Lecture 6: L2- and L1-Regularization

Contents

Atrribution: A lot of this material is adapted from CPSC 340 lecture notes.

Imports

```
import os
import sys

sys.path.append("code/.")
%matplotlib inline
import matplotlib.pyplot as plt
import mglearn
import numpy as np
import numpy.linalg as npla
import numpy.random as npr
import pandas as pd
from plotting_functions import *
from sklearn import datasets
from sklearn.dummy import DummyClassifier, DummyRegressor
from sklearn.impute import SimpleImputer
from sklearn.linear_model import LinearRegression, LogisticRegression, Ridge,
from sklearn.model_selection import cross_val_score, cross_validate, train_tes
from sklearn.preprocessing import PolynomialFeatures, StandardScaler
pd.set_option("display.max_colwidth", 200)
```

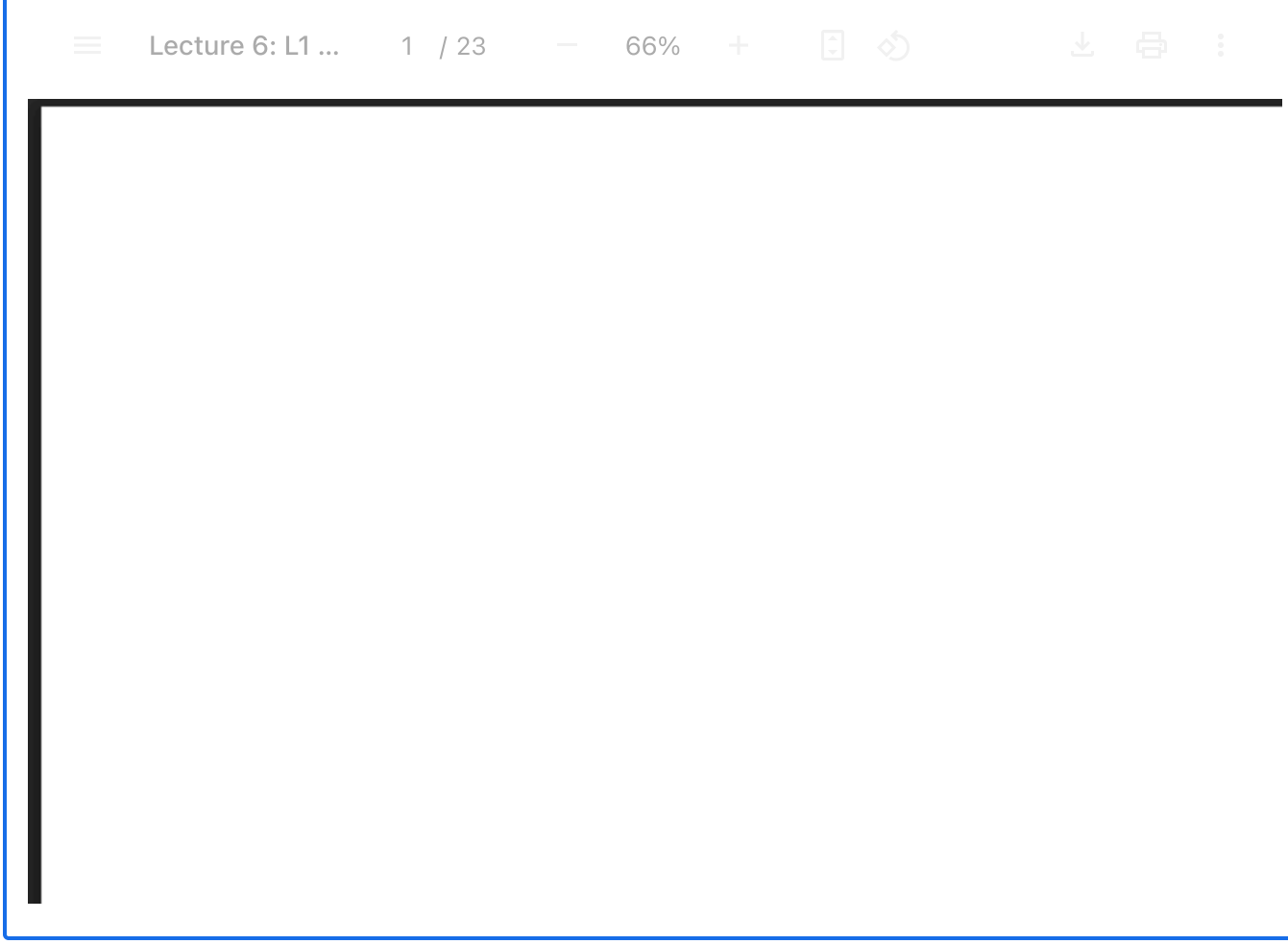
Learning outcomes

From this lecture, students are expected to be able to:

- Broadly explain L2 regularization (Ridge).
- Use L2 regularization (Ridge) using `sklearn`.
- Compare L0- and L2-regularization.
- Explain the relation between the size of regression weights, overfitting, and complexity hyperparameters.
- Explain the effect of training data size and effect of regularization.
- Explain the general idea of L1-regularization.
- Learn to be skeptical about interpretation of the coefficients.
- Use L1-regularization (Lasso) using `sklearn`.
- Discuss sparsity in L1-regularization.
- Compare L0-, L1-, and L2-regularization.
- Use L1 regularization for feature selection.
- Explain the importance of scaling when using L1- and L2-regularization
- Broadly explain how L1 and L2 regularization behave in the presence of collinear features.

Lecture slides

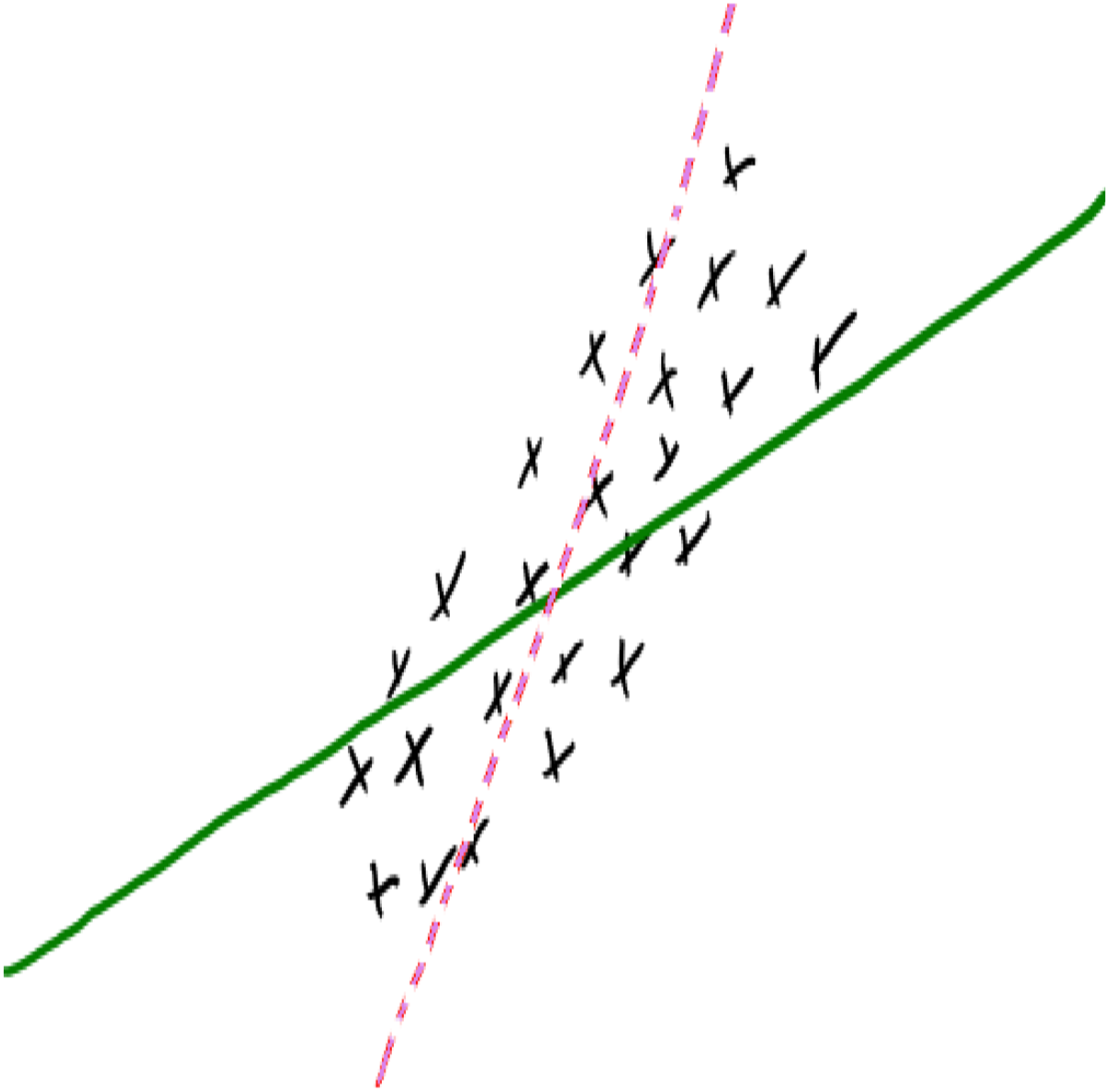
Section 1 slides | Section 2 slides



Recap

Idea of regularization: Pick the line/hyperplane with smaller slope

- Assuming the models below (dashed and solid green lines) have the same training error and if you are forced to choose one of them, which one would you pick?
  - **Pick the solid green line because its slope is smaller.**
  - Small change in x_i has a smaller change in prediction y_i
  - Since w is less sensitive to the training data, it's likely to generalize better.



