Machine Learning in Practise

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Resampling: Bootstrapping

- In practice (unlike in theory), we have only ONE training set S.
- We can simulate multiple training sets by bootstrap replicates
  - S' = {x | x is drawn at random with replacement from S} and |S'| = |S|

Original	Bootstrap1	Bootstrap2	Bootstrap3	Bootstrap4
1	1	2	1	1
2	1	3	2	1
3	3	3	3	1
4	3	3	5	4
5	5	4	5	5

Bootstrapping Sample: Example

- Numerical: $X = \{10, 27, 31, 40, 46\}$
- Calculate bootstrap samples
- Are these valid bootstrap samples?
  - $X_1 = \{10, 10, 31, 31, 46\}$?
  - $X_2 = \{10, 27, 31, 10\}$?
  - $X_3 = \{31, 31, 31, 31\}$?
  - $X_4 = \{31, 31, 31, 31, 31\}$?

Procedure: Measuring Bias and Variance

- Construct B bootstrap replicates of S (e.g., Construct B bootstrap replicates of S (e.g., b = 200): $S_1, \ldots, S_B$
- Apply learning algorithm to each replicate S_b to obtain hypothesis h_b
- Let $T = S \setminus S_b$ be the data points that do not appear in any $S_1..S_B$ (out of bag points).
- Compute predicted value $h_b(x)$ for each x in T
- Alternately, set T could also be a hold out set created from S before constructing bootstrap samples
- For each data point x in T, we will now have the observed corresponding value y and several predictions $y_1, \ldots, y_B$

Procedure: Measuring Bias and Variance

- Compute the average prediction $\underline{h}$.
  - $\underline{h} = \Sigma_b h_b(x)/B$
- Estimate bias as $(\underline{h} - y)$
- Estimate variance as
  - $\Sigma_b (y_b - \underline{h})^2/(B - 1)$
- Assume noise is 0
- Assumptions:
  - Bootstrap replicates are not real data
  - We ignore the noise

Practice Question

Given data points: {76,60,82,12,38,73,82,17}, construct **8** bootstrap samples. Report the standard error between the true mean and the average of means of bootstrapped samples.

Linear Regression Revisited

- Objective Function: An optimization problem

$$\underset{\theta}{\text{minimize}} \quad J(\theta)$$

- Minimize sum of costs over all input/output pairs

$$J(\Theta) = 1/M \sum_{i=1}^{M} (\Theta^T \Phi(x_i) - y_i)^2 \qquad \frac{1}{M} \sum_{i=1}^{M} \left[\sum_{j=0}^{p} \theta_j x_j^{(i)} - y^{(i)} \right]$$

- Gradient Descent

$$\theta_j = \theta_j - \alpha \frac{\partial J(\theta)}{\partial \theta_j}, \text{ for all } j$$

Regularization

- To overcome underfitting:
  - Add new parameters to our model
  - Increase the model complexity
- To overcome overfitting:
  - Reduce the model complexity
  - Regularization/shrinkage
    - Change the error function to penalize hypothesis complexity

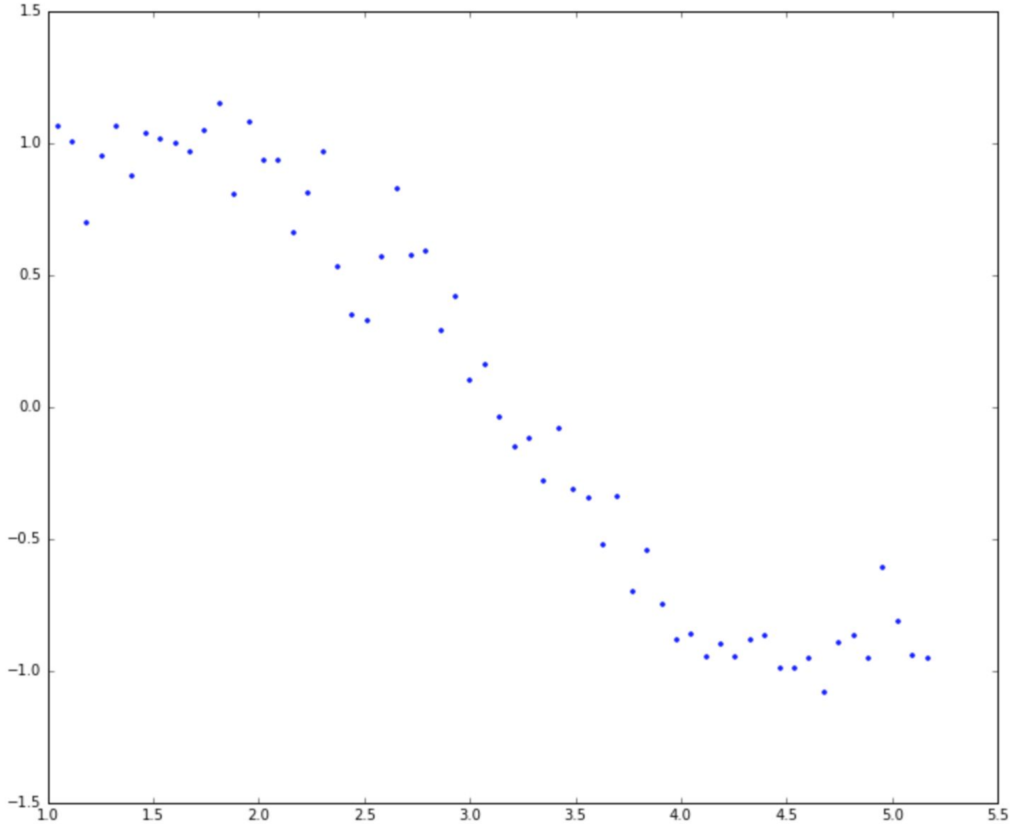
$$J(\Theta) = J_w(\Theta) + \lambda J_{pen}(\Theta)$$

