Machine Learning

Regularization - Lasso

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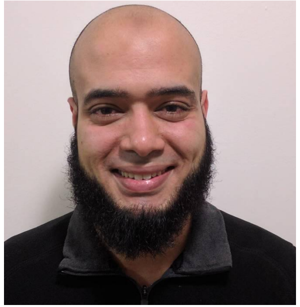


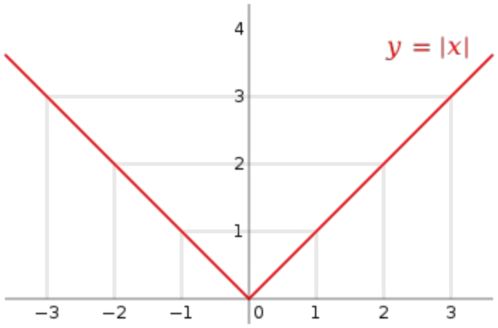
Question!

- Assume we have 1000 features for our N examples
- We trained a **regularized** linear regression and it works great on train/val/test
- However, on investigation, we found that 950 of the weights were all zeros
- What does this imply? What kind of actions we can take?

- The model doesn't depend on these features for its computations
- So we can consider **removing** them and trained with less features
- This is an example of how regularization can help with feature selection
- **Feature selection** is the process of reducing the number of input variables
- While Ridge regularization doesn't typically have this property, Lasso regularization is known for its ability to perform feature selection

Lasso Regression (L1 Regularization)

$$\underset{W}{\text{minimize}} \frac{1}{2N} \sum_{n=1}^{N} (y(X^n, W) - t^n)^2 + \frac{\lambda}{2} \sum_{i=1}^{M} |W_i|$$



- Another popular choice is L1 regularization
  - Instead of squaring each weight value, the absolute value is taken
  - This may seem similar to Ridge, but there are important implications to consider
- Is the absolute function a differentiable function?
- It is differentiable **everywhere** except for x = 0.

Lasso Regression vs Ridge

- Assume we have 2 weights w1 = -0.1 and w2 = 4
- Which one assigns a higher penalty: Lasso or Ridge?

- For w1: $(-0.1)^2 = 0.01$ while $|-0.1| = 0.1$ ⇒ Lasso assigns a higher penalty
  - For |weights| < 1, Lasso pushes them toward zero more strongly than Ridge
- For w2: $(4)^2 = 16$ while $|4| = 4$ ⇒ Ridge assigns a higher penalty
  - Side note: the squared L2 norm is sensitive to outliers in the error computation of the data (y-t)
    - If predict_price(home) is 1000 and the ground_truth(home) is 1001000, this would be considered an outlier

Lasso Regression vs Ridge

- Assume we have w1 = 10 and w2 = 20
- Does ridge **prioritize** the parameter equally? What about lasso?

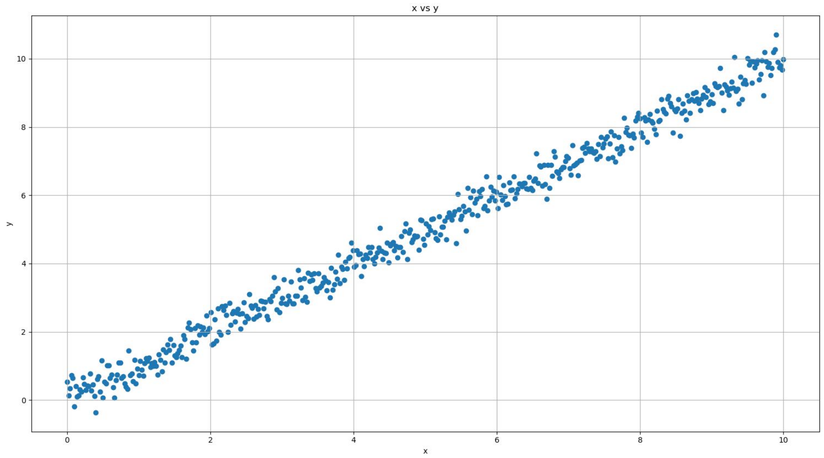
- For Ridge, the current cost is: $10^2 + 20^2 = 500$
  - If we reduce w1 by 1 the cost is: $9^2 + 20^2 = 481$ ⇒ a drop of 19
  - If we reduce w2 by 1 the cost is: $10^2 + 19^2 = 461$ ⇒ a drop of 39: a bigger effect
  - Ridge minimizes the weights **proportionally relative** to their **magnitude**
    - Larger weights lose **more**, smaller ones lose **less** ($dw^2 = w$)
    - For more mathematical treatment: *See Introduction to Statistical Learning: ch6*
- For Lasso, the current cost is: 10 + 20 = 30
  - If we reduce w1 by 1 the cost is: 9 + 20 = 29 ⇒ a drop of 1 ($dw = 1$)
  - If we reduce w2 by 1 the cost is: 10 + 19 = 29 ⇒ a drop of 1 also
  - Lasso does not favor a specific weight to reduce (treating 5 is the same as 500)