- Regularization is a technique for controlling model complexity.
  - Instead of minimizing just the Loss, minimize **Loss + λ Model complexity**
  - Loss: measures how well the model fits the data.
  - Model complexity: measures model complexity (also referred to as **regularization term**)
  - A scalar λ decides the overall impact of the regularization term.

How to quantify model complexity?

- Total number of features with non-zero weights
  - L0 regularization: quantify model complexity as $||w||_0$, L0 norm of w.
- As a function of weights: A feature weight with high absolute value is more complex than the feature weight with low absolute value.

- L2 regularization: quantify model complexity as $\|w\|_2^2$, square of the L2 norm of w.
- L1 regularization: quantify model complexity as $\|w\|_1$, L1 norm of w.

L0-regularization

- L0-regularization.

$$J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_0$$

- Regularization parameter λ controls the strength of regularization.
- To increase the degrees of freedom by one, need to decrease the error by λ.
- Prefer smaller degrees of freedom if errors are similar.
- Can't optimize because the function is discontinuous in $\|w\|_0$
  - Search over possible models

L2-regularization

- Standard regularization strategy is L2-regularization.
- Also referred to as **Ridge**.
- The loss function has an L2 penalty term.

$$J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_2^2$$

- Regularization parameter λ controls the strength of regularization.
  - bigger $\lambda \rightarrow$ more regularization $\rightarrow$ lower weights
- Setting $\lambda = 0$ is the same as using OLS
  - Low training error, high variance, bigger weights, likely to overfit
- Setting λ to a large value leads to smaller weights
  - Higher training error, low variance, high bias, smaller weights, likely to underfit
- We want to strike a balance between these two extremes, which we can control by optimizing the value for λ.

`sklearn`'s `Ridge` or L2 regularization

Let's bring back `sklearn's` California housing dataset.

```
from sklearn.datasets import fetch_california_housing
from sklearn.preprocessing import PolynomialFeatures

housing = fetch_california_housing(as_frame=True)
X = housing["data"]
y = housing["target"]

pf = PolynomialFeatures(degree=2, include_bias=False)
X = pf.fit_transform(X)
X_train_poly, X_test_poly, y_train, y_test = train_test_split(X, y, random_sta

ss = StandardScaler()
X_train = ss.fit_transform(X_train_poly)
X_test = ss.transform(X_test_poly)
```

```
X_train.shape
```

```
(15480, 44)
```

Let's explore L2 regularization with this dataset.

Example: L2-Regularization "Shrinking"

- λ in the formulation above is `alpha` in `sklearn`.
- We get least squares with $\lambda = 0$.
- As we increase α
  - $\|y - Xw\|_2^2$ goes $\uparrow$
  - $\|w\|_2^2$ goes $\downarrow$
  - Though individual w_j can increase or decrease with lambda because we use the L2-norm, the large ones decrease the most.

```
def lr_loss_squared(w, X, y): # define OLS loss function
    return np.sum((y - X @ w) ** 2)
```

```
from numpy.linalg import norm
from collections import defaultdict
alphas = [0, 0.01, 0.1, 1.0, 10, 100, 1000, 1000000]
weight_shrinkage_data = defaultdict(list) #{'alpha':[], '||Xw - y||^2':[], '||

for (i, alpha) in enumerate(alphas):
    r = Ridge(alpha=alpha)
    r.fit(X_train, y_train)
    weight_shrinkage_data['alpha'].append(alpha)
    OLS = np.round(lr_loss_squared(r.coef_, X_train, y_train), 4)
    l2_term = np.round(norm(r.coef_, 2)**2, 4)
    intercept = np.round(r.intercept_,4)
    weight_shrinkage_data['||y - Xw||^2'].append(OLS)
    weight_shrinkage_data['||w||^2'].append(l2_term)
    weight_shrinkage_data['total_loss'].append(OLS + l2_term * alpha)
    weight_shrinkage_data['intercept'].append(intercept)
    weight_shrinkage_data['train score'].append(np.round(r.score(X_train, y_tr
    weight_shrinkage_data['test score'].append(np.round(r.score(X_test, y_test

pd.DataFrame(weight_shrinkage_data)
```

	alpha	||y - Xw||^2	||w||^2	total_loss	intercept	train score	test score
0	0.00	73099.4882	7634.4579	73099.488200	2.0744	0.69	-0.73
1	0.01	73113.1963	4239.9359	73155.595659	2.0744	0.69	-0.17
2	0.10	73222.8589	888.3987	73311.698770	2.0744	0.68	0.62
3	1.00	73437.3112	77.0152	73514.326400	2.0744	0.67	0.02
4	10.00	73597.9629	8.4983	73682.945900	2.0744	0.66	-3.80
5	100.00	73777.7373	2.5195	74029.687300	2.0744	0.65	-3.37
6	1000.00	74363.2804	0.7118	75075.080400	2.0744	0.62	0.10
7	1000000.00	85565.9420	0.0008	86365.942000	2.0744	0.08	0.08

In this example, as `alpha` goes up

- $||Xw - y||_2^2$ is increasing
- $||w||_2^2$ is decreasing; weight become smaller and smaller
- The intercept stays the same. (Since our standardization included centering the features by subtracting the mean, the intercept is now the mean of the target – dummy model prediction.)
- We are getting best test score for `alpha=0.10`.

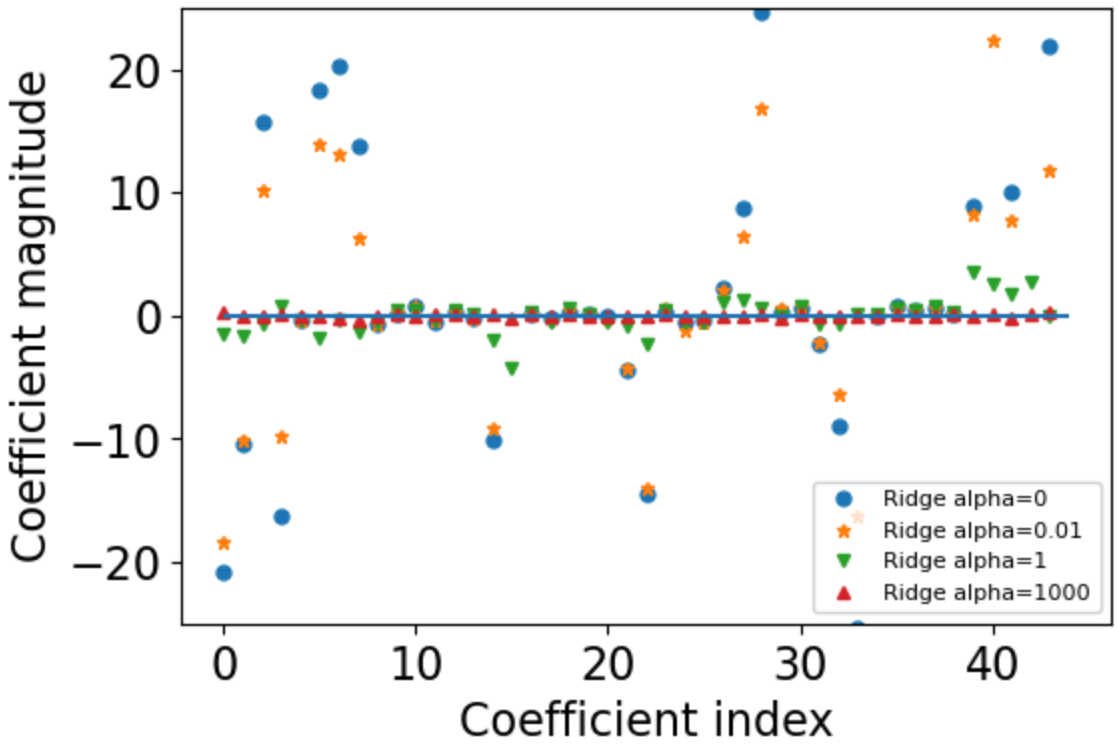
- The total loss is worse than OLS but it's helping with generalization.

The weights become smaller but do not become zero

- As `alpha` goes up, we increase the regularization strength.
- The weights become smaller and smaller but tend not to become exactly zero.

```
alphas = [0, 0.01, 1, 1000]
```

```
plt.figure(figsize=(6, 4))
markers = ['o','*', 'v','^']
ridge_models = {}
for (i, alpha) in enumerate(alphas):
    r = Ridge(alpha = alpha)
    r.fit(X_train, y_train)
    plt.plot(r.coef_, markers[i], markersize=5, label="Ridge alpha="+ str(alph
plt.xlabel("Coefficient index")
plt.ylabel("Coefficient magnitude")
plt.hlines(0, 0, len(r.coef_))
plt.ylim(-25, 25)
plt.legend(loc="best",fontsize=8);
```



Let's try a very large `alpha` value, which is likely to make weights very small.

```
ridge10000 = Ridge(alpha=10000).fit(X_train, y_train)
print("Total number of features", X_train.shape[1])
print("Number of non-zero weights: ", np.sum(ridge10000.coef_ != 0))
```

```
Total number of features 44
Number of non-zero weights:  44
```

All features have non-zero weights.