Regularization

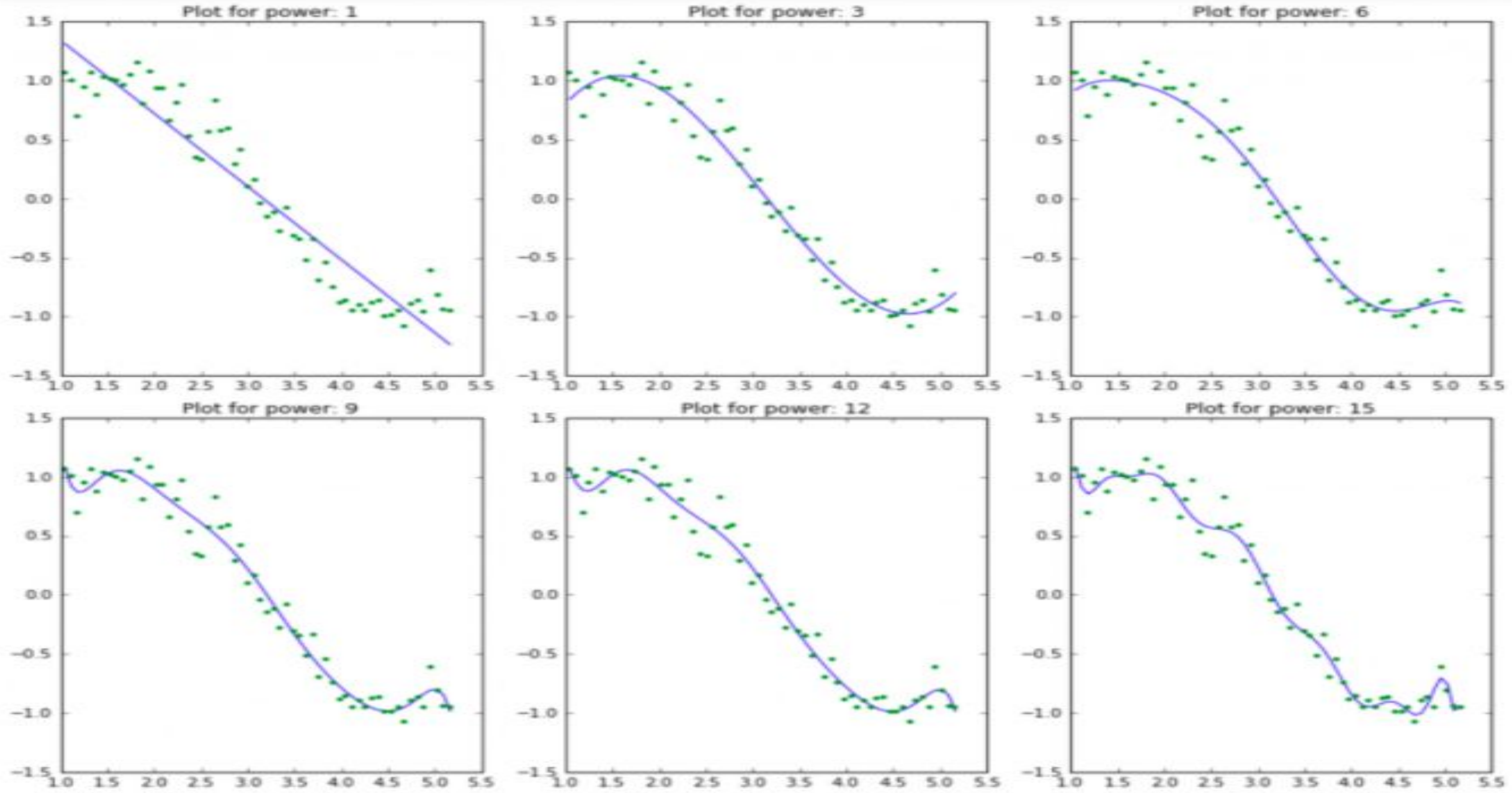
- Regularization constraints or regularizes the coefficient estimates
  - shrinks the coefficient estimates towards zero

- Shrinking the coefficient estimates can significantly reduce their variance.