Lasso Regression: Sparsity

- With a higher λ, Lasso may push several weights toward being exactly zero
  - Why zero? Why with a higher λ? Later
- This implies the following:
- Lasso can help us do feature selection (cancel features of **zero weights**)
  - Why matter?
- Lasso is performing 2 things simultaneously: regularization and selection
  - The acronym Lasso stands for Least Absolute **Shrinkage and Selection** Operator

Lasso Regression vs Ridge Regression

- Let's generate simple simple data with 500 values for y = x + noise
  - Optimal values: c = 0 and m = 1
- Clearly we can fit the data with a single feature
- However, we will add 3 random (entirely useless) features for each value
  - Input data: [500 x 4] and output is 1 feature
- Let's explore Ridge vs Lasso
  - We can see if Lasso recognizes the useless features



Lasso Regression vs Ridge Regression

```
    lasso 7    : MSE 5.896 - intercept 4.20- Weights 0.159 0.000 0.000 0.000
    lasso 5    : MSE 3.028 - intercept 3.00- Weights 0.398 0.000 0.000 0.000
    lasso 3    : MSE 1.115 - intercept 1.81- Weights 0.637 0.000 0.000 0.000
    lasso 1    : MSE 0.159 - intercept 0.61- Weights 0.876 0.000 0.000 0.000
    lasso 0.1  : MSE 0.041 - intercept 0.08- Weights 0.984 0.000 0.000 0.000
Q2  lasso 0.01 : MSE 0.040 - intercept 0.02- Weights 0.994 0.000 0.001 0.000
Q1  lasso 0.001: MSE 0.039 - intercept 0.02- Weights 0.995 0.001 0.011 0.007

    Ridge 7    : MSE 0.040 - intercept 0.03- Weights 0.994 0.002 0.013 0.008
    Ridge 1    : MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008
    Ridge 0.1  : MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008
    Ridge 0.01 : MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008
    Ridge 0.001: MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008
```

- Q1) Which λ will cross validation choose for the Lasso method?
- Q2) Which λ will inform you about the useless features while having fair error?

Lasso Regression: Careful with Cross-Validation

- There is a blocking problem when using cross-validation for lasso λ
- The last 2 questions reveal 2 different goals:
  - Minimum prediction error (max accuracy) vs most-removed features
- The goal of cross-validation is to find the minimum prediction error
- The goal of feature selection is to find the λ that eliminates the most unnecessary features
- No guarantee their lambda matches!
  - In practice, typically λ_cross_prediction < λ_most_useless_features
    - Recall, higher λ cancels more features
  - This inconsistency is mathematically [proven](#) in the paper:
    - High-dimensional graphs and variable selection with the Lasso By Nicolai Meinshausen and Peter Buhlmann, 2006
- So, overall we don't use cross validation to determine λ if we want to select important features

Lasso Regression: Improving the Performance

- Sometimes people try to improve their models further
- Here are 2 possible approaches:
- Two-stage procedure
  - 1) Using Lasso with several lambda values to perform feature selection (without cross validation)
  - 2) Applying another model (such as Lasso, Ridge, or Linear Regression)
- Use Elastic net regularization
  - It linearly combines the L1 and L2 penalties (with two hyperparameters)
    - Deep learning solutions typically have multiple linearly combined error functions

$$\underset{W}{\text{minimize}} \frac{1}{2N} \sum_{n=1}^{N} (y(X^n, W) - t^n)^2 + \frac{\lambda 1}{2} \sum_{i=1}^{M} |W_i| + \frac{\lambda 2}{2} \sum_{i=1}^{M} W_i^2$$