Regularization path

Let's trace the journey of coefficients of a few features with different values of `alpha`.

```
feature_names = pf.get_feature_names_out()
```

Let's examine the coefficients

```
r10 = Ridge(alpha=0.10)
r10.fit(X_train, y_train)
coefs = (
    pd.DataFrame(r10.coef_, feature_names, columns=["coef"])
    .query("coef != 0")
    .sort_values("coef")
    .reset_index()
    .rename(columns={"index": "variable"})
)
```

```
coefs.style.background_gradient('PuOr')
```

	variable	coef
0	MedInc Longitude	-16.762873
1	MedInc	-10.178537
2	HouseAge Longitude	-9.608717
3	HouseAge	-6.986869
4	MedInc Latitude	-5.683734
5	HouseAge Latitude	-2.931366
6	AveBedrms Longitude	-2.152434
7	AveBedrms Latitude	-1.934514
8	Longitude	-1.637599
9	AveRooms AveBedrms	-1.571689
10	AveBedrms AveOccup	-1.536152
11	MedInc^2	-0.540772
12	AveRooms Population	-0.518624
13	HouseAge AveOccup	-0.414707
14	HouseAge AveRooms	-0.376728
15	MedInc AveBedrms	-0.280714
16	Population	-0.106295
17	MedInc AveOccup	-0.072894
18	AveBedrms	-0.067099
19	Population^2	0.050877
20	HouseAge Population	0.076735
21	AveOccup^2	0.177787
22	HouseAge^2	0.197444
23	MedInc HouseAge	0.292222
24	MedInc Population	0.358598
25	HouseAge AveBedrms	0.495107
26	MedInc AveRooms	0.544633

	variable	coef
27	Population Latitude	0.573911
28	Population AveOccup	0.603423
29	AveBedrms^2	0.620403
30	AveBedrms Population	0.780217
31	AveRooms	0.908226
32	AveRooms^2	0.940577
33	Longitude^2	0.944154
34	Population Longitude	1.199605
35	AveRooms AveOccup	1.697423
36	AveOccup	2.478821
37	AveRooms Latitude	2.523284
38	AveRooms Longitude	3.693662
39	Latitude	3.830685
40	Latitude^2	4.330258
41	AveOccup Latitude	6.270548
42	AveOccup Longitude	9.143782
43	Latitude Longitude	10.627639

```
feats = ['MedInc', 'AveBedrms',  'Population', 'MedInc Longitude', 'Population
```

```
msk = [feat in feats for feat in feature_names]
```

```
r10.coef_[msk]
```

```
array([-10.17853657,  -0.06709887,  -0.10629543, -16.7628735 ,
         1.19960525,  10.6276393 ])
```

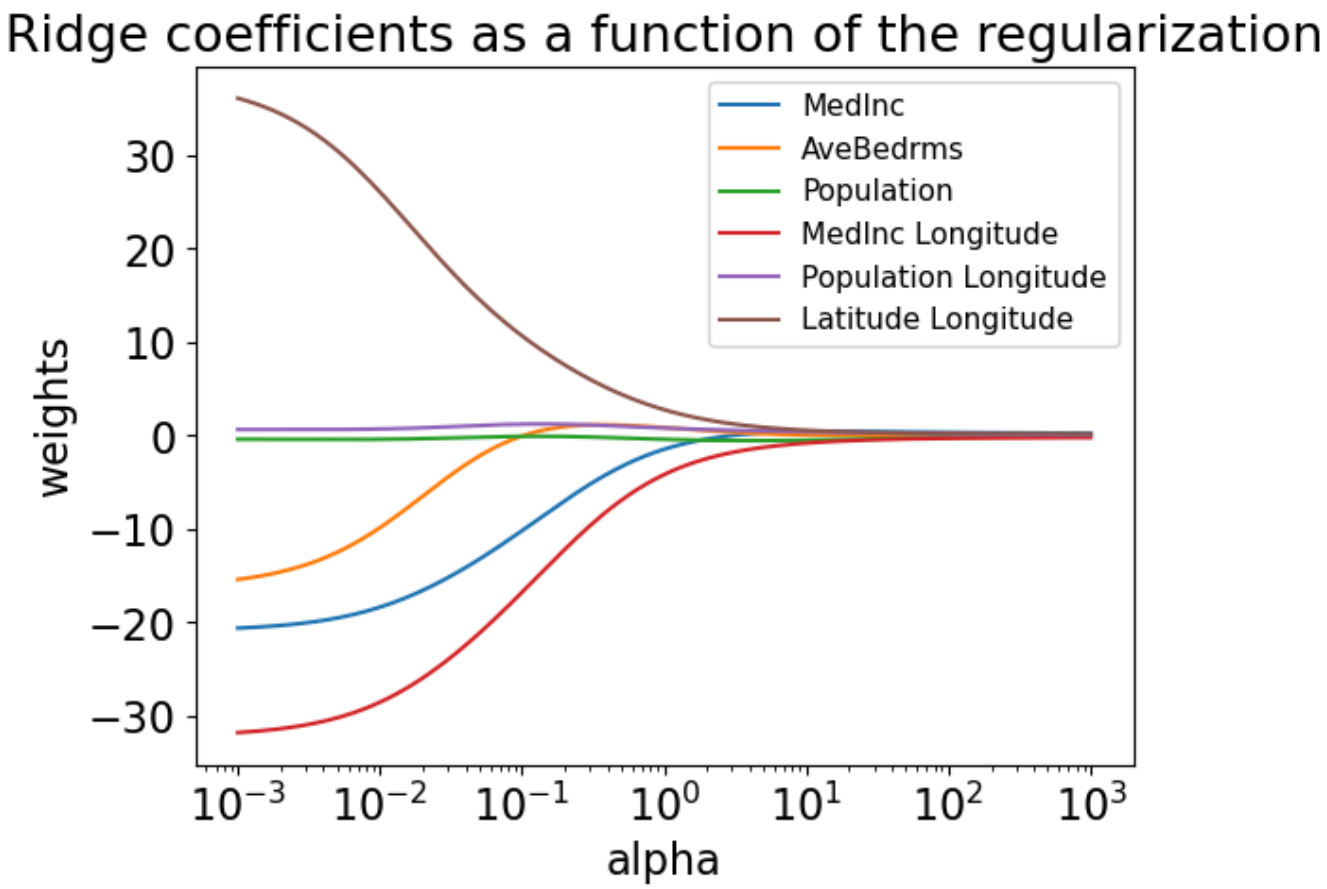
```
# Attribution: Code adapted from here: https://scikit-learn.org/stable/auto_ex
import numpy as np
import matplotlib.pyplot as plt
from sklearn import linear_model

n_alphas = 200
alphas = np.logspace(-3, 3, n_alphas)

coefs = []
for a in alphas:
    ridge = linear_model.Ridge(alpha=a, fit_intercept=False)
    ridge.fit(X_train, y_train)
    coefs.append(ridge.coef_[msk])

ax = plt.gca()
ax.plot(alphas, coefs)

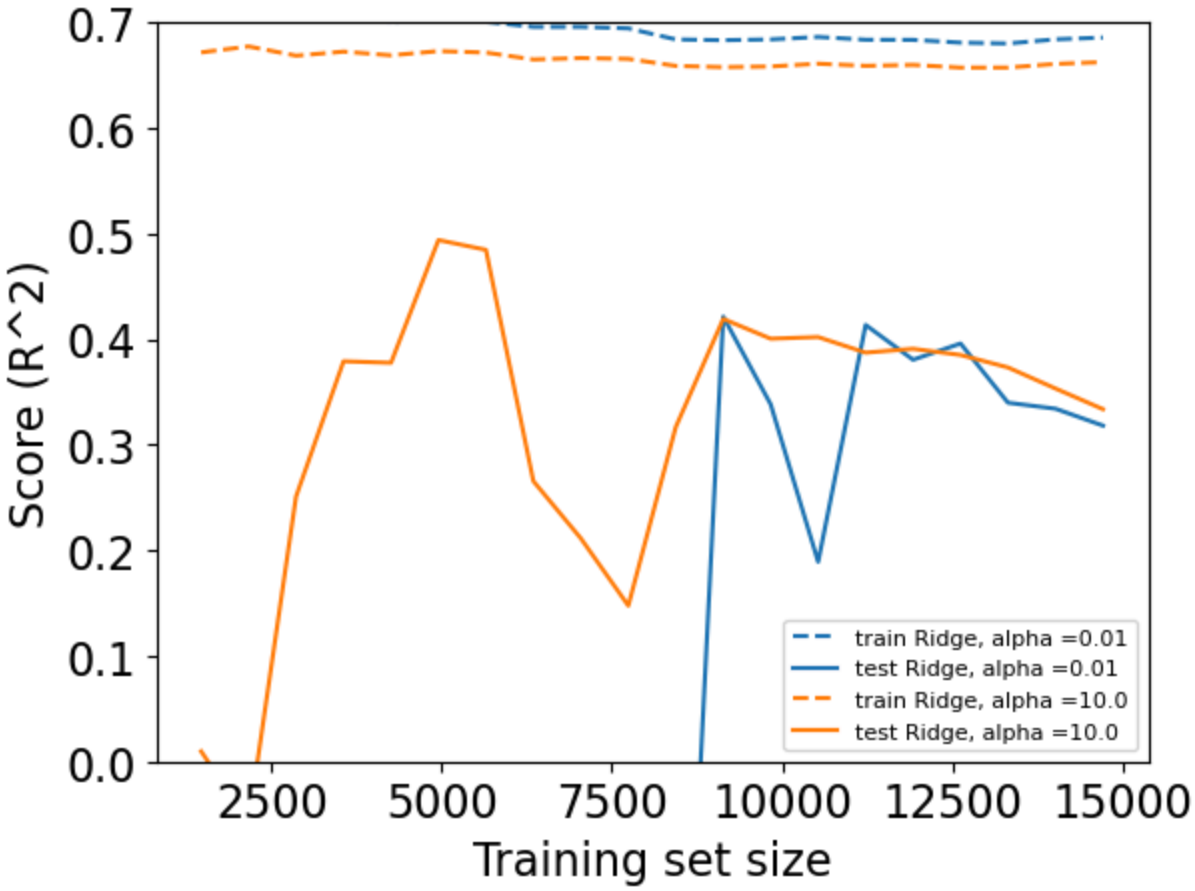
ax.set_xscale("log")
#ax.set_xlim(ax.get_xlim()[::-1])  # reverse axis
plt.xlabel("alpha")
plt.ylabel("weights")
plt.title("Ridge coefficients as a function of the regularization")
plt.axis("tight")
ax.legend(feats, loc="best", fontsize=11)
plt.show()
```