SINE Curve: Noisy Data



Regression – Without any penalisation



Coefficients increase exponentially

	rss	intercept	coef_x_1	coef_x_2	coef_x_3	coef_x_4	coef_x_5	coef_x_6	coef_x_7	coef_x_8	coef_x_9	coef_x_10	coef_x_11	c
model_pow_1	3.3	2	-0.62	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	N
model_pow_2	3.3	1.9	-0.58	-0.006	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	N
model_pow_3	1.1	-1.1	3	-1.3	0.14	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	N
model_pow_4	1.1	-0.27	1.7	-0.53	-0.036	0.014	NaN	NaN	NaN	NaN	NaN	NaN	NaN	N
model_pow_5	1	3	-5.1	4.7	-1.9	0.33	-0.021	NaN	NaN	NaN	NaN	NaN	NaN	N
model_pow_6	0.99	-2.8	9.5	-9.7	5.2	-1.6	0.23	-0.014	NaN	NaN	NaN	NaN	NaN	N
model_pow_7	0.93	19	-56	69	-45	17	-3.5	0.4	-0.019	NaN	NaN	NaN	NaN	N
model_pow_8	0.92	43	-1.4e+02	1.8e+02	-1.3e+02	58	-15	2.4	-0.21	0.0077	NaN	NaN	NaN	N
model_pow_9	0.87	1.7e+02	-6.1e+02	9.6e+02	-8.5e+02	4.6e+02	-1.6e+02	37	-5.2	0.42	-0.015	NaN	NaN	N
model_pow_10	0.87	1.4e+02	-4.9e+02	7.3e+02	-6e+02	2.9e+02	-87	15	-0.81	-0.14	0.026	-0.0013	NaN	N
model_pow_11	0.87	-75	5.1e+02	-1.3e+03	1.9e+03	-1.6e+03	9.1e+02	-3.5e+02	91	-16	1.8	-0.12	0.0034	N
model_pow_12	0.87	-3.4e+02	1.9e+03	-4.4e+03	6e+03	-5.2e+03	3.1e+03	-1.3e+03	3.8e+02	-80	12	-1.1	0.062	-
model_pow_13	0.86	3.2e+03	-1.8e+04	4.5e+04	-6.7e+04	6.6e+04	-4.6e+04	2.3e+04	-8.5e+03	2.3e+03	-4.5e+02	62	-5.7	0
model_pow_14	0.79	2.4e+04	-1.4e+05	3.8e+05	-6.1e+05	6.6e+05	-5e+05	2.8e+05	-1.2e+05	3.7e+04	-8.5e+03	1.5e+03	-1.8e+02	1
model_pow_15	0.7	-3.6e+04	2.4e+05	-7.5e+05	1.4e+06	-1.7e+06	1.5e+06	-1e+06	5e+05	-1.9e+05	5.4e+04	-1.2e+04	1.9e+03	-

Ridge Regularization

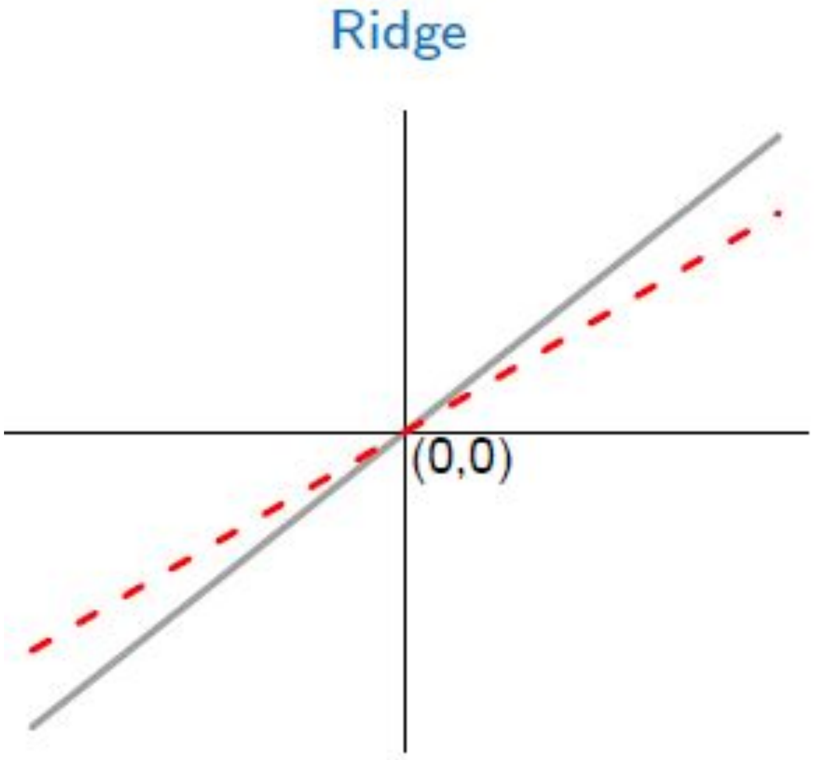
- Minimization objective = LS Obj + λ * (sum of square of slope)

$$J(\Theta) = \frac{1}{M}\sum_{i=1}^{M}(\Theta^T\Phi(x_i) - y_i)^2 + \lambda\sum_{j=1}^{p}\Theta_j^2$$

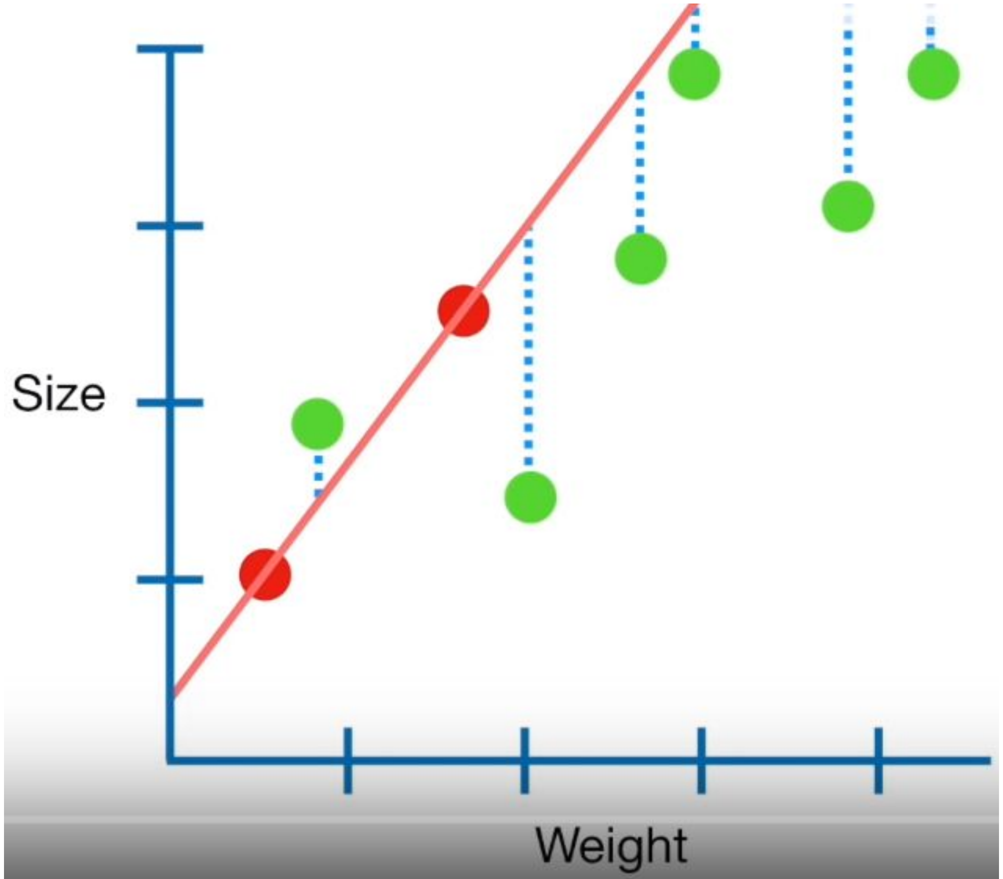
$$\frac{\partial J}{\partial \Theta} = \frac{2}{M}\sum_{i=1}^{M}(\Theta_T\Phi(x_i) - y_i)\Phi(x_i) + 2\lambda\Theta_j$$

