UNIVERSITY AT ALBANY
STATE UNIVERSITY OF NEW YORK

CSI 436/536 (Spring 2025)

Machine Learning

Lecture 10: Regularization

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Announcement

- Homework 2 is due next Mon, Mar 3!

- Midterm exam on Mon Mar 10.
  - TA will lead the homework 1 and 2 review next Wednesday.
  - Come to our office hours!

- Midterm presentations on Wed Mar 12.
  - I'll give a quick tutorial on presentations today.

Recap: Two problems of supervised learning

	Classification		Regression
	Binary classification	Multi-class classification	
Feature space	$\mathbb{R}^d$	$\mathbb{R}^d$	$\mathbb{R}^d$
Label space	{-1, 1}	{1, 2, 3, …, K}	$\mathbb{R}$
Performance metric	Classification error (0-1 loss) for test data	Classification error (0-1 loss) for test data	Mean Square Error
Popular surrogate loss (for training)	Logistic loss / exponential loss / square loss	Multiclass logistic loss (Cross-Entropy loss)	Square loss

Today

- SGD for linear regression
- Linear regression in curve fitting
- Problem of overfitting
- Regularization prevents overfitting
- Quick tutorial on course project presentation

The objective function for learning linear regression under square loss

- $\widehat{w} = \text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} (x_i^T w - y_i)^2 = \text{argmin}_w \|Xw - y\|_2^2$
  - aka: Ordinary Least Square (OLS)
- Direct solver: setting gradient to 0.

Derive the SGD algorithm

- Problem:
- $\widehat{w} = \text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} (x_i^T w - y_i)^2 = \text{argmin}_w \|Xw - y\|_2^2$

- Step 1: Calculate the gradient of the square loss

- Step 2: Write the SGD update rule

Checkpoint: How to solve linear regression?

- Challenges:
  - We don’t have access to future data for prediction!
  - We also don’t have access to ground truth
- By solving an optimization problem that minimizes the loss function on the **training data**, and hope that it generalizes.
  - We can verify if it generalizes or not using hold-out / cross-validation …
- The least square optimization problem using square loss function:

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2$$

Checkpoint: Linear regression

- Stochastic Gradient Descent (SGD)
  - Using a stochastic approximation of the gradient:

$$\theta_{t+1} = \theta_t - \eta_t \hat{\nabla} f(\theta_t)$$

  - Calculated by one data point randomly sampled from dataset
- Linear regression
  - $\widehat{w} = \text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} (x_i^T w - y_i)^2 = \text{argmin}_w \|Xw - y\|_2^2$
  - Direct solver: $\widehat{w} = (X^T X)^{-1} X^T y$
  - GD: $w \leftarrow w - 2\eta X^T (Xw - y)$
  - SGD: $w \leftarrow w - 2\eta {x_i}^T (x_i^T w - y_i)$

Checkpoint: Time complexity

- Direct solver
  - $O(nd^2 + d^3)$
- GD:
  - $O(ndT)$
- SGD:
  - $O(dT)$

- $T = \text{n\_iterations}$

Example of regression - Curve fitting: How to train a function fitting blue dots?

- Input:

  $x \in \mathcal{X} = [0, 1] \subset \mathbb{R}$

- Output:

  $y \in \mathcal{Y} = \mathbb{R}$

- Data:

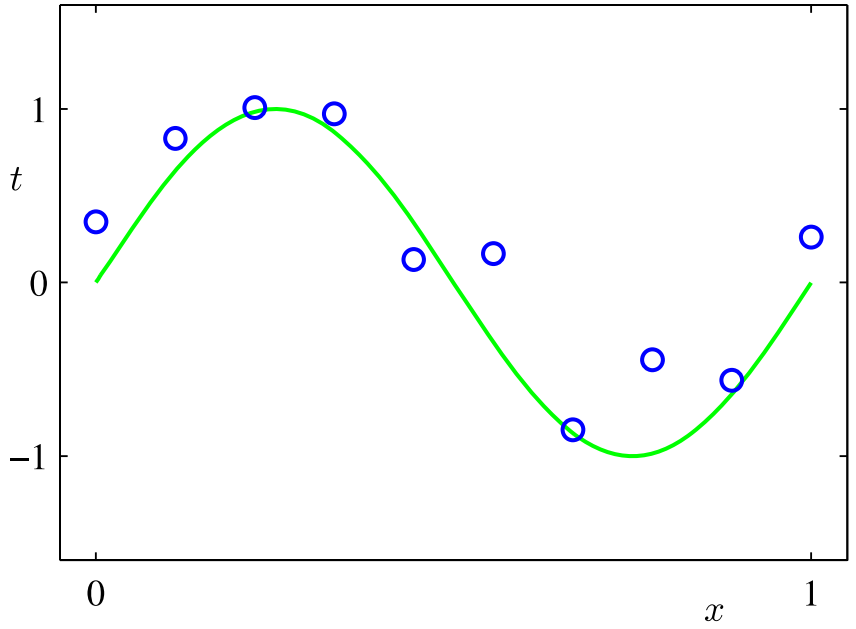
  $(x_1, y_1), ..., (x_n, y_n)$

- Ground truth:

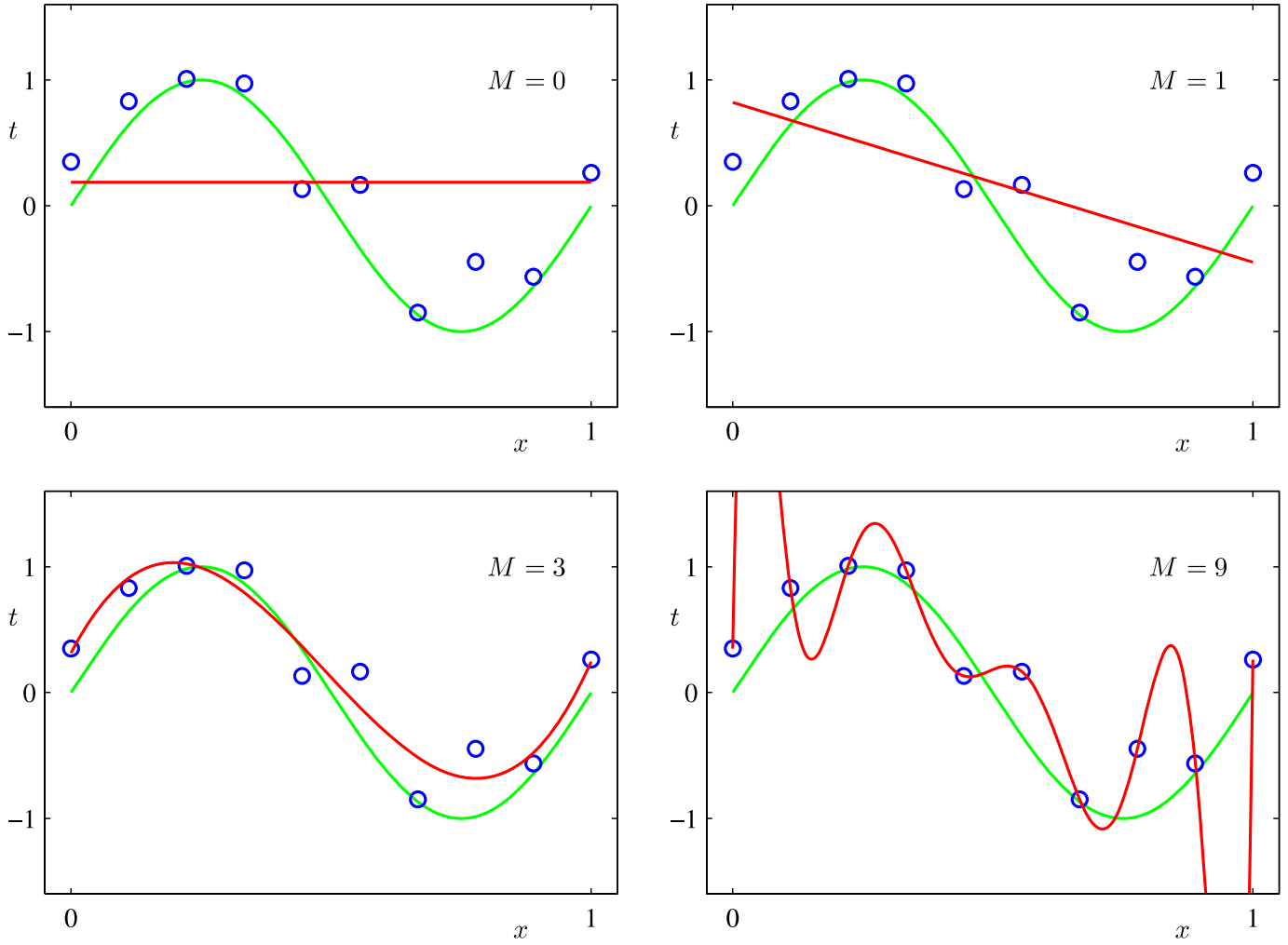
  $f_0(x) = \sin(2\pi x)$

- Hypothesis (model)

  $f(x) = w_0 + w_1 x + w_2 x^2 + ... + w_M x^M$

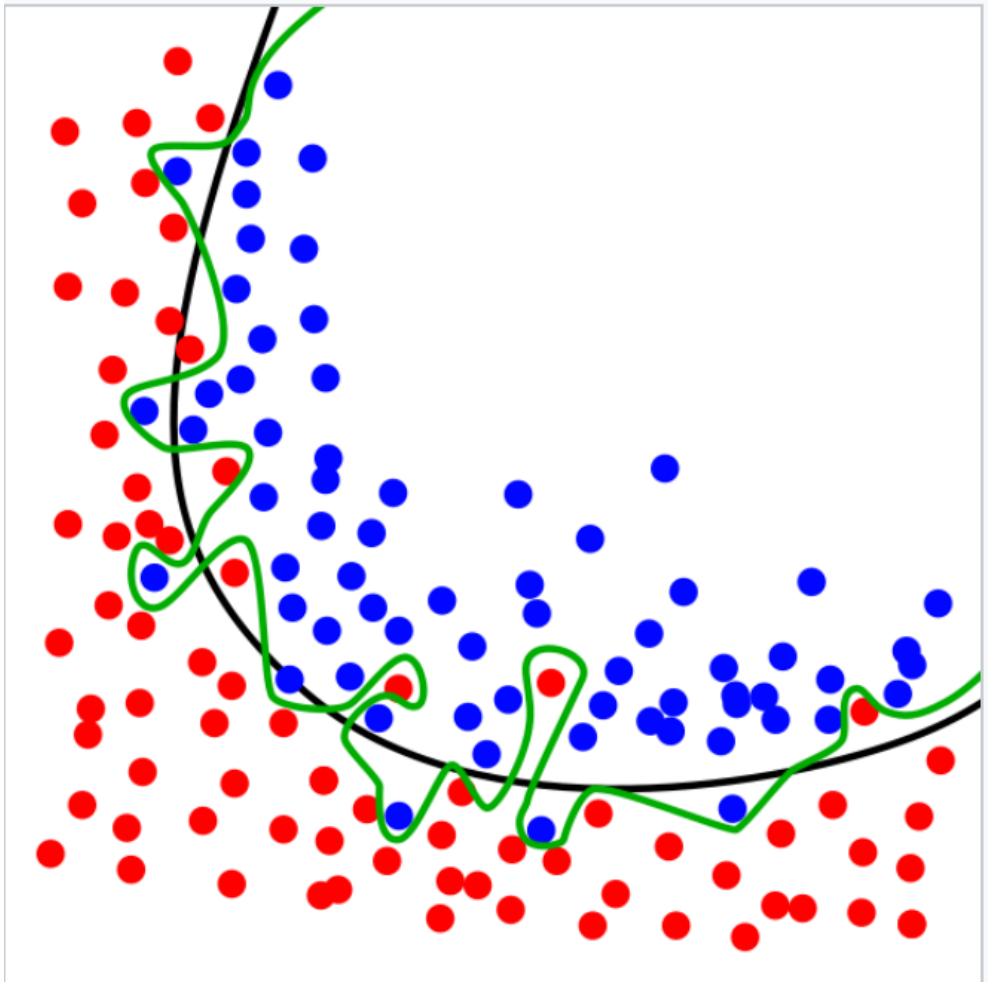


Polynomial regression under square loss



Problem of overfitting!