Lasso Regression: Why Sparsity

- For **mathematical** details:
  - ‘Machine Learning A Probabilistic Perspective’ book ch 13.3
  - ‘An Introduction to Statistical Learning’ book ch 6.2.2 (inventor of Lasso)
- First, we re-formulate the penalty as a constraint

$$\underset{W}{\text{minimize}} \frac{1}{2N} \sum_{n=1}^{N} (y(X^n, W) - t^n)^2 \quad \text{subject to} \quad \frac{\lambda}{2} \sum_{i=1}^{M} |W_i| \leq s$$

- Now we have 2 separate contours: cost function and constraint
- **Theory of constrained optimization**: solution to the constrained optimization lies at the **intersection** between the contours of the two functions

Lasso Regression: Why Sparsity

- The cost function is represented by the red ellipses in the illustration
- The shadowed region represents the contours of the penalty constraint
- Lasso constraint has **corners** at each of the **axes**, and so the ellipse often intersects the constraint region at an axis
- Ridge regression has a circular constraint without any sharp points

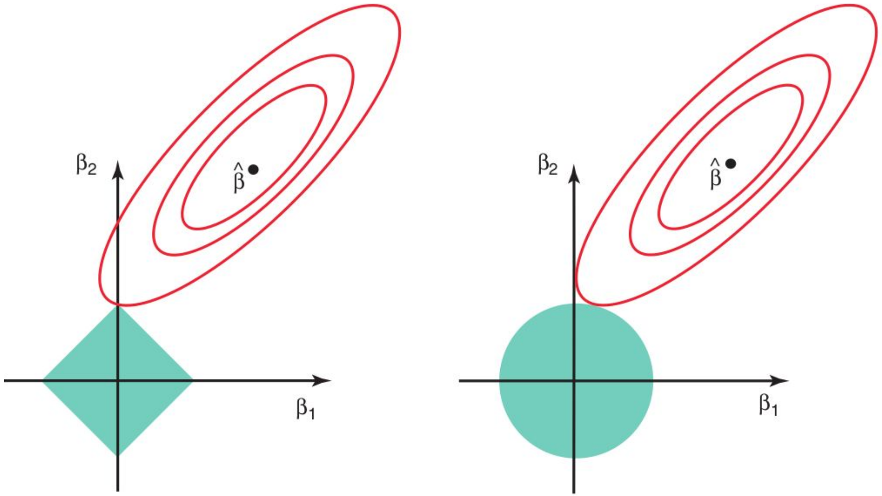
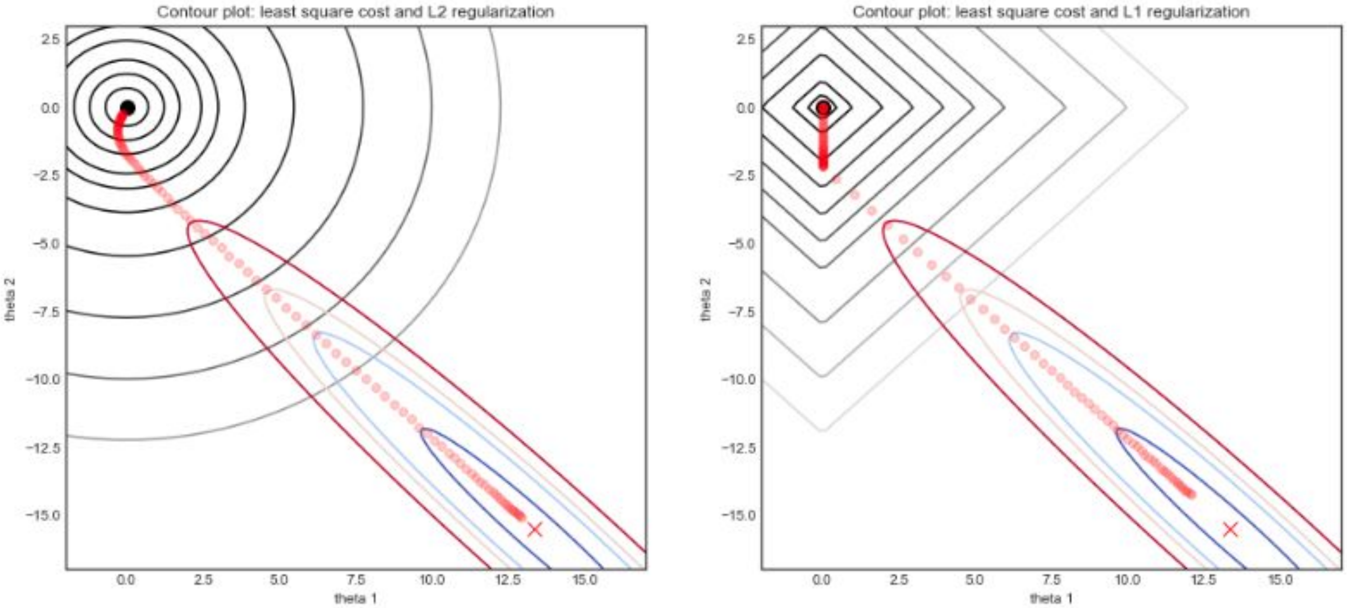


