W4995 Applied Machine Learning

Linear models for Regression

02/01/17

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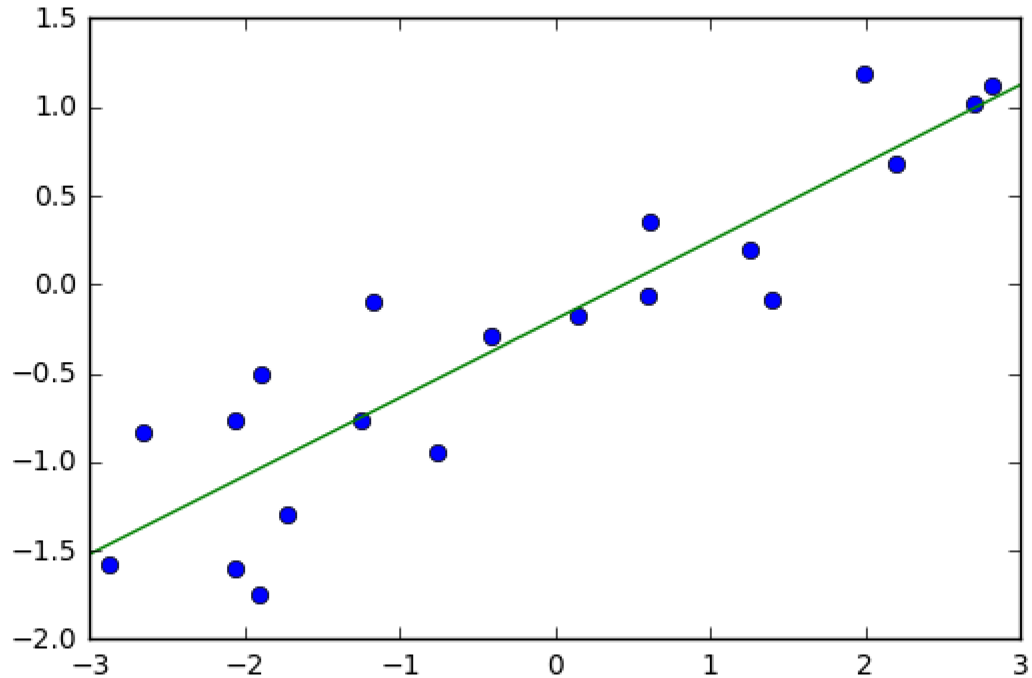
Linear Models for Regression



$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^{p} w_i x_i + b$$

Linear Regression
Ordinary Least Squares

$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^{p} w_i x_i + b$$

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^{p} ||w^T \mathbf{x}_i - y_i||^2$$

Unique solution if $\mathbf{X} = (\mathbf{x}_1, ...\mathbf{x}_n)^T$ has full rank.

Ridge Regression

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^{n} ||w^T x_i - y_i||^2 + \alpha ||w||^2$$

Always has a unique solution.
Has tuning parameter alpha

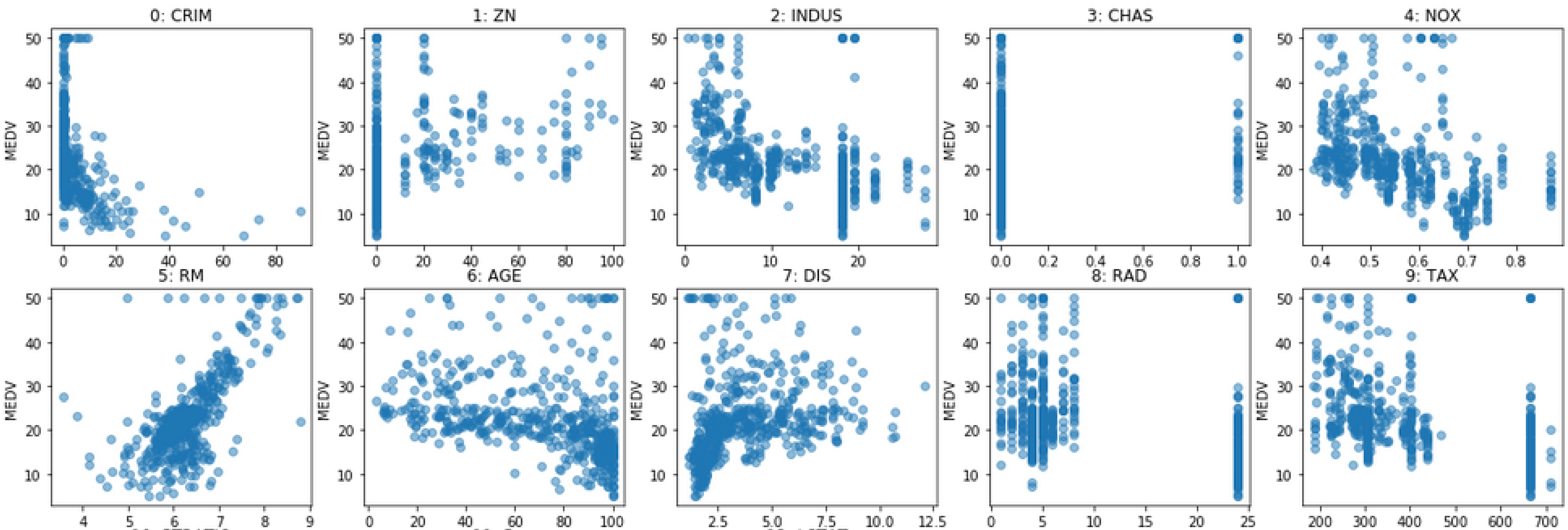
(regularized) Empirical Risk Minimization

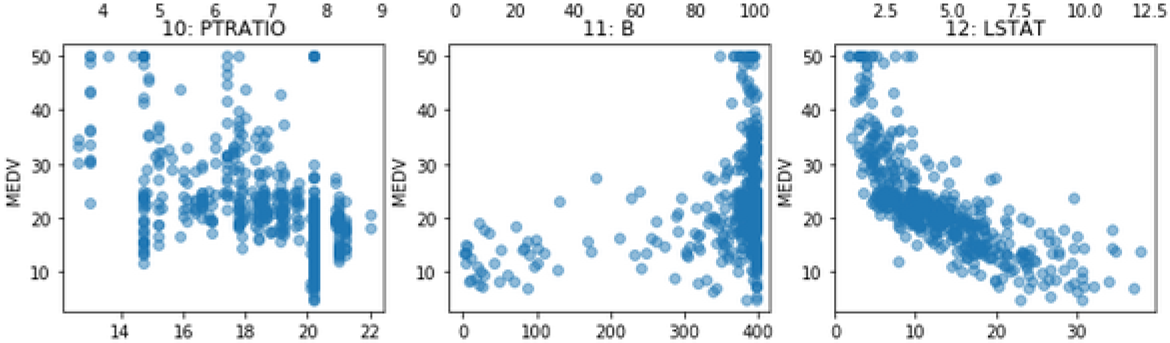
$$min_{f \in F} \sum_{i=1}^{n} L(f(\mathbf{x}_i), y_i) + \alpha R(f)$$

Data fitting

Regularization

Boston Housing Dataset






```
print(X.shape)
print(y.shape)
```

```
(506, 13)
(506,)
```

```python
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
```

```python
np.mean(cross_val_score(LinearRegression(), X_train, y_train, cv=5))
```

```
0.69844164175864798
```

```python
np.mean(cross_val_score(Ridge(), X_train, y_train, cv=5))
```