$$\Theta_(j+1) = (1 - 2\lambda\alpha)\Theta_j - \frac{2\alpha}{M}\sum_{i=1}^{M}(\Theta^T\Phi(x_i) - y_i)\Phi(x_i)$$

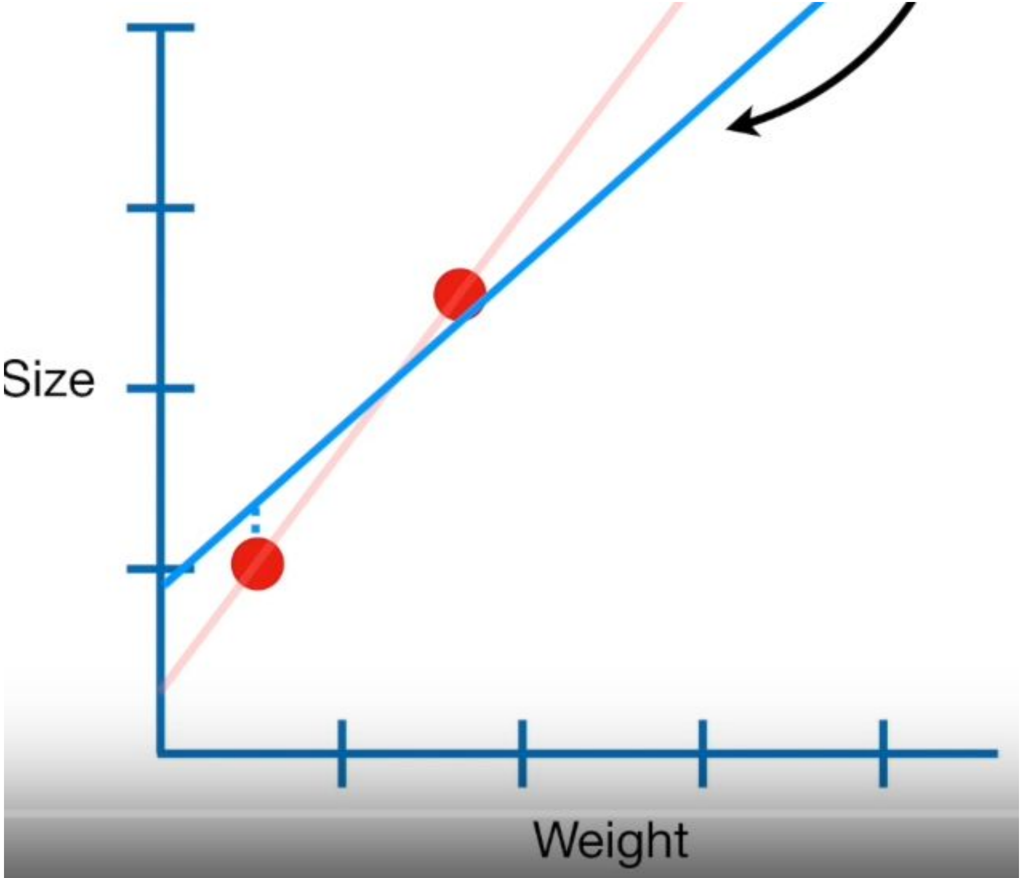
Ridge Regularization



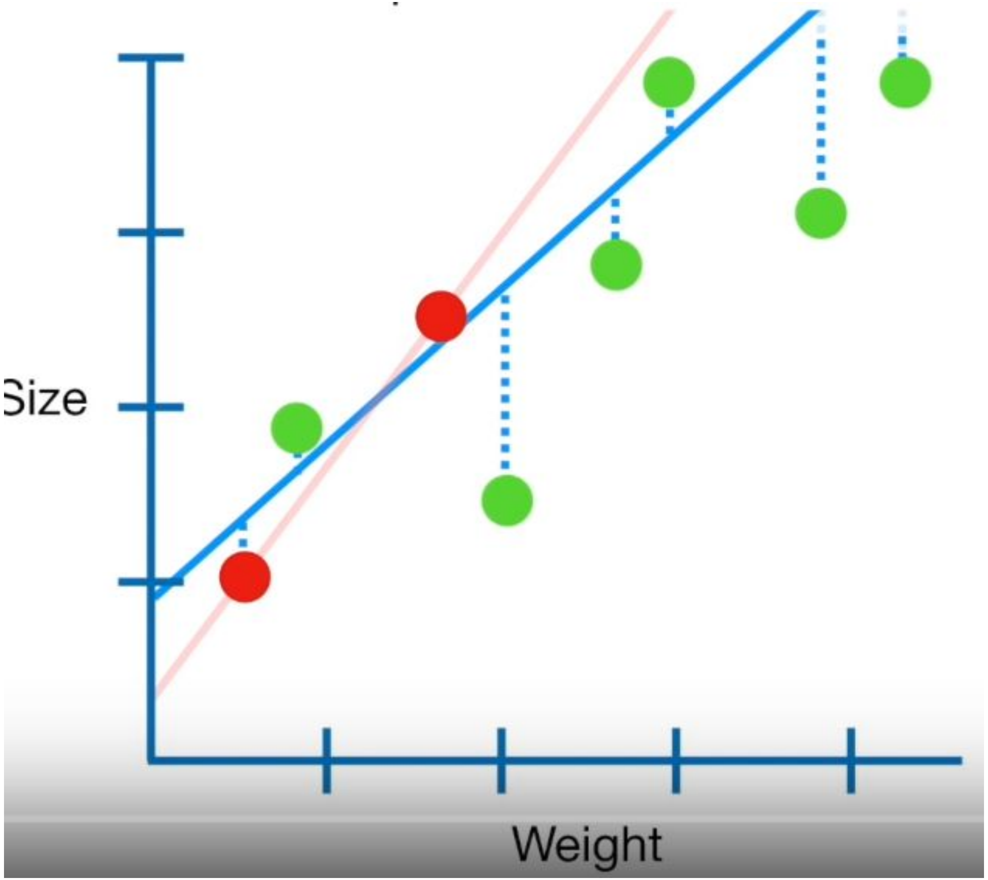
Low Bias and High Variance: Overfit



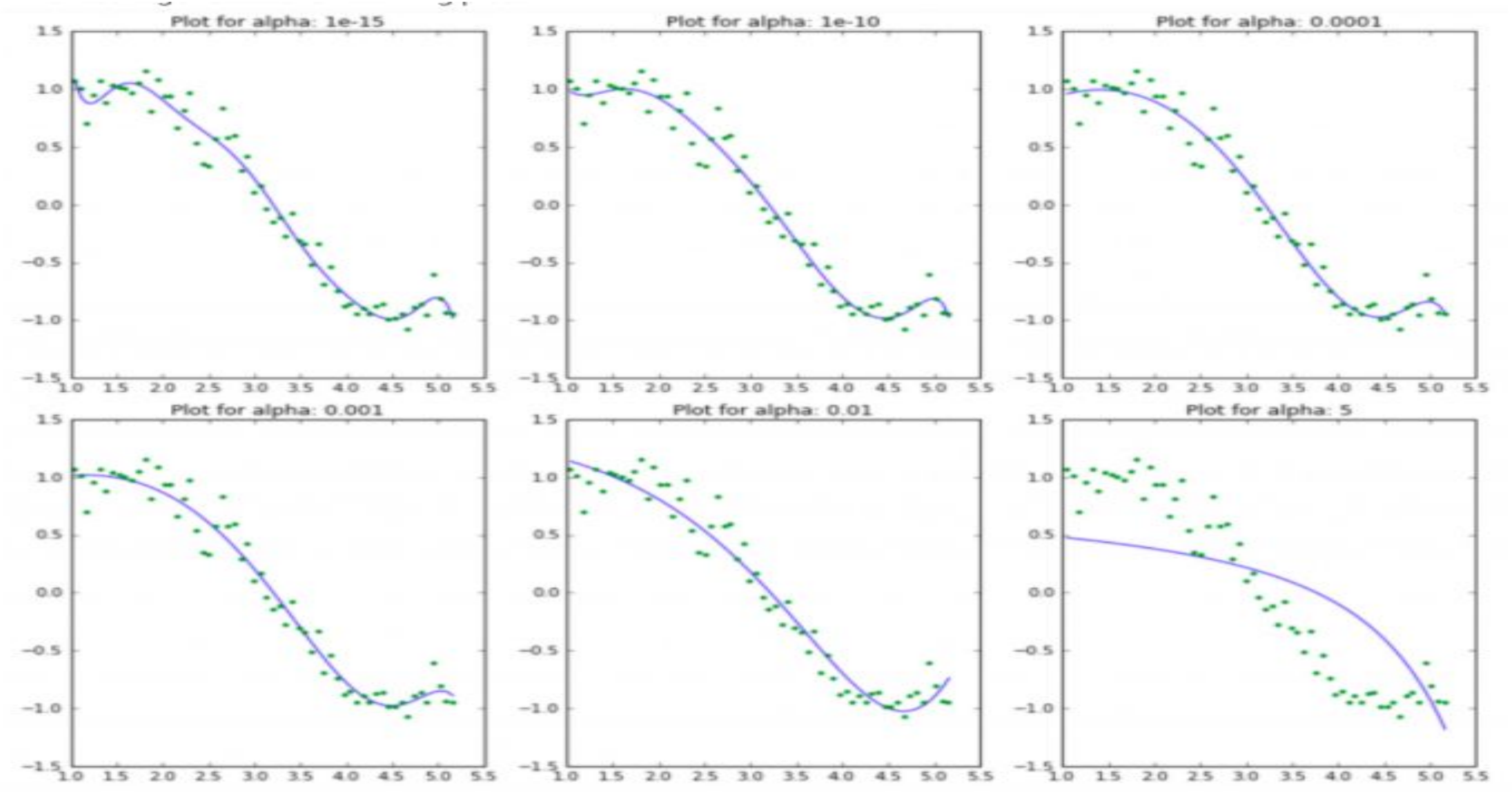
Ridge Regression



Ridge Regression



Regression - Ridge Regression



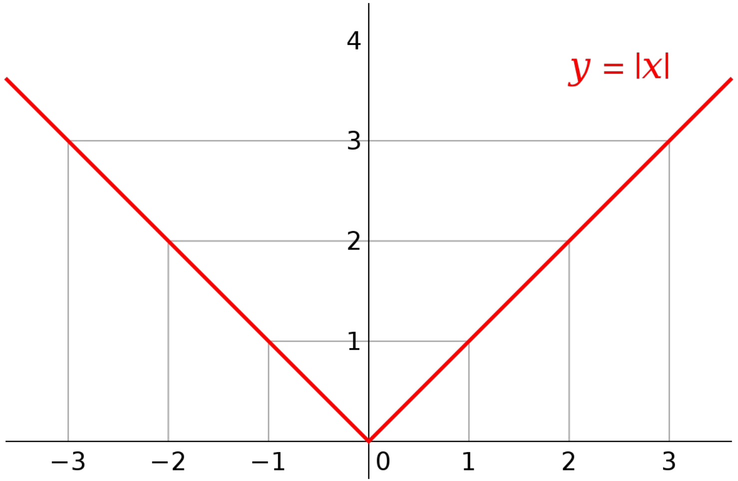
Regression - Ridge Regression

	rss	intercept	coef_x_1	coef_x_2	coef_x_3	coef_x_4	coef_x_5	coef_x_6	coef_x_7	coef_x_8	coef_x_9	coef_x_10	coef_x_11	coe