The coefficients are very close to zero but not exactly zero. That said, they won't have much impact on prediction.

Regularization learning curves

```
plot_learning_curve(Ridge(alpha=0.01), X_train, y_train)
plot_learning_curve(Ridge(alpha=10.0), X_train, y_train)
```



- As one would expect, the training score is higher than the test score for all dataset sizes
- Training score of `Ridge` with `alpha=0.01` > Training score of `Ridge` with `alpha=10` (more regularization)
- However, the test score of `Ridge` with `alpha=10` > Test score of `Ridge` with `alpha=0.01` for smaller training sizes.
- As more and more data becomes available to the model, both models improve. Ridge with less regularization catches up with ridge with more regularization and actually

performs better.

How to pick λ?

- Theory: as n grows λ should be in the range $O(1)$ to $\sqrt{n}$.
- Practice: optimize validation set or cross-validation error.
    - Almost always decreases the test error.

(Optional) Should we regularize the y-intercept?

- No!
    - Why encourage it to be closer to zero? (It could be anywhere.)
    - You should be allowed to shift function up/down globally.
- Yes!
    - Useful for optimization; It makes the solution unique and it easier to compute w
- Compromise: regularize by a smaller amount than other variables. $
$J(w) = ||Xw + w_0 - y||^2 + \frac{\lambda_1}{2}||w||^2 + \frac{\lambda_2}{2}w_0^2$$

Some properties of L2-regularization

1. Solution w is unique. It has to do with the smoothness of the function.
    - We are not going into mathematical details. If interested see slide 20 from CPSC 340.
2. **Almost always improves the validation error.**
3. No collinearity issues.
4. Less sensitive to changes in X.
5. Gradient descent (optimization algorithm) converges faster (bigger λ means fewer iterations). (You'll learn about Grafient descent in 572.)
6. Worst case: just set λ small and get the same performance

Summary: L2-regularization

- Change the loss function by adding a continuous L2-penalty on the model complexity.

- Best parameter λ almost already leads to improved validation error.
  - L2-regularized least squares is also called "ridge regression".
  - Can be solved as a linear system like least squares.
- Some benefits of L2 regularization
  - Solution is unique.
  - Less sensitive to data.
  - Fast.

❓❓ Questions for you (recap)

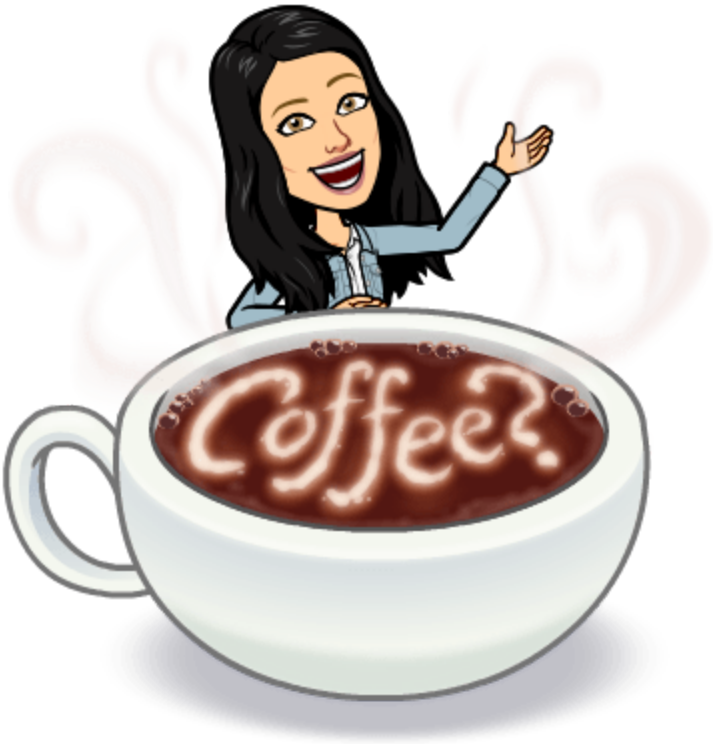
iClicker Exercise 6.1

Select all of the following statements which are TRUE.

- (A) Introducing L2 regularization to the model means making it less sensitive to changes in X.
- (B) Introducing L2 regularization to the model can results in worse performance on the training set.
- (C) L2 regularization shrinks the weights but all w_js tend to be non-zero.

V's answers: A, B, C

Break (~5 mins)



L1 regularization

- An alternative to `Ridge` (L2-regularization for least squares) is `Lasso`.
- Instead of L0- or L2-norm, regularize with L1-norm.

$$J(w) = \sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda \sum_{j=1}^{d}|w_j| \text{ or}$$

$$J(w) = \|y - Xw\|_2^2 + \lambda\|w\|_1$$

- $\lambda \rightarrow$ regularization strength
- $\|w\|_1 \rightarrow$ L1-norm of w
- Objective balances getting low error vs. having small values for w_j

Similarities with L2-regularization

- L1-regularization $J(w) = ||Xw - y||_2^2 + \lambda||w||_1$
- L2-regularization $J(w) = ||Xw - y||_2^2 + \lambda||w||_2^2$
- Both shrink weights.
- Both result in lower validation error.

Do not confuse the L1 loss (absolute loss) with L1-regularization!

Terminology and notation: Ridge and Lasso

- Linear regression model that uses L2 regularization is called **Ridge** or Tikhonov regularization.
  - `scikit-learn` Ridge
- Linear regression model that uses L1 regularization is called **Lasso**.
  - `scikit-learn` Lasso

> class sklearn.linear_model.Lasso(alpha=1.0, fit_intercept=True, normalize=False, precompute=False, copy_X=True, max_iter=1000, tol=0.0001, warm_start=False, positive=False, random_state=None, selection='cyclic')

L1-regularization

- The consequence of using L1-norm is that some features are exactly zero, which means that the features are entirely ignored by the model.
- This can be considered as a form of feature selection!!
- L1-regularization simultaneously regularizes and selects features.
- Very fast alternative to search and score methods

Let's apply `Lasso` on the California housing data.

```
X_train.shape
```

```
(15480, 44)
```

```
from sklearn.linear_model import Lasso

lasso = Lasso().fit(X_train, y_train)
print("Training set score: {:.2f}".format(lasso.score(X_train, y_train)))
print("Test set score: {:.2f}".format(lasso.score(X_test, y_test)))
print("Number of features used:", np.sum(lasso.coef_ != 0))
```

```
Training set score: 0.00
Test set score: -0.00
Number of features used: 0
```

- That's strange. It's not using any features – like dummy model. It's underfitting.
- Similar to `Ridge` it also has a regularization hyperparameter `alpha`.
- Let's decrease it to reduce underfitting.