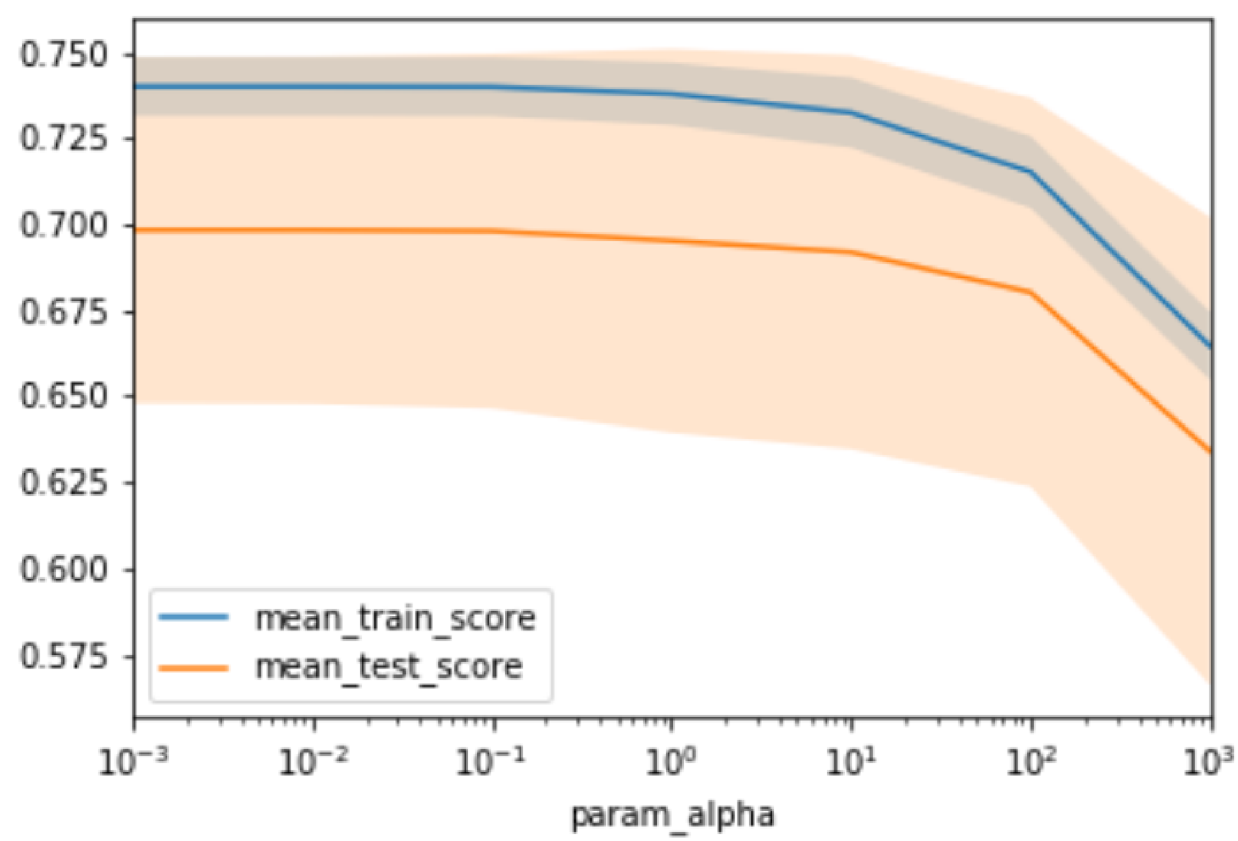
```
0.69530615273465046
```

Score is always R^2 for regression!

```python
from sklearn.model_selection import GridSearchCV
param_grid = {'alpha': np.logspace(-3, 3, 7)}
print(param_grid)
```

```
{'alpha': array([  1.00000000e-03,   1.00000000e-02,   1.00000000e-01,
         1.00000000e+00,   1.00000000e+01,   1.00000000e+02,
         1.00000000e+03])}
```

```python
grid = GridSearchCV(Ridge(), param_grid, cv=5)
grid.fit(X_train, y_train)
```



Adding features

```
from sklearn.preprocessing import PolynomialFeatures, scale
X_poly = PolynomialFeatures(include_bias=False).fit_transform(scale(X))
print(X_poly.shape)
X_train, X_test, y_train, y_test = train_test_split(X_poly, y, random_state=42)
```

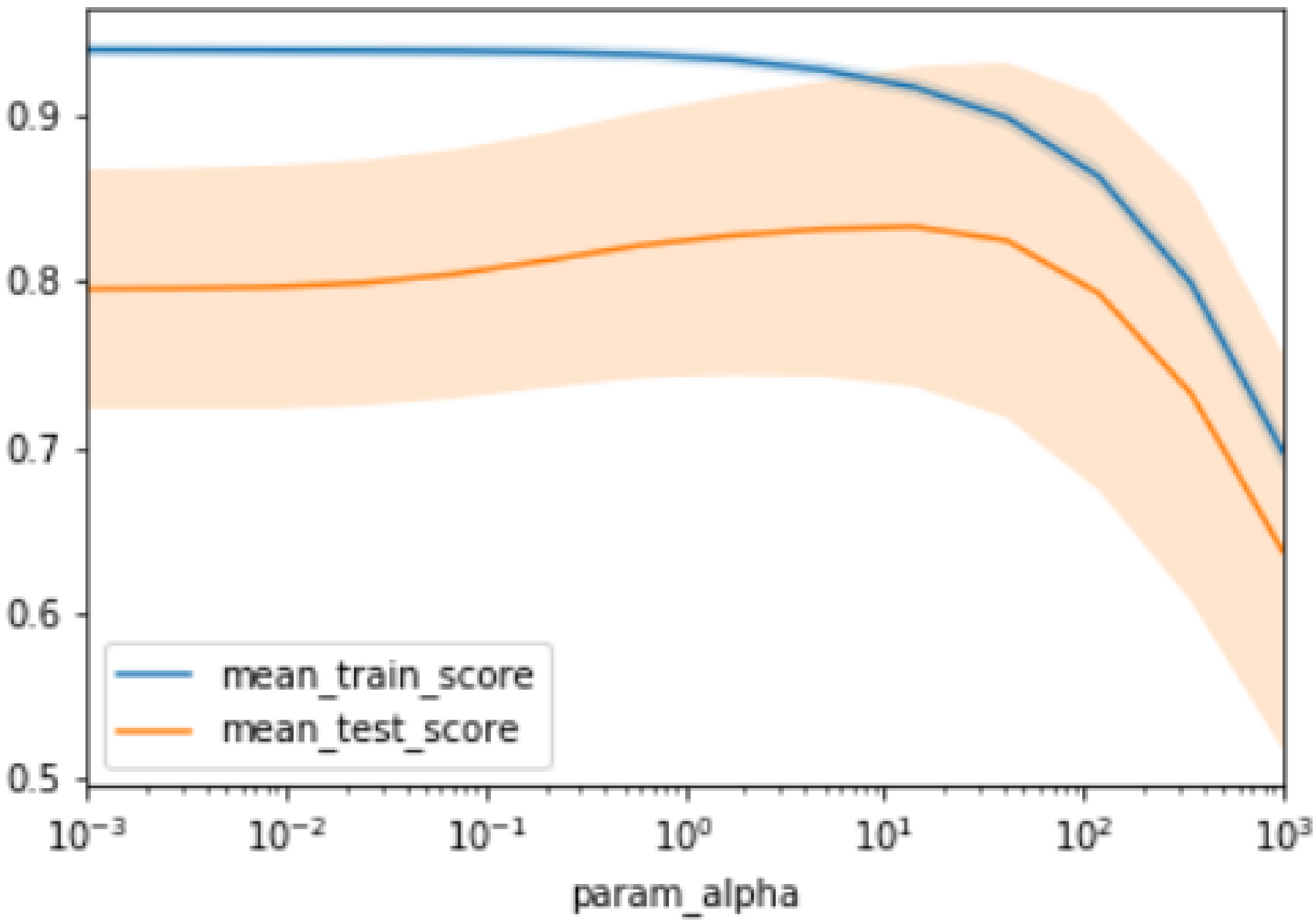
```
(506, 104)
```

```
np.mean(cross_val_score(LinearRegression(), X_train, y_train, cv=10))
```

```
0.79424725375805638
```

```
np.mean(cross_val_score(Ridge(), X_train, y_train, cv=10))
```

```
0.82530611400699261
```