Recap: The problem of Overfitting



The green line represents an overfitted model.

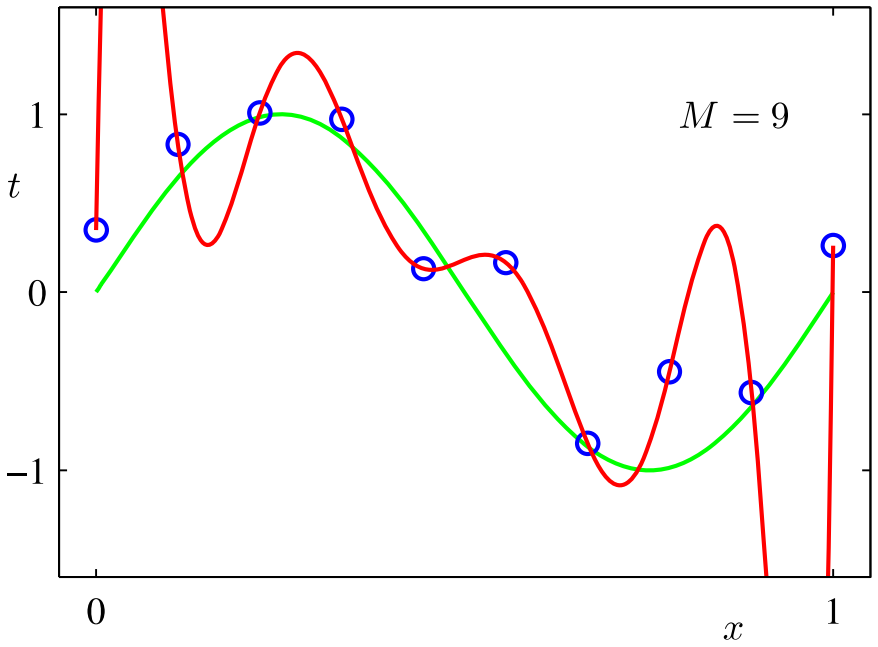
1. Best follows the training data
2. Too dependent on training data
3. More likely to fail (higher error rate) than black line on new unseen test data

Discussion: examples of overfitting in our learning as human beings?

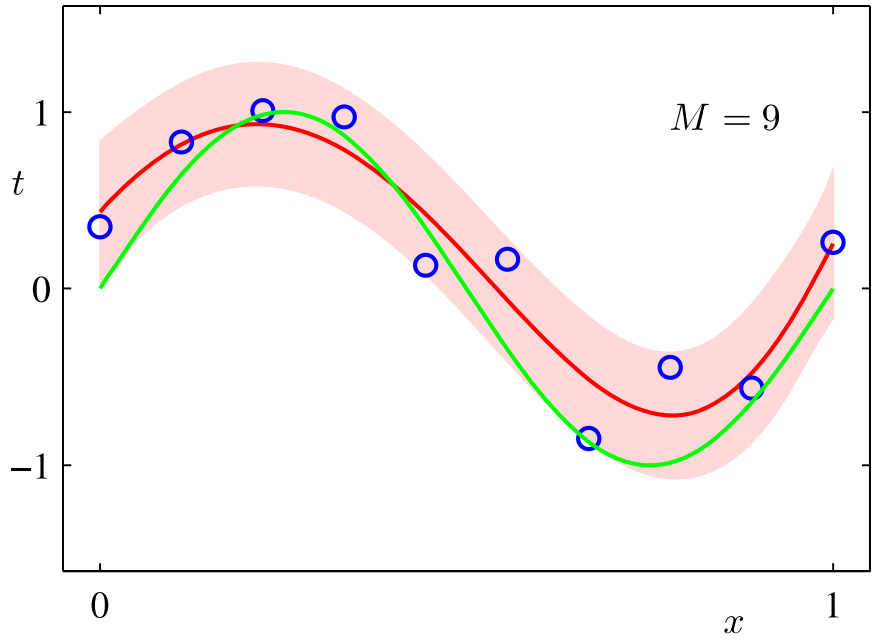
Regularization prevents overfitting!