- Let's examine weight shrinkage for l1 regularization
- Lasso loss is not a smooth function.
- Slower compared to Ridge.

```
from numpy.linalg import norm
alphas = [0, 0.0001, 0.01, 0.1, 1]
weight_shrinkage_data = {'alpha':[], '||Xw - y||^2':[], '||w||_1':[], 'interce

for (i, alpha) in enumerate(alphas):
    print('alpha: ', alpha)
    l = Lasso(alpha=alpha, max_iter=10000)
    l.fit(X_train, y_train)
    weight_shrinkage_data['alpha'].append(alpha)
    OLS = np.round(lr_loss_squared(l.coef_, X_train, y_train), 4)
    l1_term = np.round(norm(l.coef_, 1), 4)
    intercept = np.round(l.intercept_, 4)
    weight_shrinkage_data['||Xw - y||^2'].append(OLS)
    weight_shrinkage_data['||w||_1'].append(l1_term)
    weight_shrinkage_data['intercept'].append(intercept)
    weight_shrinkage_data['train score'].append(np.round(l.score(X_train, y_tr
    weight_shrinkage_data['test score'].append(np.round(l.score(X_test, y_test
```

```
alpha:  0
```

```
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/base.py:14
  return fit_method(estimator, *args, **kwargs)
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/linear_mod
  model = cd_fast.enet_coordinate_descent(
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/linear_mod
  model = cd_fast.enet_coordinate_descent(
```

```
alpha:  0.0001
```

```
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/linear_mod
  model = cd_fast.enet_coordinate_descent(
```

```
alpha:  0.01
alpha:  0.1
alpha:  1
```

Note the warning we see about the algorithm not converging with alpha=0. Here we are including alpha=0 for demonstration purposes, but if you would even use this in a real world scenario (although this scenario is rare), it is better to use the LinearRegression estimator instead.

```
pd.DataFrame(weight_shrinkage_data)
```

	alpha	||Xw - y||^2	||w||_1	intercept	train score	test score
0	0.0000	73398.6742	52.1039	2.0744	0.67	0.52
1	0.0001	73462.0080	33.8967	2.0744	0.67	0.20
2	0.0100	74463.3147	3.2798	2.0744	0.62	0.33
3	0.1000	76723.2012	0.8035	2.0744	0.51	0.48
4	1.0000	87271.1329	0.0000	2.0744	0.00	-0.00

```
r = Ridge(alpha = 0.1).fit(X_train, y_train)
print("Training set score: {:.2f}".format(r.score(X_train, y_train)))
print("Test set score: {:.2f}".format(r.score(X_test, y_test)))
print("Number of features used:", np.sum(r.coef_ != 0))
```

```
Training set score: 0.68
Test set score: 0.62
Number of features used: 44
```

```
lasso = Lasso(alpha=0.1, max_iter=10000).fit(X_train, y_train)
print("Training set score: {:.2f}".format(lasso.score(X_train, y_train)))
print("Test set score: {:.2f}".format(lasso.score(X_test, y_test)))
print("Number of features used:", np.sum(lasso.coef_ != 0))
```

```
Training set score: 0.51
Test set score: 0.48
Number of features used: 3
```

- In this case we are not really getting better results with Lasso.
- In fact, Lasso is not able to do better than linear regression.
- Often you might see better scores than `Ridge` with fewer features.
- If `alpha` is too low, we reduce the effect of overfitting and the results are similar to linear regression.

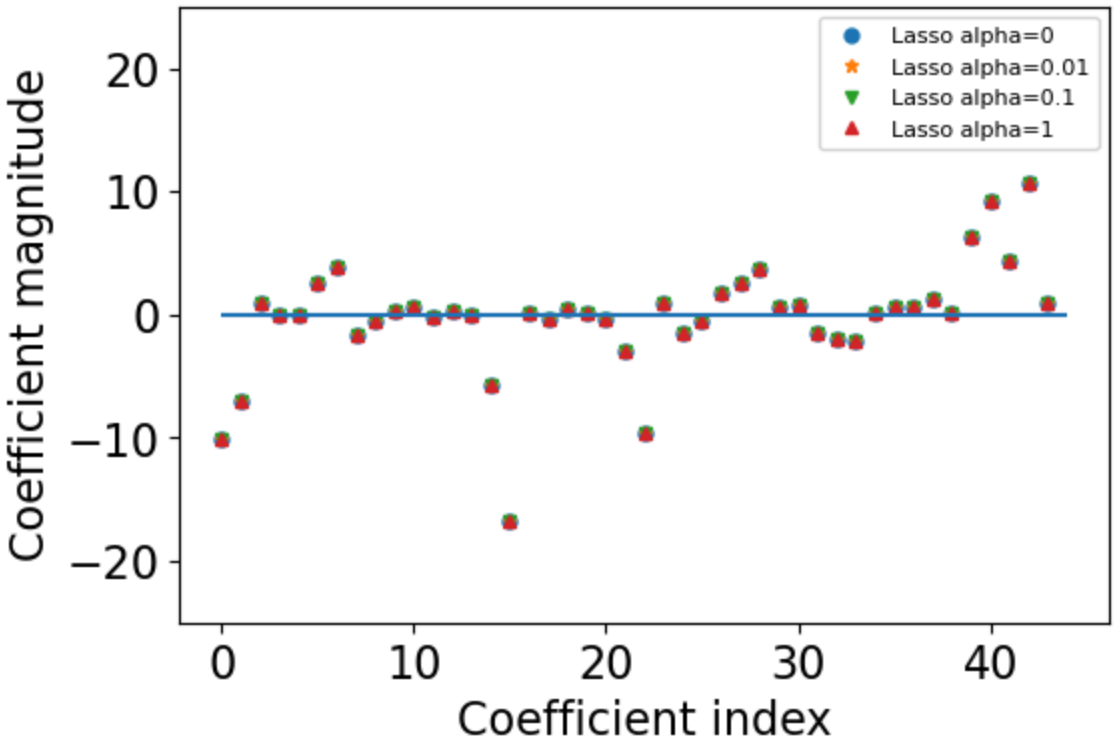
The weights become smaller and eventually become zero.

Let's plot coefficients of `Lasso`.

```
alphas = [0, 0.01, 0.1, 1]
```

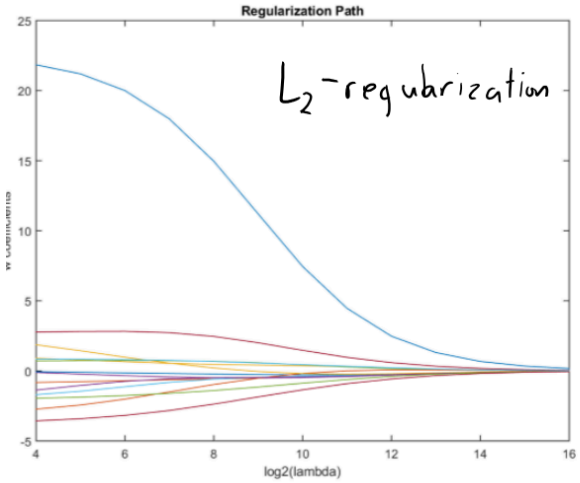
```
plt.figure(figsize=(6, 4))
markers = ['o','*', 'v','^']
lasso_models = {}
for (i, alpha) in enumerate(alphas):
    lasso = Lasso(alpha = alpha, max_iter=10000)
    lasso.fit(X_train, y_train)
    plt.plot(r.coef_, markers[i], markersize=5, label="Lasso alpha="+ str(alph
plt.xlabel("Coefficient index")
plt.ylabel("Coefficient magnitude")
plt.hlines(0, 0, len(lasso.coef_))
plt.ylim(-25, 25)
plt.legend(loc="best",fontsize=8);
```

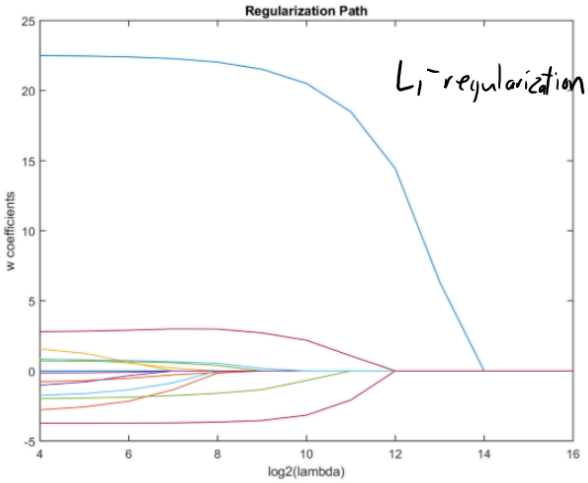
```
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/base.py:14
  return fit_method(estimator, *args, **kwargs)
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/linear_mod
  model = cd_fast.enet_coordinate_descent(
/home/joel/miniconda3/envs/573/lib/python3.12/site-packages/sklearn/linear_mod
  model = cd_fast.enet_coordinate_descent(
```



- For `alpha = 100` most of the coefficients are zero.
- With smaller values of `alpha` we get less and less regularization.

- I'm not showing L1 regularization path on our data because it takes too long to run.
- But you're likely to see this type of plots in the context of regularization.





Terminology and notation: Sparsity

- We say a linear function is sparse if most of the coefficients are zero.
- Example: Here only 2 out of 8 coefficients are non-zero and so it is a sparse function. $ $0x_1 + 0.45x_2 + 0x_3 + 0x_4 + 1.2x_5 + 0x_6 + 0x_7 + 0x_8$$
- L0- and L1-regularization encourage sparsity.

Example: L0 vs. L1 vs. L2

Consider problem where 3 vectors can get minimum training error:

$$w^1 = \begin{bmatrix}100\\0.02\end{bmatrix}, w^2 = \begin{bmatrix}100\\0\end{bmatrix}, w^3 = \begin{bmatrix}99.99\\0.02\end{bmatrix}$$

- Without regularization, we could choose any of these 3.
- We are assuming that all have the same error, so regularization will "break tie".
- Which one would you choose with each of L0, L1, L2 regularization?