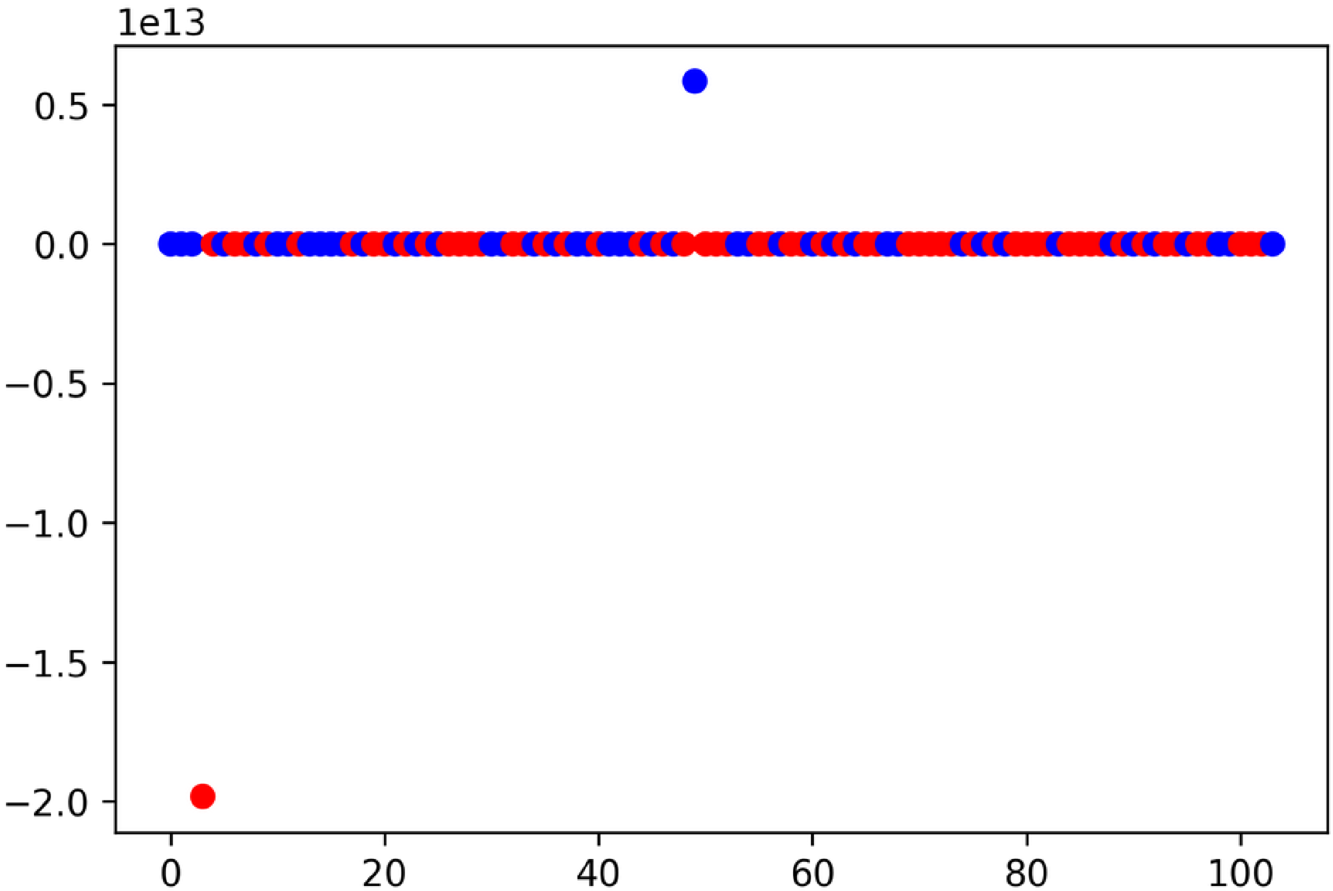



```
print(grid.best_params_)
print(grid.best_score_)
```

```
{'alpha': 14.251026703029993}
0.833124993262
```

Plotting coefficient values (LR)

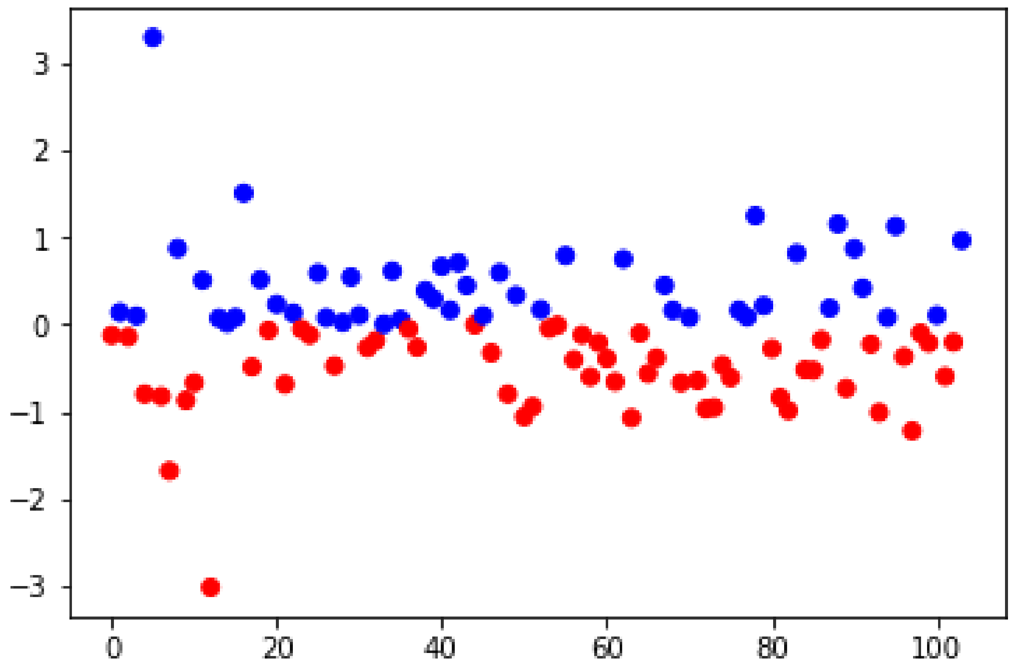
```
lr = LinearRegression().fit(X_train, y_train)
plt.scatter(range(X_poly.shape[1]), lr.coef_, c=np.sign(lr.coef_), cmap="bwr_r")
```



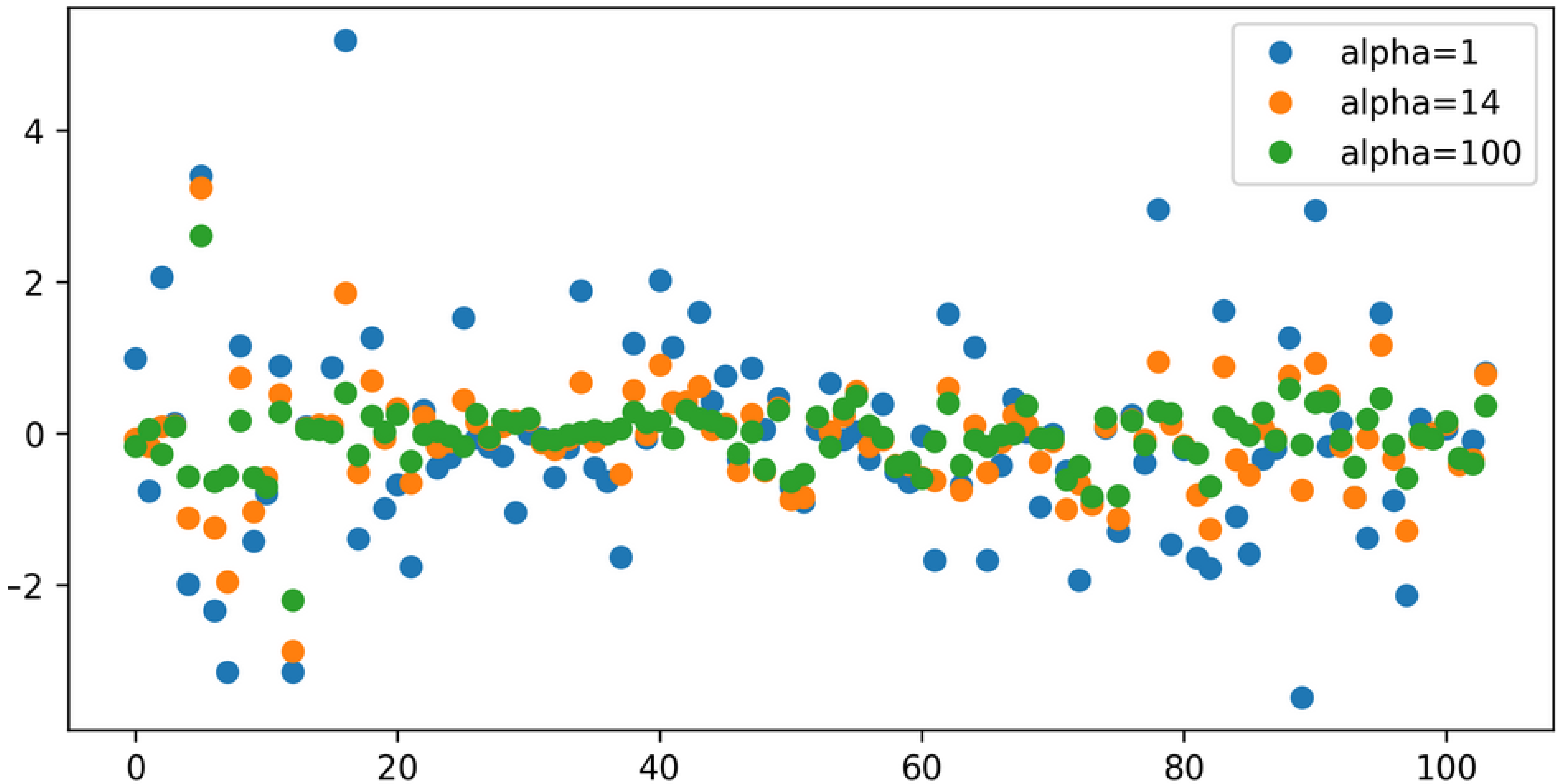
Ridge Coefficients

```
ridge = grid.best_estimator_
plt.scatter(range(X_poly.shape[1]), ridge.coef_, c=np.sign(ridge.coef_), cmap="bwr_r")
```