alpha_1e-15	0.87	95	-3e+02	3.8e+02	-2.4e+02	66	0.96	-4.8	0.64	0.15	-0.026	-0.0054	0.00086	0.0
alpha_1e-10	0.92	11	-29	31	-15	2.9	0.17	-0.091	-0.011	0.002	0.00064	2.4e-05	-2e-05	-4.
alpha_1e-08	0.95	1.3	-1.5	1.7	-0.68	0.039	0.016	0.00016	-0.00036	-5.4e-05	-2.9e-07	1.1e-06	1.9e-07	2e-
alpha_0.0001	0.96	0.56	0.55	-0.13	-0.026	-0.0028	-0.00011	4.1e-05	1.5e-05	3.7e-06	7.4e-07	1.3e-07	1.9e-08	1.9
alpha_0.001	1	0.82	0.31	-0.087	-0.02	-0.0028	-0.00022	1.8e-05	1.2e-05	3.4e-06	7.3e-07	1.3e-07	1.9e-08	1.7
alpha_0.01	1.4	1.3	-0.088	-0.052	-0.01	-0.0014	-0.00013	7.2e-07	4.1e-06	1.3e-06	3e-07	5.6e-08	9e-09	1.1
alpha_1	5.6	0.97	-0.14	-0.019	-0.003	-0.00047	-7e-05	-9.9e-06	-1.3e-06	-1.4e-07	-9.3e-09	1.3e-09	7.8e-10	2.4
alpha_5	14	0.55	-0.059	-0.0085	-0.0014	-0.00024	-4.1e-05	-6.9e-06	-1.1e-06	-1.9e-07	-3.1e-08	-5.1e-09	-8.2e-10	-1.
alpha_10	18	0.4	-0.037	-0.0055	-0.00095	-0.00017	-3e-05	-5.2e-06	-9.2e-07	-1.6e-07	-2.9e-08	-5.1e-09	-9.1e-10	-1.
alpha_20	23	0.28	-0.022	-0.0034	-0.0006	-0.00011	-2e-05	-3.6e-06	-6.6e-07	-1.2e-07	-2.2e-08	-4e-09	-7.5e-10	-1.

LASSO Regression

- Minimization objective = LS Obj + λ* (sum of absolute value of slope)

$$J(\Theta) = \frac{1}{M}\sum_{i=1}^{M}(\Theta^T\Phi(x_i) - y_i)^2 + \lambda\sum_{j=1}^{p}|\Theta_j|$$