Which one would you choose with L0 regularization?

$$w^1 = \begin{bmatrix}100\\-0.02\end{bmatrix}, w^2 = \begin{bmatrix}100\\0\end{bmatrix}, w^3 = \begin{bmatrix}99.99\\0.02\end{bmatrix}$$

- What are the L0 norms of different weight vectors?
  - $||w^1||_0 = 2$
  - $||w^2||_0 = 1$
  - $||w^3||_0 = 2$

- L0 regularization would choose w^2.

Which one would you choose with L1 regularization?

$$w^1 = \begin{bmatrix}100\\0.02\end{bmatrix}, w^2 = \begin{bmatrix}100\\0\end{bmatrix}, w^3 = \begin{bmatrix}99.99\\0.02\end{bmatrix}$$

- What are the L1 norms of different weight vectors?
  - $||w^1||_1 = 100.02$
  - $||w^2||_1 = 100$
  - $||w^3||_1 = 100.01$

- L1-regularization would pick w^2
- L1-regularization focuses on decreasing all w_j until they are 0.

Which one would you choose with L2 regularization?

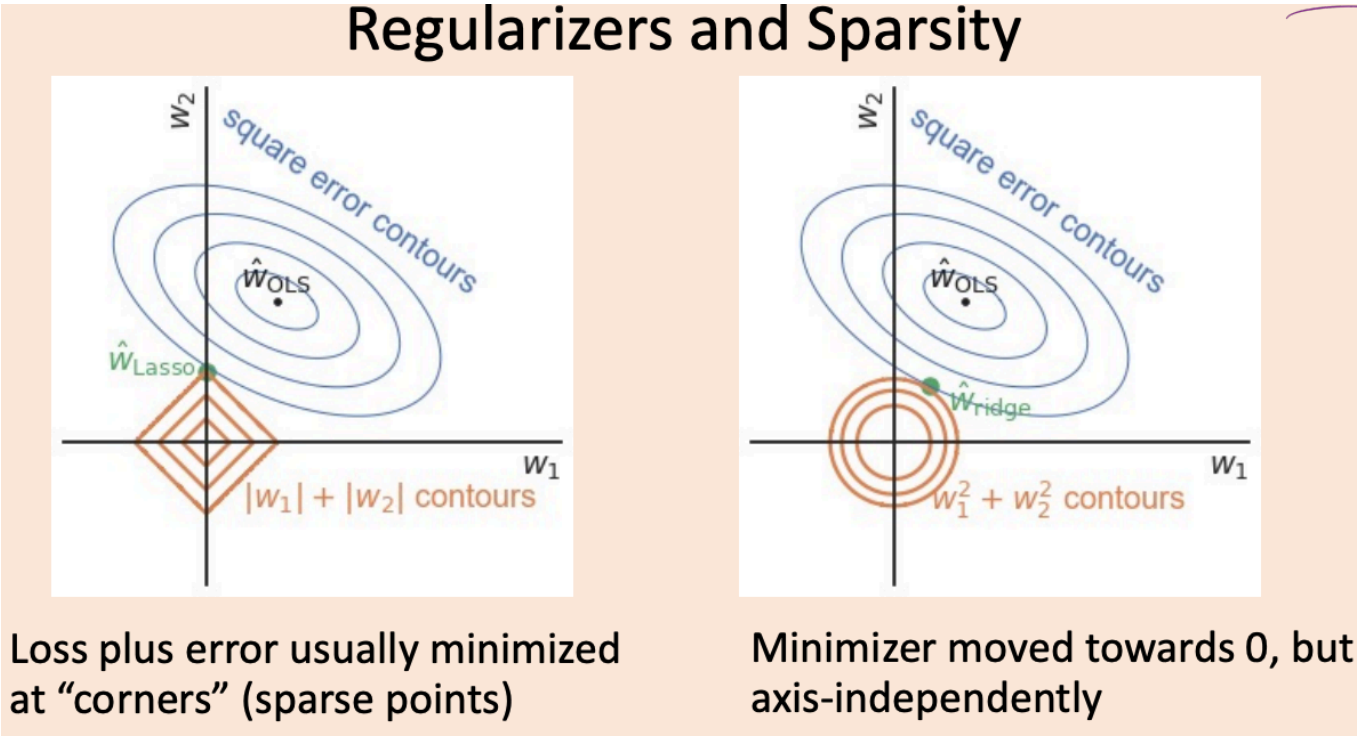
$$w^1 = \begin{bmatrix}100\\0.02\end{bmatrix}, w^2 = \begin{bmatrix}100\\0\end{bmatrix}, w^3 = \begin{bmatrix}99.99\\0.02\end{bmatrix}$$

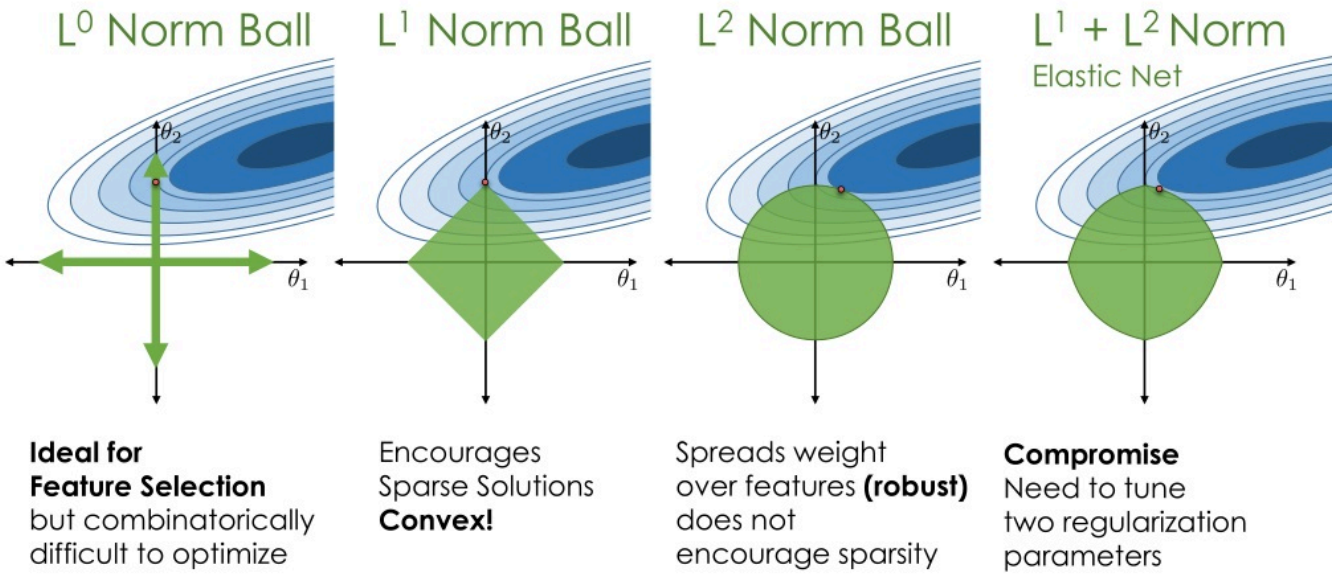
- What are the L2 norms of different weight vectors?
  - $||w^1||_2^2 = (100)^2 + (0.02)^2 = 10000.0004$
  - $||w^2||_2^2 = (100)^2 = 10000$
  - $||w^3||_2^2 = (99.99)^2 + (0.02)^2 = 9998.0005$

- L2-regularization would pick w^3
- L2-regularization focuses on decreasing largest w_j smaller