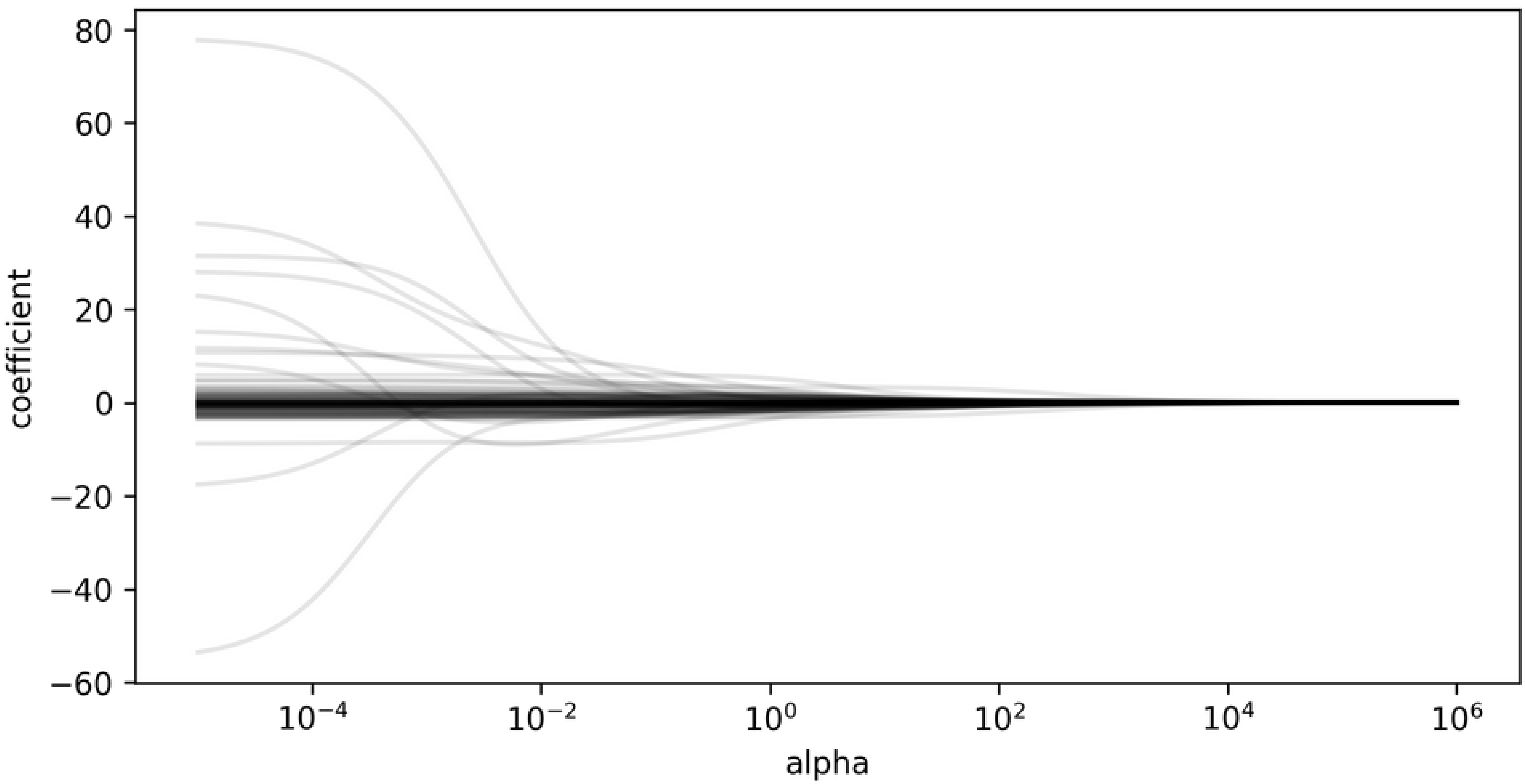
```
<matplotlib.collections.PathCollection at 0x7fda1025c780>
```



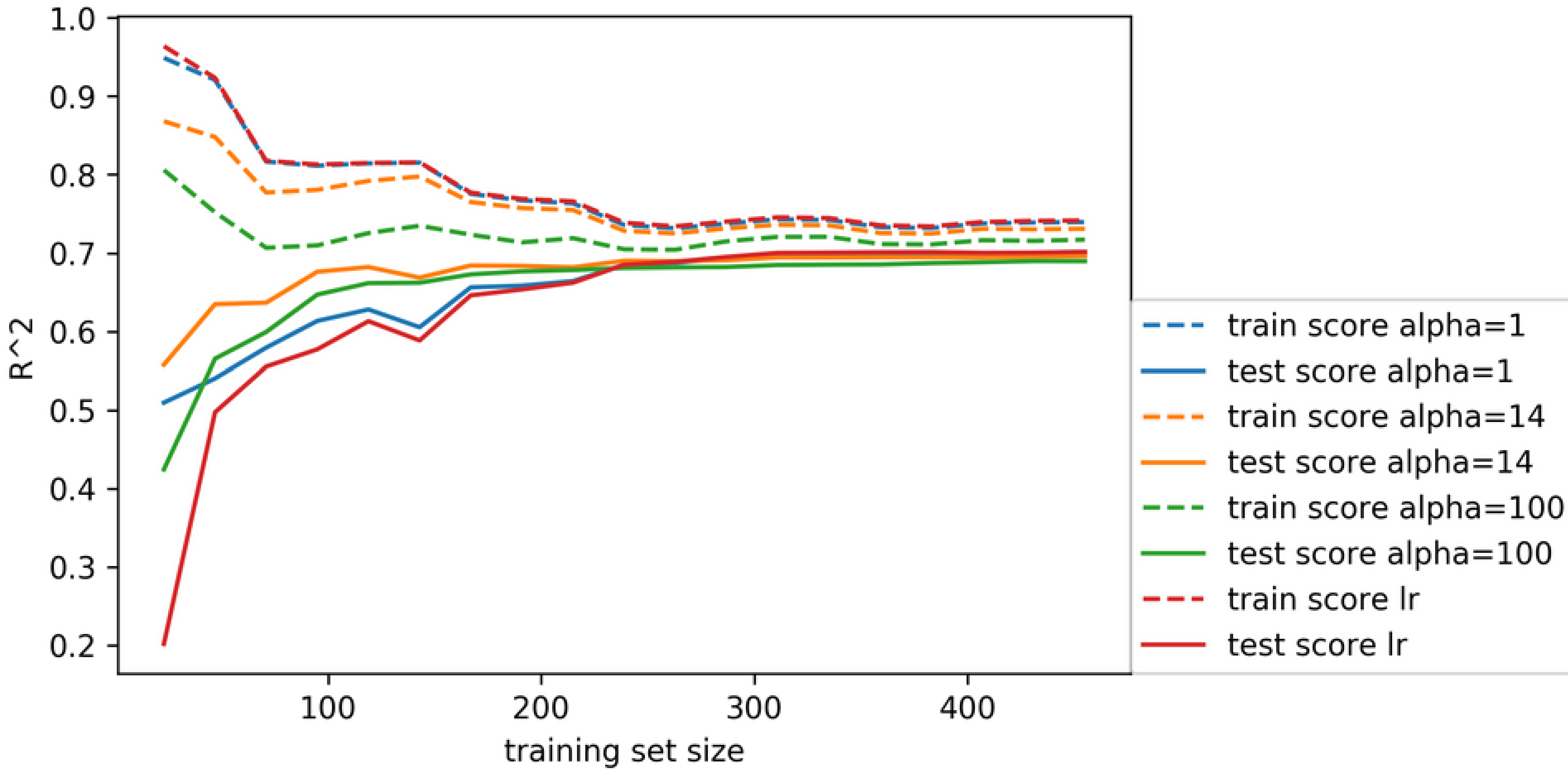
```
ridge100 = Ridge(alpha=100).fit(X_train, y_train)
ridge1 = Ridge(alpha=1).fit(X_train, y_train)
plt.figure(figsize=(8, 4))

plt.plot(ridge1.coef_, 'o', label="alpha=1")
plt.plot(ridge.coef_, 'o', label="alpha=14")
plt.plot(ridge100.coef_, 'o', label="alpha=100")
plt.legend()
```



Coefficient Paths



Learning Curve



Lasso Regression

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^{n} ||w^T \mathbf{x}_i - y_i||^2 + \alpha ||w||_1$$

Shrinks w towards zero like Ridge
Sets some w exactly to zero - automatic feature selection!

