasso
- Groups Features:
    - When predictors are highly correlated, Elastic Net:
        - Tends to select them together rather than choosing one arbitrarily
        - Shrinks their coefficients toward each other using the Ridge-like penalty
    - This behavior arises because Elastic Net combines:
        - L1 penalty (Lasso) for sparsity
        - L2 penalty (Ridge) for handling multicollinearity

Practical Example: Correlated Predictors

- Suppose two predictors, x_1 and x_2, are highly correlated:
  - Lasso:
    - May select only x_1 or x_2, ignoring the other entirely
  - Ridge:
    - Keeps both x_1 and x_2, but shrinks their coefficients
  - Elastic Net:
    - Selects both x_1 and x_2, but their coefficients may be reduced (shrunk) in different proportions
    - Balances between sparsity and correlation handling

Visualization of Sparse and Grouping Behavior



Description of the figure I

- Visual representation of the constraints applied by Lasso, Ridge, and Elastic Net regression
- The axes represent the coefficient of two predictors
- Shapes of Constraints
    - Lasso: A diamond-shaped constraint indicating L1 penalty, which promotes sparsity (coefficients set to zero)
    - Ridge: A circular constraint indicating L2 penalty, which shrinks coefficients uniformly but does not set them to zero
    - Elastic Net: A combination of Lasso and Ridge constraints, allowing both sparsity and handling of correlated groups

Description of the figure II

- Interpretation of Coefficient Paths
  - In Lasso, coefficients are pushed to the edges, setting some to zero
  - In Ridge, coefficients shrink but remain non-zero, resulting in a smoother path
  - Elastic Net provides a balance, with paths that follow the L1 and L2 constraints, enabling feature selection and correlation handling

Key Takeaways

- Elastic Net combines the best of Lasso and Ridge:
  - Sparsity: Sets some coefficients to zero for simpler models
  - Handles Correlated Predictors: Selects groups of features rather than one arbitrarily
- Ideal for:
  - High-dimensional datasets with multicollinearity
  - Applications requiring both feature selection and robust performance

Selection of Regression Models

Method	Library	Model Name
Linear Regression	sklearn.linear_model	LinearRegression
Elastic Net Regression	sklearn.linear_model	ElasticNet
Stochastic Gradient Descent Regression	sklearn.linear_model	SGDRegressor
Bayesian Ridge Regression	sklearn.linear_model	BayesianRidge
Lasso Regression	sklearn.linear_model	Lasso
Support Vector Machine	sklearn.svm	SVR
Kernel Ridge Regression	sklearn.kernel_ridge	KernelRidge
Gradient Boosting Regression	sklearn.ensemble	GradientBoostingRegressor
XGBoost Regressor	xgboost	XGBRegressor
CatBoost Regressor	catboost	CatBoostRegressor
LGBM Regressor	lightgbm	LGBMRegressor

Bibliography I

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  Regression shrinkage and selection via the lasso.
  Journal of the Royal Statistical Society: Series B (Methodological), 58(1):267–288, 1996.