(Optional) Sparsity and Regularization

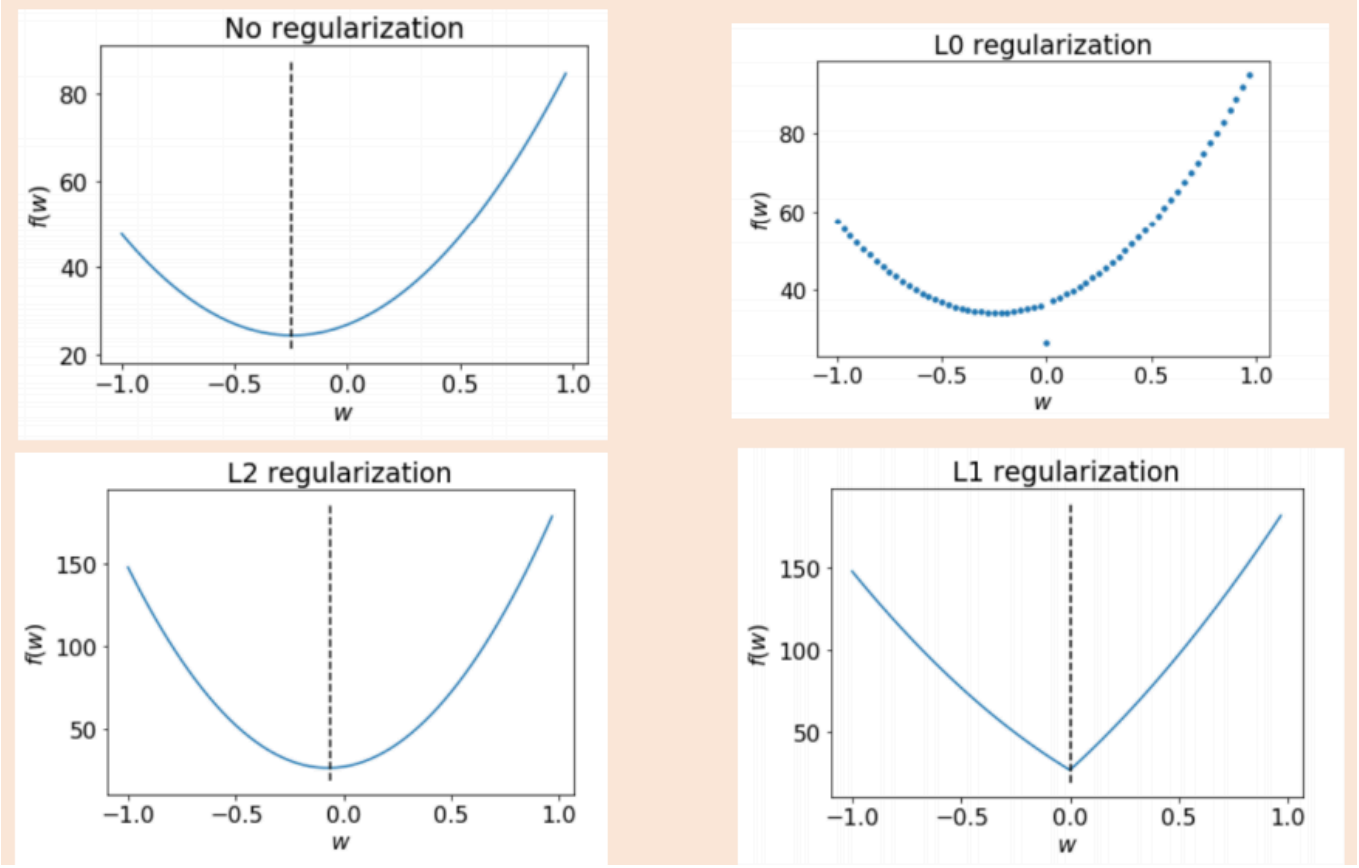
- Minimizing $||Xw - y||_2^2 + \lambda||w||_2^2$ is equivalent to minimizing $||Xw - y||_2^2$ subject to the constraint that $||w||_2^2 \leq t(\delta)$





source

(Optional) Sparsity and Regularization (with d=1)



Some properties of L1 regularization

1. Almost always improves the validation error.
2. Can learn with exponential number of irrelevant features.
3. Less sensitive to changes in X.
4. The solution is not unique. (If interested in more explanation on this, see slide 43 in this slide deck.)

Feature selection using L1 regularization

- Feature selection methods we have seen so far:
  - RFE
  - Search and score with L0-regularization (e.g., forward search)

- An effective way of feature selection: L1-regularization

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.feature_selection import SelectFromModel
from sklearn.linear_model import Lasso, LassoCV

housing = fetch_california_housing(as_frame=True)
X = housing["data"]
y = housing["target"]
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
pipe_l1_rf = make_pipeline(
    StandardScaler(),
    SelectFromModel(Lasso(alpha=0.01, max_iter=100000)),
    RandomForestRegressor(),
)

X.shape
```

```
(20640, 8)
```

```
pipe_l1_rf.fit(X_train, y_train)
pipe_l1_rf.score(X_train, y_train)
```

```
0.9729726892678439
```

```
print("Training set score: {:.2f}".format(pipe_l1_rf.score(X_train, y_train)))
print("Test set score: {:.2f}".format(pipe_l1_rf.score(X_test, y_test)))
```

```
Training set score: 0.97
Test set score: 0.79
```

```
print(
    "Number of features used:",
    np.sum(pipe_l1_rf.named_steps["selectfrommodel"].estimator_.coef_ != 0),
)
```

```
Number of features used: 7
```

Regularized models for classification

Regularized logistic regression

- Regularization is not limited to least squares.
- We can add L1 and L2 penalty terms in other loss functions as well.
- Let's look at logistic regression with L1- and L2-regularization.

```
from sklearn.datasets import load_breast_cancer

breast_cancer = load_breast_cancer()
# print(breast_cancer.keys())
# print(breast_cancer.DESCR)
```

```
breast_cancer_df = pd.DataFrame(breast_cancer.data, columns=breast_cancer.feat
breast_cancer_df["target"] = breast_cancer.target
train_df, test_df = train_test_split(breast_cancer_df, test_size=0.2, random_s

X_train, y_train = train_df.drop(columns=["target"]), train_df["target"]
X_test, y_test = test_df.drop(columns=["target"]), test_df["target"]
```

```
X_train.head()
```

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity
560	14.05	27.15	91.38	600.4	0.09929	0.11260	0.04462
428	11.13	16.62	70.47	381.1	0.08151	0.03834	0.01369
198	19.18	22.49	127.50	1148.0	0.08523	0.14280	0.11140
203	13.81	23.75	91.56	597.8	0.13230	0.17680	0.15580
41	10.95	21.35	71.90	371.1	0.12270	0.12180	0.10440

5 rows × 30 columns

```
y_train.value_counts(normalize=True)
```

```
target
1    0.632967
0    0.367033
Name: proportion, dtype: float64
```

```
from sklearn.metrics import f1_score, make_scorer, recall_score

custom_scorer = make_scorer(
    f1_score, pos_label=0
)  # note the syntax to change the positive label for f1 score
scoring_metric = custom_scorer

results_classification = {}
```

Let's try `DummyClassifier`

```
dummy = DummyClassifier()
results_classification["dummy"] = mean_std_cross_val_scores(
    dummy,
    X_train,
    y_train,
    return_train_score=True,
    scoring=scoring_metric,
)
pd.DataFrame(results_classification)
```

	dummy
fit_time	0.001 (+/- 0.000)
score_time	0.002 (+/- 0.000)
test_score	0.000 (+/- 0.000)
train_score	0.000 (+/- 0.000)

- In `sklearn`, by default logistic regression uses L2 regularization.
- The `C` hyperparameter decides the strength of regularization.
- Unfortunately, interpretation of `C` is inverse of `lambda`.

```
pipe_lgr_l2 = make_pipeline(StandardScaler(), LogisticRegression())
results_classification["Logistic Regression L2"] = mean_std_cross_val_scores(
    pipe_lgr_l2, X_train, y_train, return_train_score=True, scoring=scoring_me
)
```

```
pd.DataFrame(results_classification)
```

	dummy	Logistic Regression L2
fit_time	0.001 (+/- 0.000)	0.007 (+/- 0.002)
score_time	0.002 (+/- 0.000)	0.003 (+/- 0.001)
test_score	0.000 (+/- 0.000)	0.970 (+/- 0.011)
train_score	0.000 (+/- 0.000)	0.985 (+/- 0.005)

Weights are small but all of them are non-zero.

```
pipe_lgr_l2.fit(X_train, y_train)
l2_coefs = pipe_lgr_l2.named_steps["logisticregression"].coef_.flatten()
df = pd.DataFrame(l2_coefs, index=X_train.columns, columns=["l2_coefs"])
df
```

	l2_coefs
mean radius	-0.542448
mean texture	-0.252004
mean perimeter	-0.496523
mean area	-0.608907
mean smoothness	-0.170162
mean compactness	0.577409
mean concavity	-0.659992
mean concave points	-0.980380
mean symmetry	0.117937
mean fractal dimension	0.402504
radius error	-1.248832
texture error	-0.101663
perimeter error	-0.731364
area error	-0.927143
smoothness error	-0.232258
compactness error	0.618787
concavity error	-0.035918
concave points error	-0.203528
symmetry error	0.270964
fractal dimension error	0.739704
worst radius	-1.041989
worst texture	-1.097127
worst perimeter	-0.884671
worst area	-1.022599
worst smoothness	-0.925732
worst compactness	-0.071176
worst concavity	-0.767299

	l2_coefs
worst concave points	-0.738242
worst symmetry	-0.667742
worst fractal dimension	-0.523832

- Let's try logistic regression with L1 regularization.
- Note that I'm using a different solver (optimizer) here because not all solvers support L1-regularization.

```
pipe_lgr_l1 = make_pipeline(
    StandardScaler(), LogisticRegression(solver="liblinear", penalty="l1")
)
results_classification["Logistic Regression L1"] = mean_std_cross_val_scores(
    pipe_lgr_l1, X_train, y_train, return_train_score=True, scoring=scoring_me
)
```

```
pd.DataFrame(results_classification)
```

	dummy	Logistic Regression L2	Logistic Regression L1
fit_time	0.001 (+/- 0.000)	0.007 (+/- 0.002)	0.005 (+/- 0.000)
score_time	0.002 (+/- 0.000)	0.003 (+/- 0.001)	0.003 (+/- 0.000)
test_score	0.000 (+/- 0.000)	0.970 (+/- 0.011)	0.967 (+/- 0.007)
train_score	0.000 (+/- 0.000)	0.985 (+/- 0.005)	0.984 (+/- 0.006)

- The scores are more or less the same.
- But L1 regularization is carrying out feature selection; Many coefficients are 0.
- Similar scores with less features! More interpretable model!