Grid-Search for Lasso

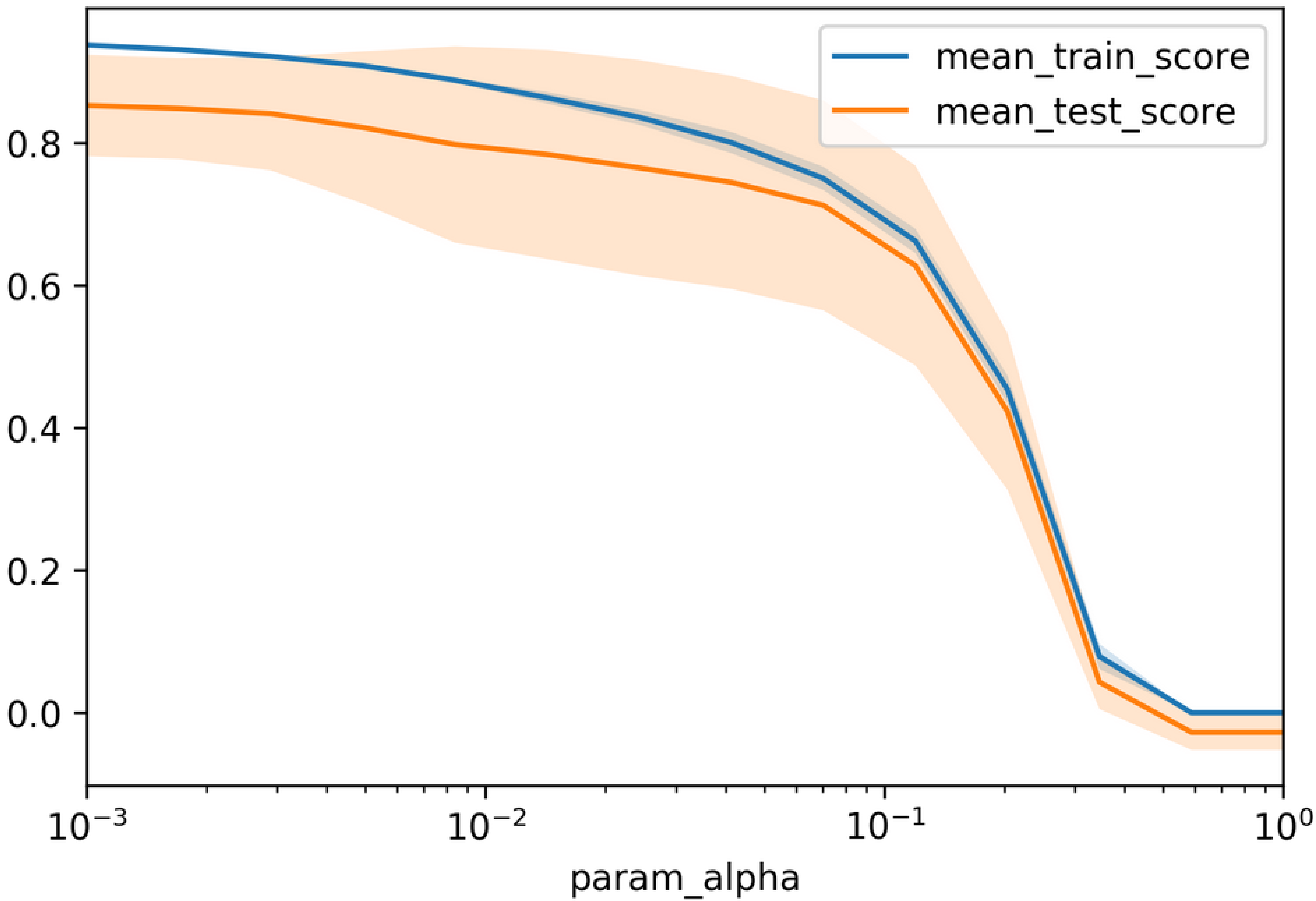
```
param_grid = {'alpha': np.logspace(-3, 0, 14)}
print(param_grid)
```

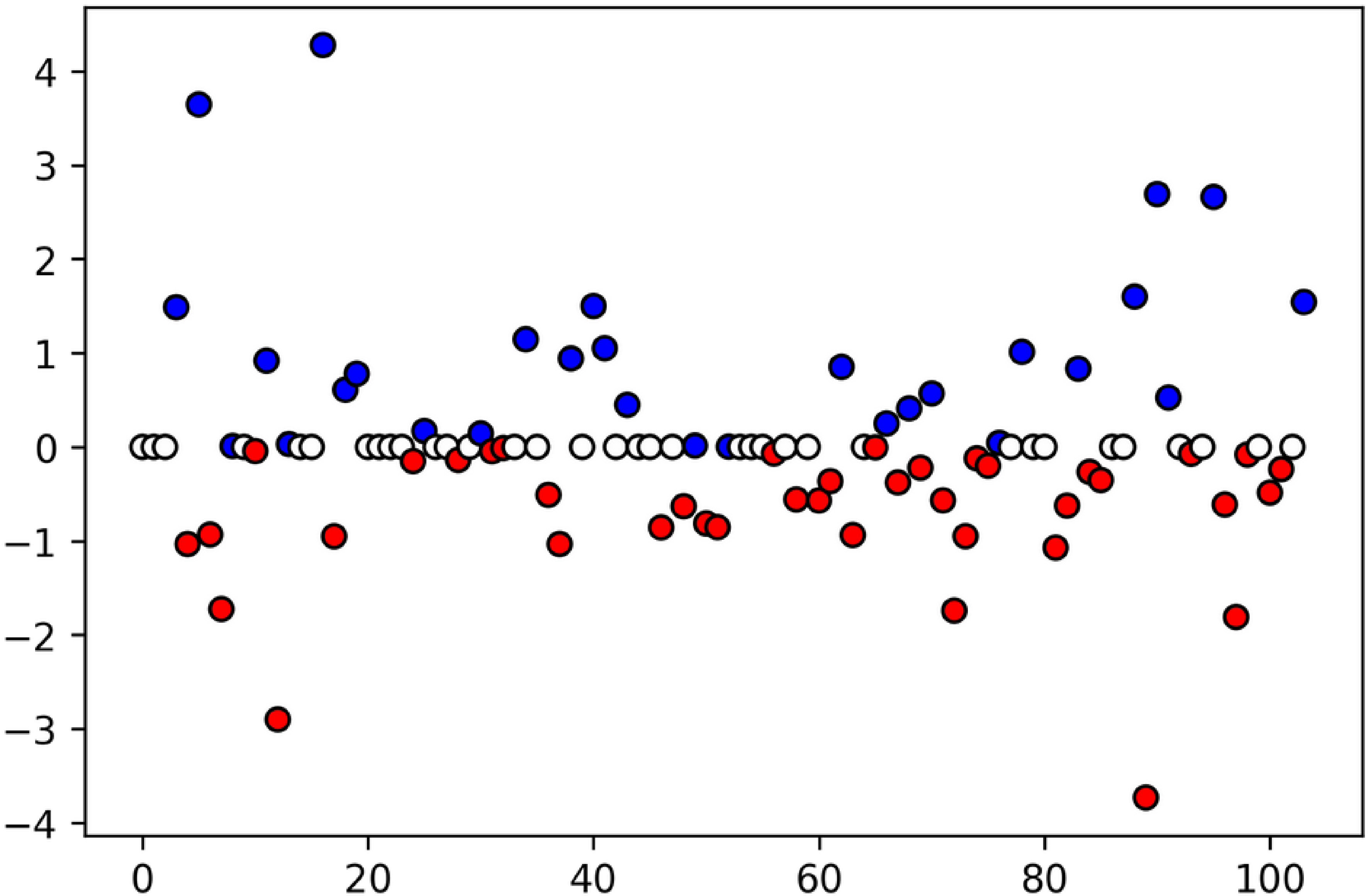
```
{'alpha': array([ 0.001     ,  0.00170125,  0.00289427,  0.00492388,  0.00837678,
        0.01425103,  0.02424462,  0.04124626,  0.07017038,  0.11937766,
        0.20309176,  0.34551073,  0.58780161,  1.        ])}
```

```
grid = GridSearchCV(Lasso(normalize=True, max_iter=1e6), param_grid, cv=10)
grid.fit(X_train, y_train)
```

```
print(grid.best_params_)
print(grid.best_score_)
```

```
{'alpha': 0.001}
0.852388809881
```


mean_train_score
mean_test_score
0.8
0.6
0.4
0.2
0.0
10^{-3}
10^{-2}
10^{-1}
10^{0}
param_alpha