LASSO Regression

- Lasso coordinate descent - closed form solution

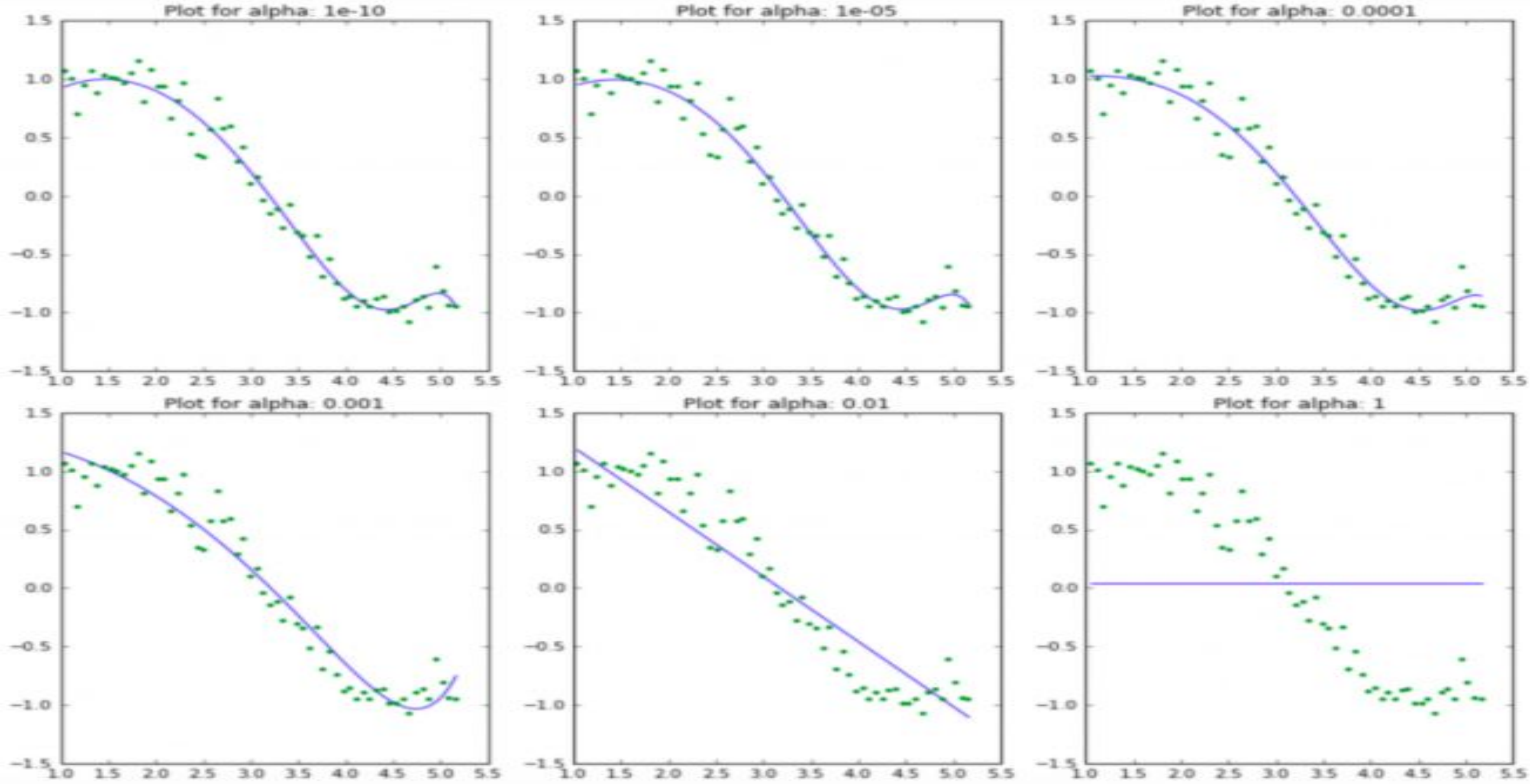
$$\begin{cases} \theta_(j+1) = \rho_j + \lambda & \text{for } \rho_j < -\lambda \\ \theta_(j+1) = 0 & \text{for } -\lambda \leq \rho_j \leq \lambda \\ \theta_(j+1) = \rho_j - \lambda & \text{for } \rho_j > \lambda \end{cases}$$

$$\rho_j = \sum_{i=1}^{m} x_j^{(i)} \left(y^{(i)} - \sum_{k \neq j}^{p} \theta_k x_k^{(i)}\right)$$

Lasso Regularization

- One significant problem of ridge regression is that the penalty term will never force any of the coefficients to be exactly zero.
- Thus, the final model will include all predictors (features), which creates a challenge in model interpretation
- The lasso works in a similar way to ridge regression, except it uses a different penalty term that shrinks some of the coefficients exactly to zero.
- Lasso performs a variable feature selection.
- $Y = m_1 * x_1 + m_2 * x_2 + m_3 * x_3 + c$