```
pipe_lgr_l1.fit(X_train, y_train)
l1_coefs = pipe_lgr_l1.named_steps["logisticregression"].coef_.flatten()
df["l1_coef"] = l1_coefs
df
```

	l2_coefs	l1_coef
mean radius	-0.542448	0.000000
mean texture	-0.252004	0.000000
mean perimeter	-0.496523	0.000000
mean area	-0.608907	0.000000
mean smoothness	-0.170162	0.000000
mean compactness	0.577409	0.000000
mean concavity	-0.659992	0.000000
mean concave points	-0.980380	-1.358428
mean symmetry	0.117937	0.000000
mean fractal dimension	0.402504	0.279743
radius error	-1.248832	-2.017323
texture error	-0.101663	0.000000
perimeter error	-0.731364	0.000000
area error	-0.927143	0.000000
smoothness error	-0.232258	-0.126395
compactness error	0.618787	0.565532
concavity error	-0.035918	0.000000
concave points error	-0.203528	0.000000
symmetry error	0.270964	0.000000
fractal dimension error	0.739704	0.205400
worst radius	-1.041989	-1.339965
worst texture	-1.097127	-1.371276
worst perimeter	-0.884671	-0.512066
worst area	-1.022599	-3.535834
worst smoothness	-0.925732	-0.982720
worst compactness	-0.071176	0.000000
worst concavity	-0.767299	-1.026726

	l2_coefs	l1_coef
worst concave points	-0.738242	-0.636031
worst symmetry	-0.667742	-0.302229
worst fractal dimension	-0.523832	0.000000

We can also carry out feature selection using L1 regularization and pass selected features to another model.

```
from lightgbm.sklearn import LGBMClassifier

pipe_lgr_lgbm = make_pipeline(
    StandardScaler(),
    SelectFromModel(LogisticRegression(solver="liblinear", penalty="l1")),
    LGBMClassifier(),
)
```

```
results_classification["L1 + LGBM"] = mean_std_cross_val_scores(
    pipe_lgr_lgbm,
    X_train,
    y_train,
    return_train_score=True,
    scoring=scoring_metric,
)
pd.DataFrame(results_classification)
```

```
[LightGBM] [Info] Number of positive: 230, number of negative: 134
[LightGBM] [Info] Auto-choosing col-wise multi-threading, the overhead of test
You can set `force_col_wise=true` to remove the overhead.
[LightGBM] [Info] Total Bins 1460
[LightGBM] [Info] Number of data points in the train set: 364, number of used
[LightGBM] [Info] [binary:BoostFromScore]: pavg=0.631868 -> initscore=0.540240
[LightGBM] [Info] Start training from score 0.540240
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
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[LightGBM] [Info] Number of positive: 230, number of negative: 134
[LightGBM] [Info] Auto-choosing col-wise multi-threading, the overhead of test:
You can set `force_col_wise=true` to remove the overhead.
[LightGBM] [Info] Total Bins 1695
```

```
[LightGBM] [Info] Number of data points in the train set: 364, number of used
[LightGBM] [Info] [binary:BoostFromScore]: pavg=0.631868 -> initscore=0.540240
[LightGBM] [Info] Start training from score 0.540240
[LightGBM] [Warning] No further splits with positive gain, best gain: -inf
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[LightGBM] [Info] Number of positive: 230, number of negative: 134
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You can set `force_col_wise=true` to remove the overhead.
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[LightGBM] [Info] Total Bins 1460
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```
/home/joel/proj/mds/DSCI_573_feat-model-select_instructors/lectures/code/./uti
  out_col.append((f"%0.3f (+/- %0.3f)" % (mean_scores[i], std_scores[i])))
```

	dummy	Logistic Regression L2	Logistic Regression L1	L1 + LGBM
fit_time	0.001 (+/- 0.000)	0.004 (+/- 0.001)	0.004 (+/- 0.001)	0.037 (+/- 0.009)
score_time	0.001 (+/- 0.000)	0.002 (+/- 0.000)	0.002 (+/- 0.000)	0.004 (+/- 0.000)
test_score	0.000 (+/- 0.000)	0.970 (+/- 0.011)	0.970 (+/- 0.001)	0.961 (+/- 0.037)
train_score	0.000 (+/- 0.000)	0.985 (+/- 0.005)	0.985 (+/- 0.005)	1.000 (+/- 0.000)

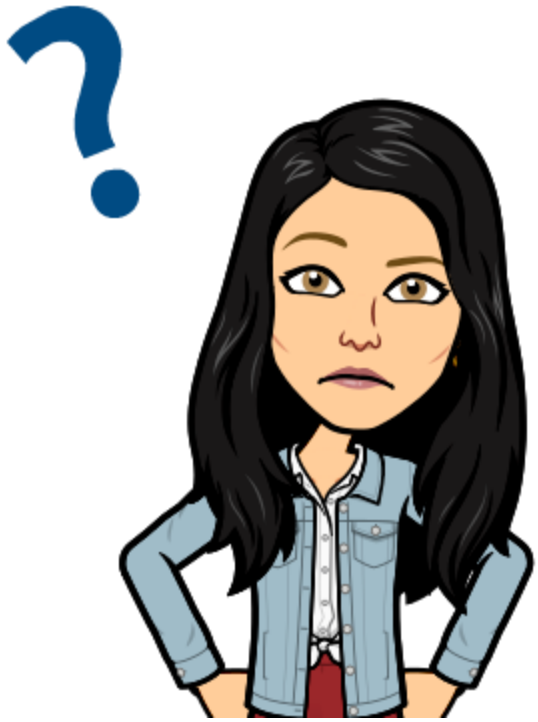
- The score went down a bit this case. But this might help in some other cases.
- The resulting model is using L1 selected features only.

How to use regularization with `scikit-learn`: some examples

- Regression
  - Least squares with L2-regularization: Ridge
  - Least squares with L1-regularization: Lasso
  - Least squares with L1- and L2-regularization: ElasticNet
  - SVR (ϵ-insensitive loss function)
    - `epsilon = 0` gives us `KernelRidge` model (least squares with RBF)
- Classification
  - SVC (supports L2-regularization)
  - LogisticRegression (support L1 and L2 with different solvers)

> penalty{'l1', 'l2', 'elasticnet', 'none'}, default='l2' Used to specify the norm used in the penalization. The 'newton-cg', 'sag' and 'lbfgs' solvers support only l2 penalties. 'elasticnet' is only supported by the 'saga' solver. If 'none' (not supported by the liblinear solver), no regularization is applied.

- Interpretations of coefficients of regularized linear models should always be taken with a grain of salt.
- With different values of the regularization parameter, sometimes even the signs of the coefficients might change!!



Regularization: scaling and collinearity

Regularization and scaling

- It doesn't matter for decision trees or naive Bayes.
  - They only look at one feature at a time.
- It doesn't matter for least squares:
  - $w_j * (100mL)$ gives the same model as $w_j * (0.1L)$ with a different w_j
- It matters for k-nearest neighbours:
  - Distance will be affected more by large features than small features.
- **It matters for regularized least squares**:
  - Penalizing w_j^2 means different things if features j are on different scales
  - Penalizing w_j means different things if features j are on different scales

Collinearity and regularization

- If you have colinear features, the weights would go crazy with regular linear regression.
- With L2 regularization: The weight will be equally distributed among all collinear features because the solution is unique.
  - Example: suppose we have three identical features with a total weight of 1
  - The weight will be distributed as 1/3, 1/3, 1/3 among the features.
- With L1 regularization: The weight will not be equally distributed; the solution is not unique.
  - Example: suppose we have three identical features with a total weight of 1
  - The weight could be distributed in many different ways
  - For example, 1/2, 1/4, 1/4 or 1.0, 0, 0 or 1/2, 1/2, 0 and so on ...

Elastic nets

- Combine good properties from both worlds

$$J(w) = \|y - Xw\|_2^2 + \lambda(l_1 ratio\|w\|_1 + (1 - l_1 ratio)\|w\|_2^2)$$

- λ control the strength of regularization
- $l_1 ratio$ controls the amount of sparsity and smoothness
- L1 promotes sparsity and the L2 promotes smoothness.
- The functional is strictly convex: the solution is unique.
- No collinearity problem
  - A whole group of correlated variables is selected rather than just one variable in the group.

You can use elastic nets using sklearn's ElasticNet.

Summary: L* regularization

- L0-regularization (AIC, BIC, Mallow's Cp, Adjusted R2, ANOVA): More on this is DSCi 562
  - Adds penalty on the number of non-zeros to select features.

$$J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_0$$

- L2-regularization (ridge regression):
  - Adding penalty on the L2-norm of w to decrease overfitting: $ $J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_2^2$$
- L1-regularization (lasso regression):
  - Adding penalty on the L1-norm decreases overfitting and selects features: $ $J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_1$$
- Interpretations of coefficients of linear models should always be taken with a grain of salt
  - Regularizing a model might change the sign of the coefficients.
- Un-regularized linear regression: not affected by scaling
- L1 or L2-regularized linear regression: both affected by scaling (and it's usually a good idea)