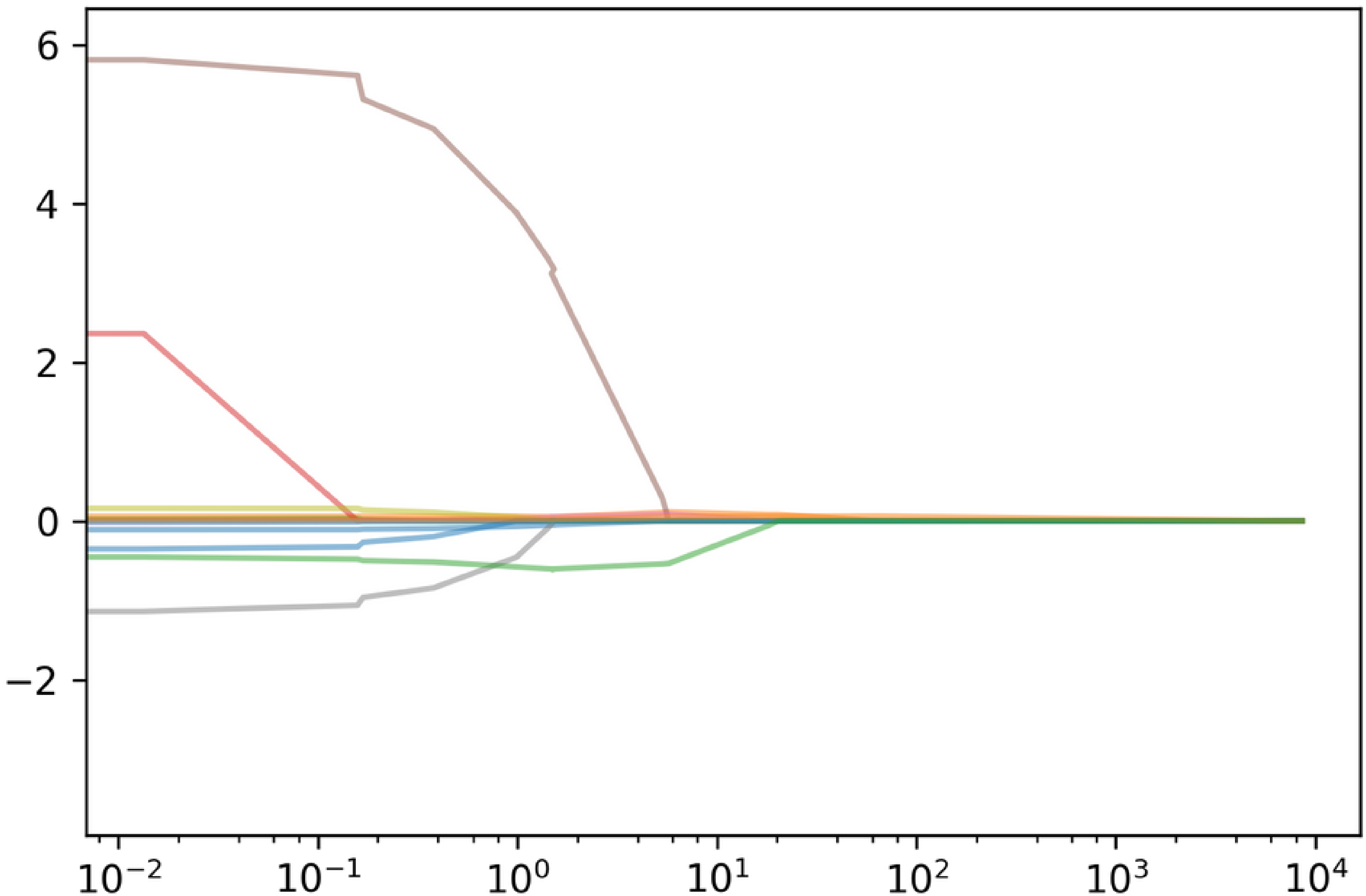
In [31]:
```
print(X_poly.shape)
np.sum(lasso.coef_ != 0)
```

```
(506, 104)
```

Out[31]: 69

```python
from sklearn.linear_model import lars_path
# lars_path computes the exact regularization path which is piecewise linear.
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
alphas, active, coefs = lars_path(X_train, y_train, eps=0.00001)
```

```python
plt.plot(alphas, coefs.T, alpha=.5)
plt.xscale("log")
```