Regression - Lasso Regression

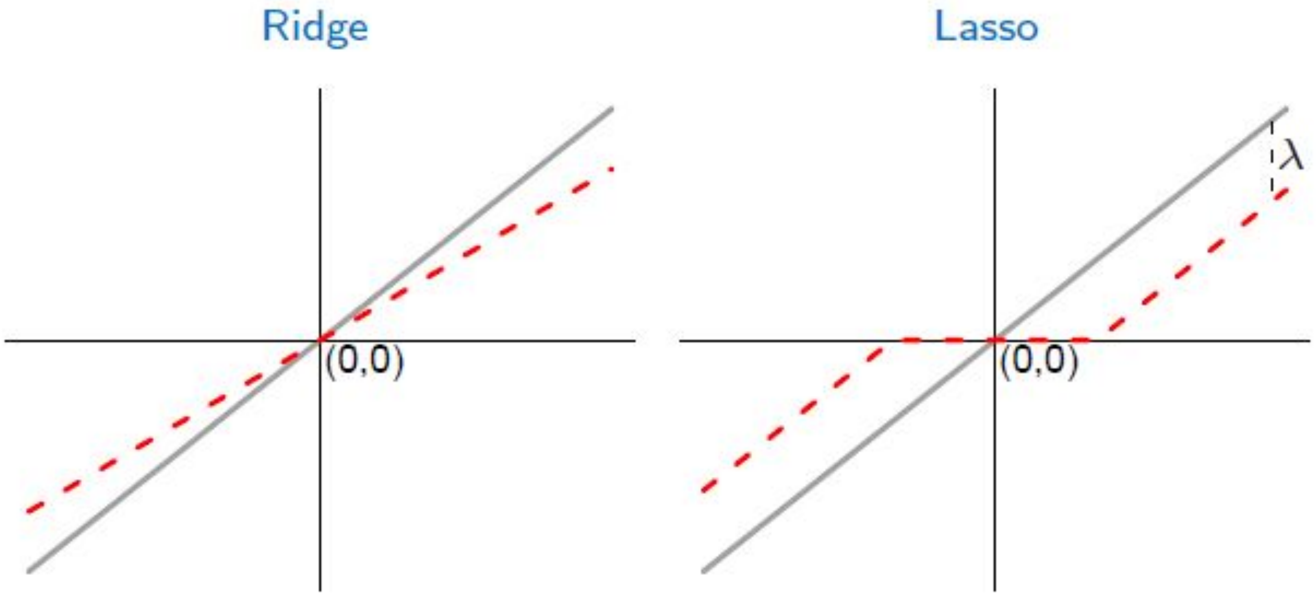


Regression - Lasso Regression

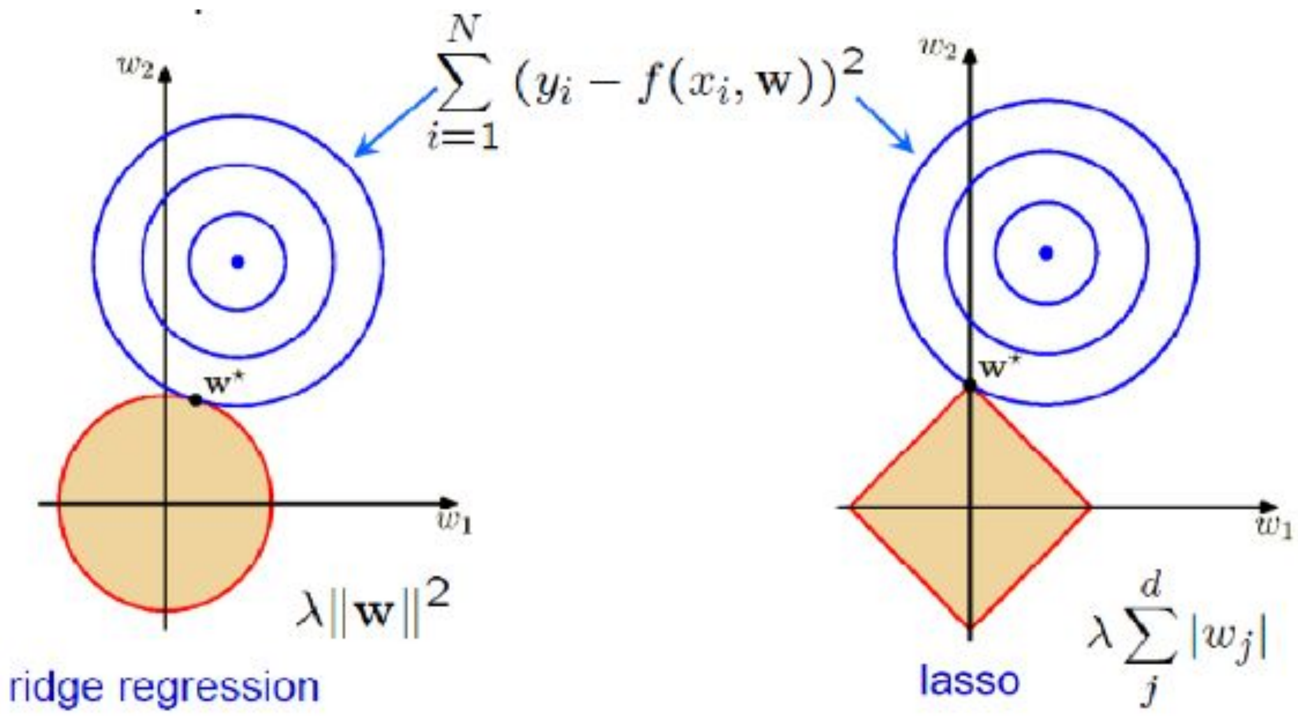
	rss	intercept	coef_x_1	coef_x_2	coef_x_3	coef_x_4	coef_x_5	coef_x_6	coef_x_7	coef_x_8	coef_x_9	coef_x_10	coef_x_11	coe
alpha_1e-15	0.96	0.22	1.1	-0.37	0.00089	0.0016	-0.00012	-6.4e-05	-6.3e-06	1.4e-06	7.8e-07	2.1e-07	4e-08	5.4
alpha_1e-10	0.96	0.22	1.1	-0.37	0.00088	0.0016	-0.00012	-6.4e-05	-6.3e-06	1.4e-06	7.8e-07	2.1e-07	4e-08	5.4
alpha_1e-08	0.96	0.22	1.1	-0.37	0.00077	0.0016	-0.00011	-6.4e-05	-6.3e-06	1.4e-06	7.8e-07	2.1e-07	4e-08	5.3
alpha_1e-05	0.96	0.5	0.6	-0.13	-0.038	-0	0	0	0	7.7e-06	1e-06	7.7e-08	0	0
alpha_0.0001	1	0.9	0.17	-0	-0.048	-0	-0	0	0	9.5e-06	5.1e-07	0	0	0
alpha_0.001	1.7	1.3	-0	-0.13	-0	-0	-0	0	0	0	0	0	1.5e-08	7.5
alpha_0.01	3.6	1.8	-0.55	-0.00056	-0	-0	-0	-0	-0	-0	-0	0	0	0
alpha_1	37	0.038	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0
alpha_5	37	0.038	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0
alpha_10	37	0.038	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0	-0

HIGH SPARSITY

RIDGE vs LASSO Regression



RIDGE vs LASSO Regression



Lasso vs Ridge Regression

- The lasso produces simpler and more interpretable models that involved only a subset of predictors.
- The lasso leads to qualitatively similar behavior to ridge regression, in that as λ increases, the variance decreases and the bias increases.
- The lasso can generate more accurate predictions compared to ridge regression.
- Cross-validation can be used in order to determine which approach is better on a particular data set.

Tuning Parameter

- Increased λ leads to increased bias but decreased variance
- $\lambda = 0$
  - The objective becomes same as simple linear regression.
- $0 < \lambda < \infty$:
  - The coefficients will be somewhere between 0 and ones for simple linear regression.

Cross-validation is used to find the parameter that results in the lowest variance.