FIGURE 6.7. *Contours of the error and constraint functions for the lasso (left) and ridge regression (right). The solid blue areas are the constraint regions, $|\beta_1| + |\beta_2| \leq s$ and $\beta_1^2 + \beta_2^2 \leq s$, while the red ellipses are the contours of the RSS.*

Lasso Regression: Why Sparsity

- Why does a large λ likely result in more sparsity than a small λ?
    - With large λ, the weights shrink which makes use closer to the narrower contours and this increase the chances of solutions at the corners of the diamond



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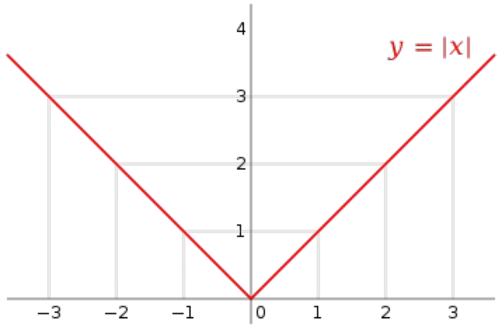
Lasso Regression: Differentiability

- The absolute function is a convex function
  - However, it is NOT differentiable at 0 (a sharp corner)
  - Hence:
    - Our cost function does not have a closed form
    - We can't apply a gradient descent
- About differentiability
  - The absolute value function is a piecewise function
  - When x > 0, we know derivative of **f(x) = x is 1**
  - When x < 0, we know derivative of **f(x) = -x is -1**
  - However, there is no derivative for f(x - 0)
    - The neighbour gradients jumps from -1 to 1
  - If there is no derivative, then we **can't update** the weights in the **multivariate** case



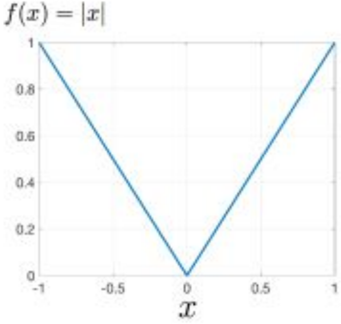
$$f(x)=\begin{cases} x; & x\geq 0 \\ -x; & x<0 \end{cases}$$

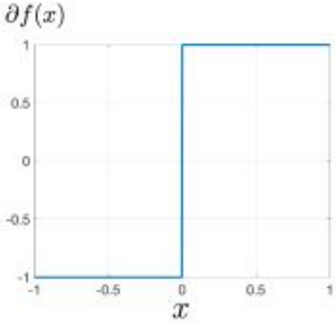
Lasso Regression: Implementation

- There are several techniques
  - Subgradient method
  - Coordinate descent
    - Update only a single weight at each step
      - Recall how Gradient descent updates all of the weights at once
    - SKLearn uses coordinate descent method to implement Lasso optimization
    - Refer to resources / internet

Implementing Lasso: Subgradient method

- We can use it for **non-differentiable** objective functions
- It is not a descent method; the function value can increase
- Optionally, refer to the math details in the resources section
- We compute some kind of gradient for the piecewise function





$$f(x) = |x| \qquad \partial f(x) = \begin{cases} \{-1\}, & \text{if } x < 0 \\ [-1, 1], & \text{if } x = 0 \\ \{1\}, & \text{if } x > 0 \end{cases}$$

- The final derivatives for absolute value function are simple
- For f(0), any value in the range [-1, 1] is accepted
  - We typically use 1
- Then it is all about the sign of f(x): positive or negative
  - **df(x) = sign(x)**
  - Multiplied by λ for lasso
    - **df(x) = sign(x)** * λ