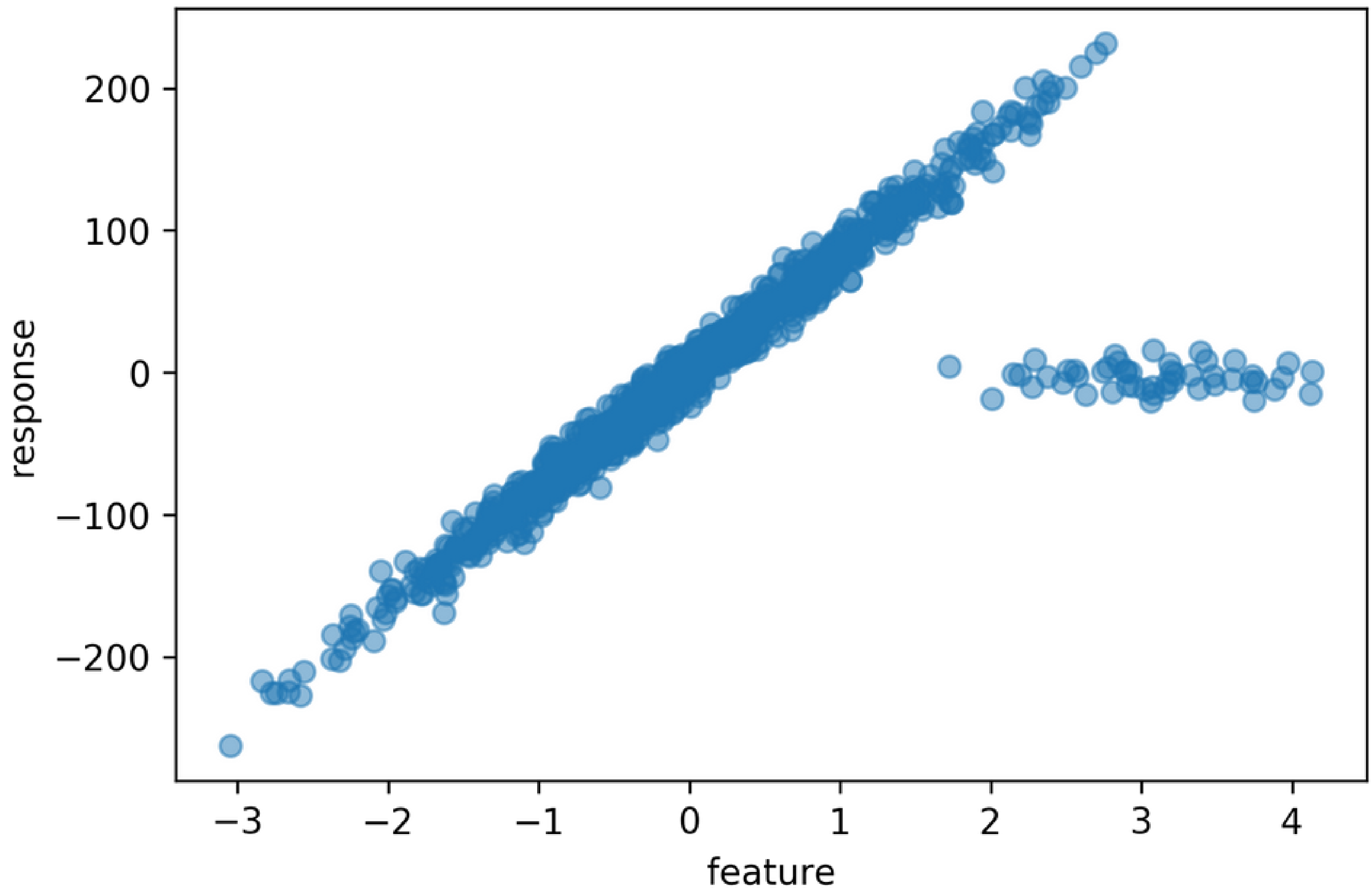


Elastic Net

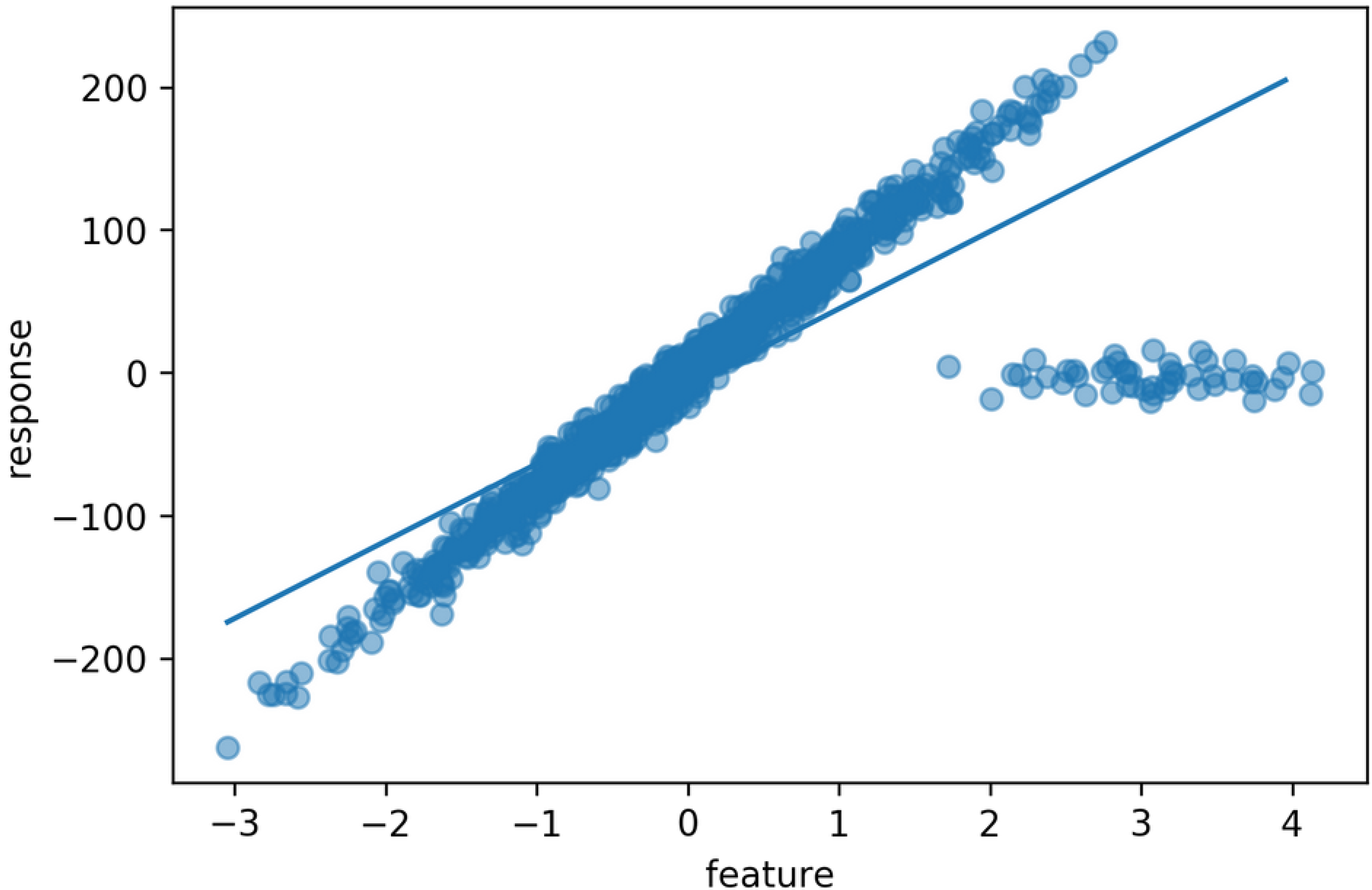
- Combines benefits of Ridge and Lasso
- two parameters to tune.

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^{n} ||w^T \mathbf{x}_i - y_i||^2 + \alpha_1 ||w||_1 + \alpha_2 ||w||_2^2$$

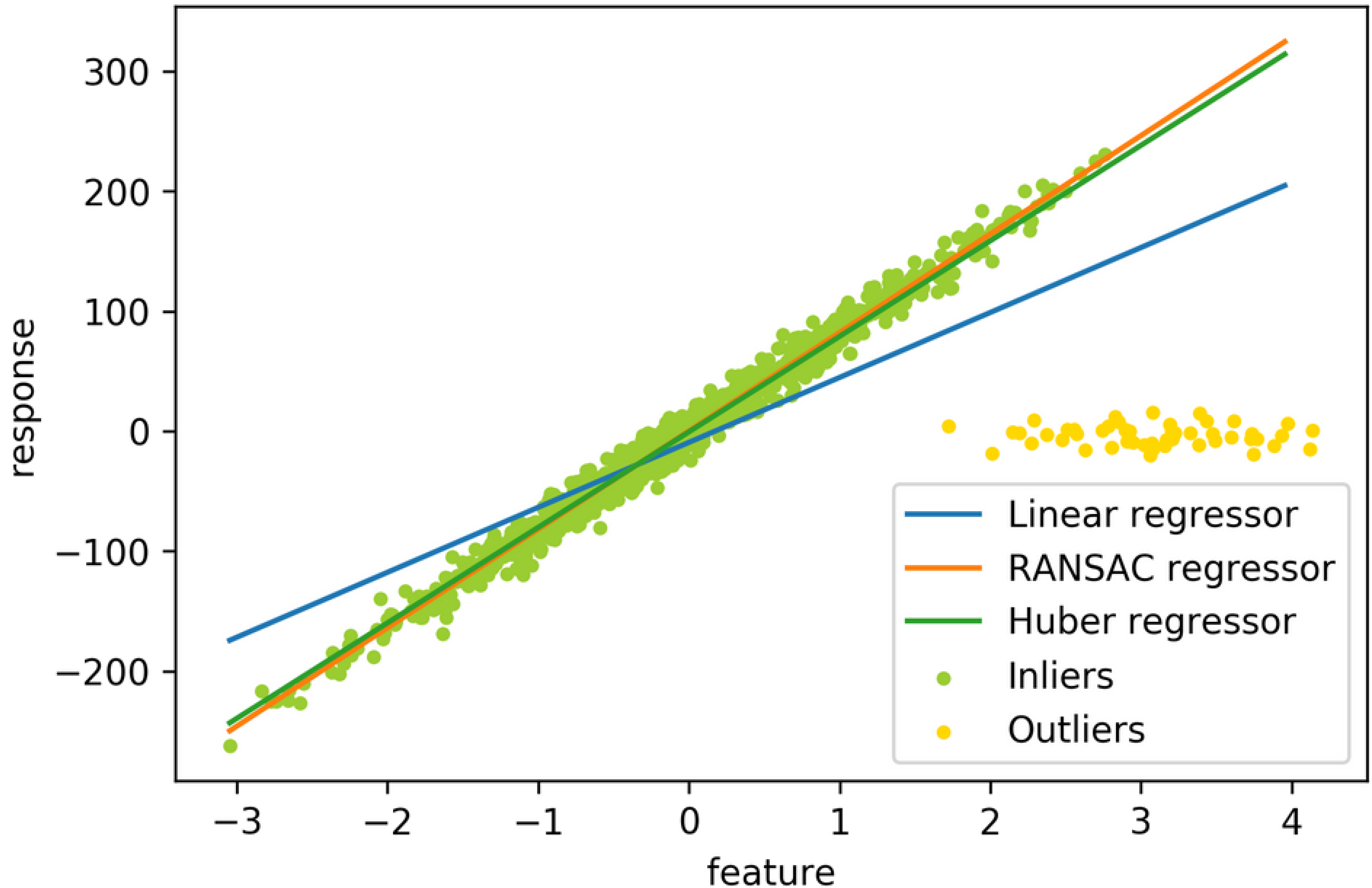
Robust Regression
RANSAC and Huber



Least Squares Fit to Outlier Data



Robust Fit

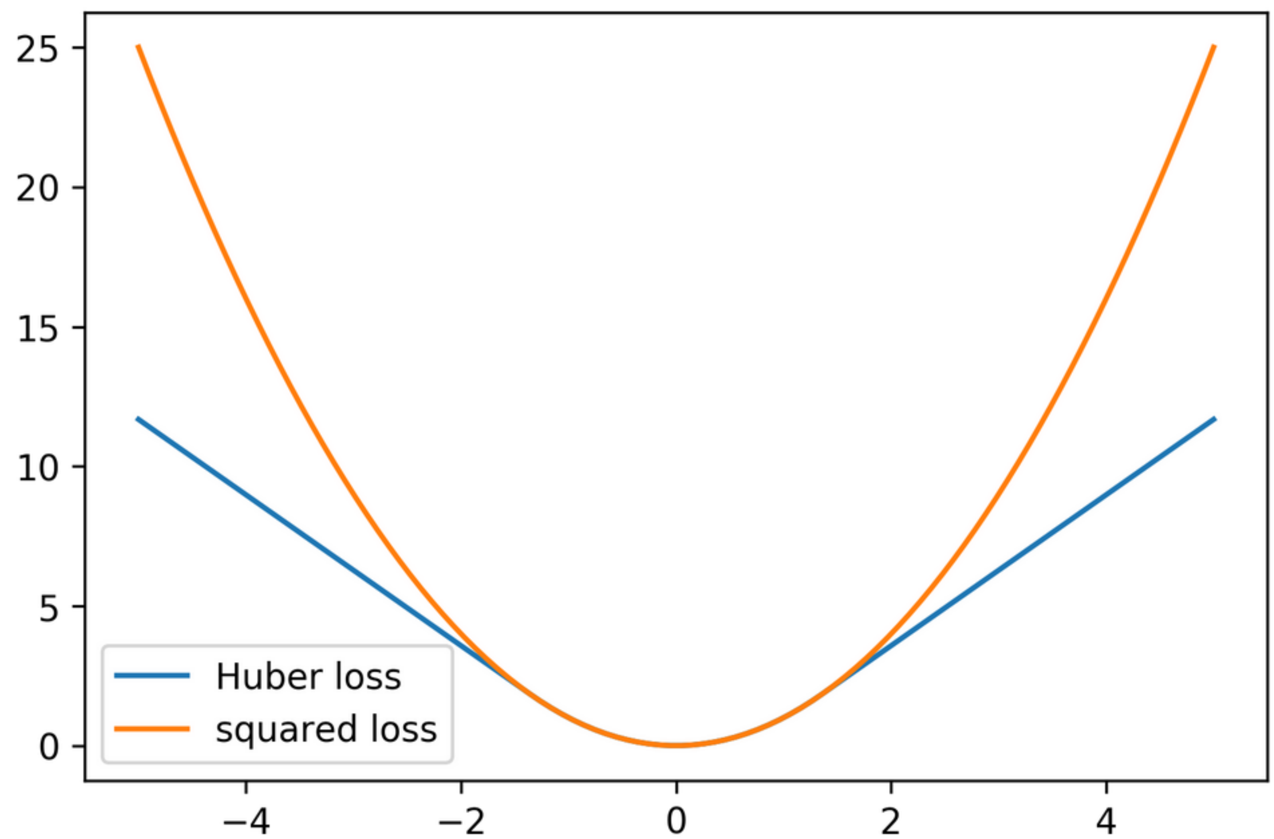


300
200
100
0
−100
−200
response
−3
−2
−1
0
1
2
3
4
feature
Linear regressor
RANSAC regressor
Huber regressor
Inliers
Outliers

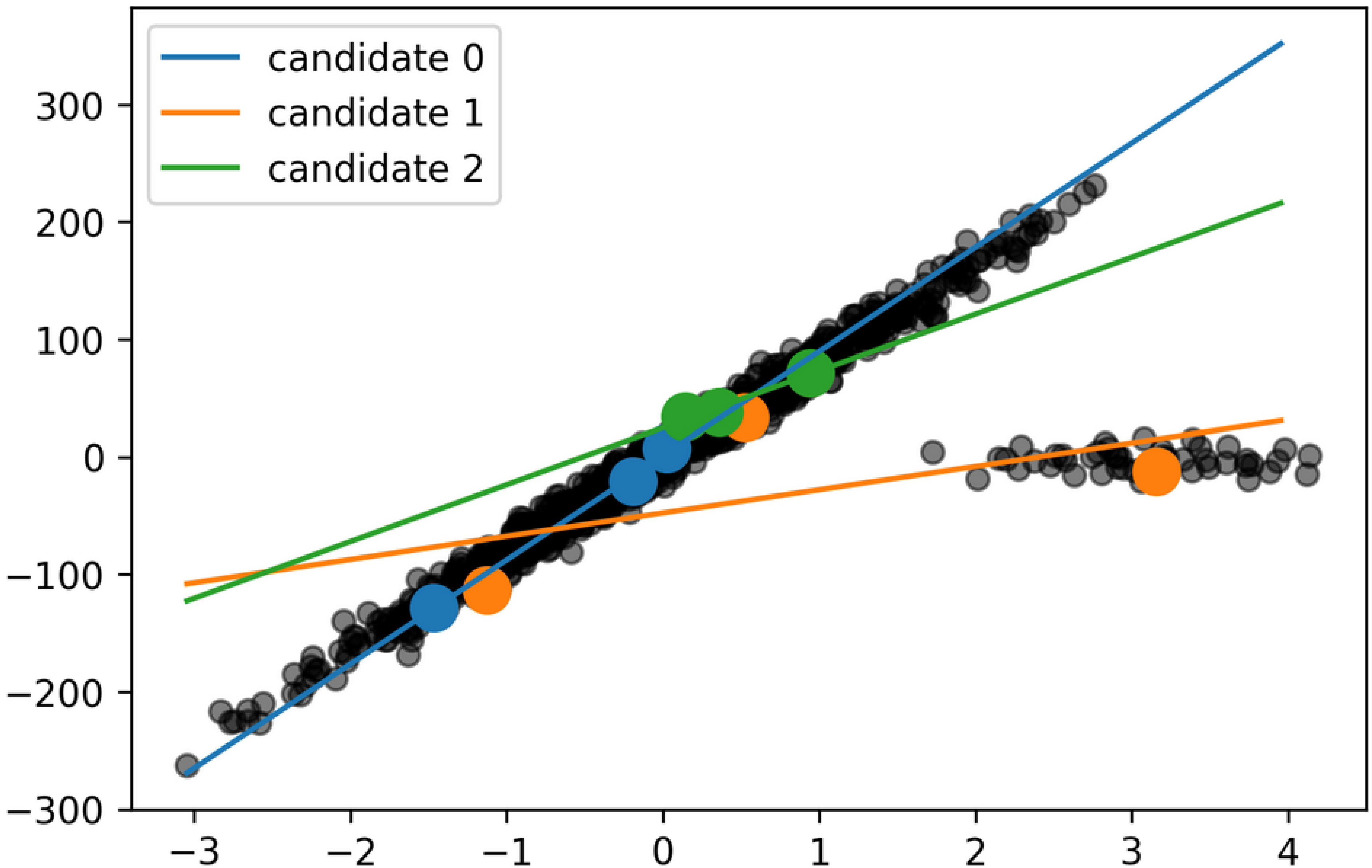
$$\min_{w,\sigma} \sum_{i=1}^{n} \left(\sigma + H_m\left(\frac{X_i w - y_i}{\sigma} \right) \sigma \right) + \alpha {||w||_2}^2$$

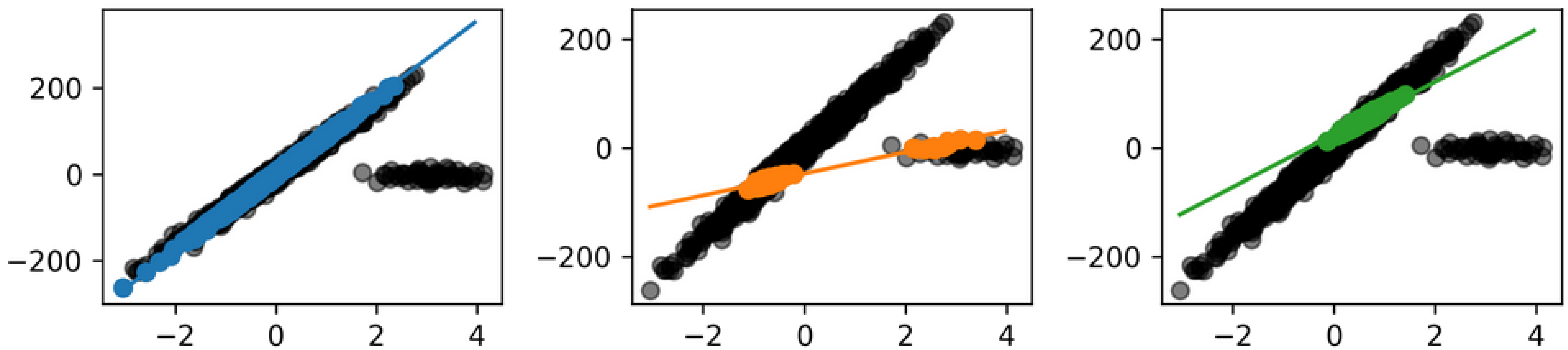
Huber Loss

$$H_m(z) = \begin{cases} z^2, & \text{if } |z| < \epsilon, \\ 2\epsilon|z| - \epsilon^2, & \text{otherwise} \end{cases}$$



RANSAC


candidate 0
candidate 1
candidate 2
300
200
100
0
−100
−200
−300
−3
−2
−1
0
1
2
3
4


200
0
−200
−2
0
2
4