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SKlearn library

- Linear regression is a **simple** and old model. Many variates were created with deep mathematical analysis around them
  - In practice, we might try them and see the best

```
def evalaute(x, t, model, name):
    model.fit(x, t)
    pred_t = model.predict(x)
    err = mean_squared_error(t, pred_t)
    w = ' '.join([f'{w:.3f}' for w in model.coef_])
    print(f'{name}: MSE {err:.3f} - intercept {model.intercept_

if __name__ == '__main__':
    x, t = get_linear_data()

    evalaute(x, t, Lasso(alpha=0.01), 'lasso 0.01 ')
    evalaute(x, t, LassoLars(alpha=0.01, normalize=False), 'Las
    evalaute(x, t, ElasticNet(alpha=0.01), 'ElasticNet 0.01 ')
    evalaute(x, t, Ridge(alpha=1), 'Ridge 1     ')
    evalaute(x, t, BayesianRidge(), 'BayesianRidge')
    evalaute(x, t, LinearRegression(), 'LinearRegression')
```

Importance of scaling

- Very Large input features require tiny weights. Very small input features require large weights. Scale/standardize your data!

```
x, t = get_linear_data()

evalaute(x, t, Lasso(alpha=0.01), 'lasso 0.01 ')
evalaute(x, t, Ridge(alpha=1), 'Ridge 1    ')
evalaute(x, t, LinearRegression(), 'LinearRegression')
print()
x /= 10 ** 5
# Tiny features require big weights.
# But weights are penalized, and regualrizer will set to 0
evalaute(x, t, Lasso(alpha=0.01), 'lasso 0.01 ')
evalaute(x, t, Ridge(alpha=1), 'Ridge 1    ')
evalaute(x, t, LinearRegression(), 'LinearRegression')
```

Importance of scaling

```
lasso 0.01 : MSE 0.040 - intercept 0.02- Weights 0.994 0.000 0.001 0.000
Ridge 1    : MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008
LinearRegression: MSE 0.039 - intercept 0.02- Weights 0.995 0.002 0.013 0.008

lasso 0.01 : MSE 8.334 - intercept 4.99- Weights 0.000 0.000 0.000 0.000
Ridge 1    : MSE 8.334 - intercept 4.99- Weights 0.042 0.000 0.001 0.000
LinearRegression: MSE 0.039 - intercept 0.02- Weights 99540.085 233.673 1257.960 813.894
```

Lasso Regression: In Practice

- We typically just try Ridge, Lasso and Elastic Net and see which one works better (**empirical** approach). Start with Ridge
- Lasso *might* works well if there are small number of significant features, while Ridge is the opposite
- Don't count on lasso features selection. Do your own investigations
  - If features D > examples N, lasso selects at most N features
  - Lasso might drop significant features that generate illogical models
  - Lasso might select only one feature from a group of **relevant** features
  - If the data is perturbed (changed) slightly, we might get different solutions
  - Then which features are the important ones?!
- Lasso is slower than ridge which is differentiable and has a closed form

Feature Selection

- Feature selection is selecting a subset of relevant features that are informative and discriminative
- In theory it can come with many advantages:
  - Dimensionality Reduction ⇒ less complex model ⇒ less overfitting
    - More features requires more weights which make the model more complex
  - Interpretability: easier to understand the factors that influence the model's predictions

Feature Selection Techniques

- Univariate Feature Selection: Investigate each feature independently (e.g. chi-square test)
- **Correlation**-based Methods: correlation between features and the target variable, as well as the intercorrelation between features (very common)
- **Lasso** (discard zero weights)
- Tree-based Methods (e.g. random forests) provides features importance
- Dimensionality reduction technique (e.g. PCA and **Autoencoders**)
- Tip: in practice, try using all of your data and run simple models first

Relevant Materials

- Lasso: Article, StatQuest, Proximal gradient, Article
- Subgradients: video, article, article, Probabilistic Perspective 13.3.2
- Coordinate descent: slides
- Deriving lasso coordinate descent: article / video coursera / code
- **Regularization path**: **plot** weights vs lambdas: article - code
- Soft thresholding: link, Probabilistic Perspective:ch:13.3.2

"Acquire knowledge and impart it to the people."

"Seek knowledge from the Cradle to the Grave."