- Same model:

$$f(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M$$



No regularization



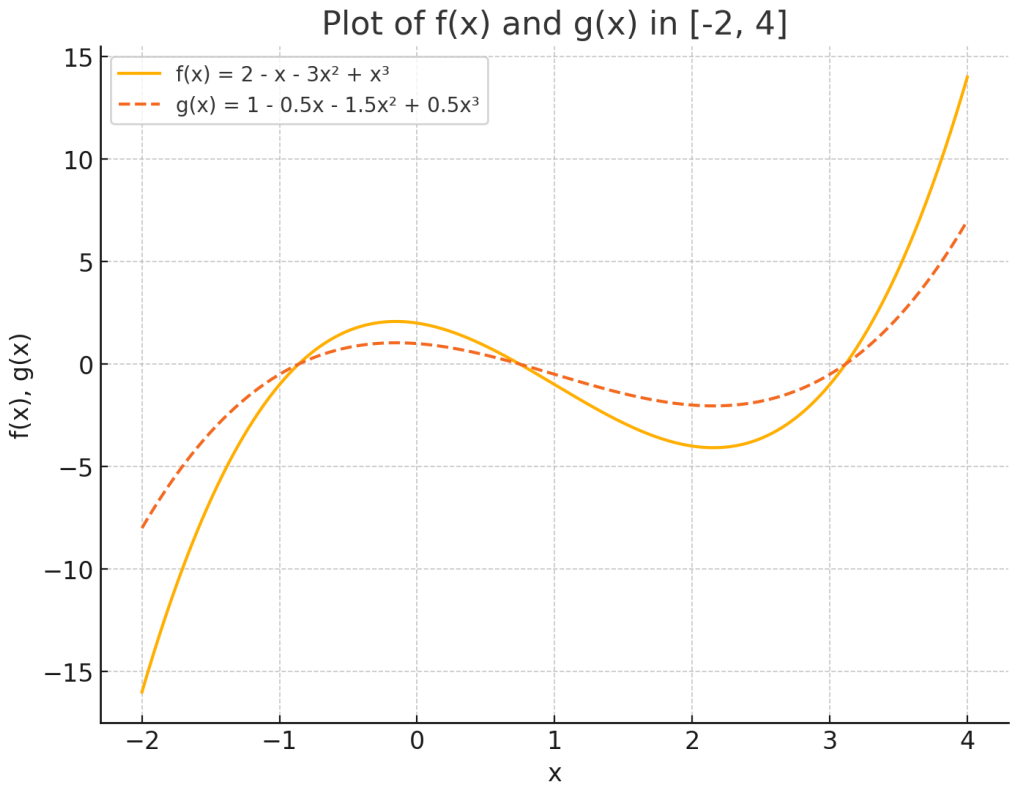
With regularization

How does regularization work?

- Regularization controls the parameter complexity (norms of parameter).
  - p-norm regularized least square

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n}\|X\theta - y\|_2^2 + \lambda\|\theta\|_p^p$$

- In-class exercise:
  - Find L-2 norm of $x = [2, -1, -3, 1]$ and $x' = [1, -0.5, -1.5, 0.5]$
  - Plot $f(x) = 2 - x - 3x^2 + x^3$ and $g(x) = 1 - 0.5x - 1.5x^2 + 0.5x^3$ in $[-2, 4]$



Different choices of regularization

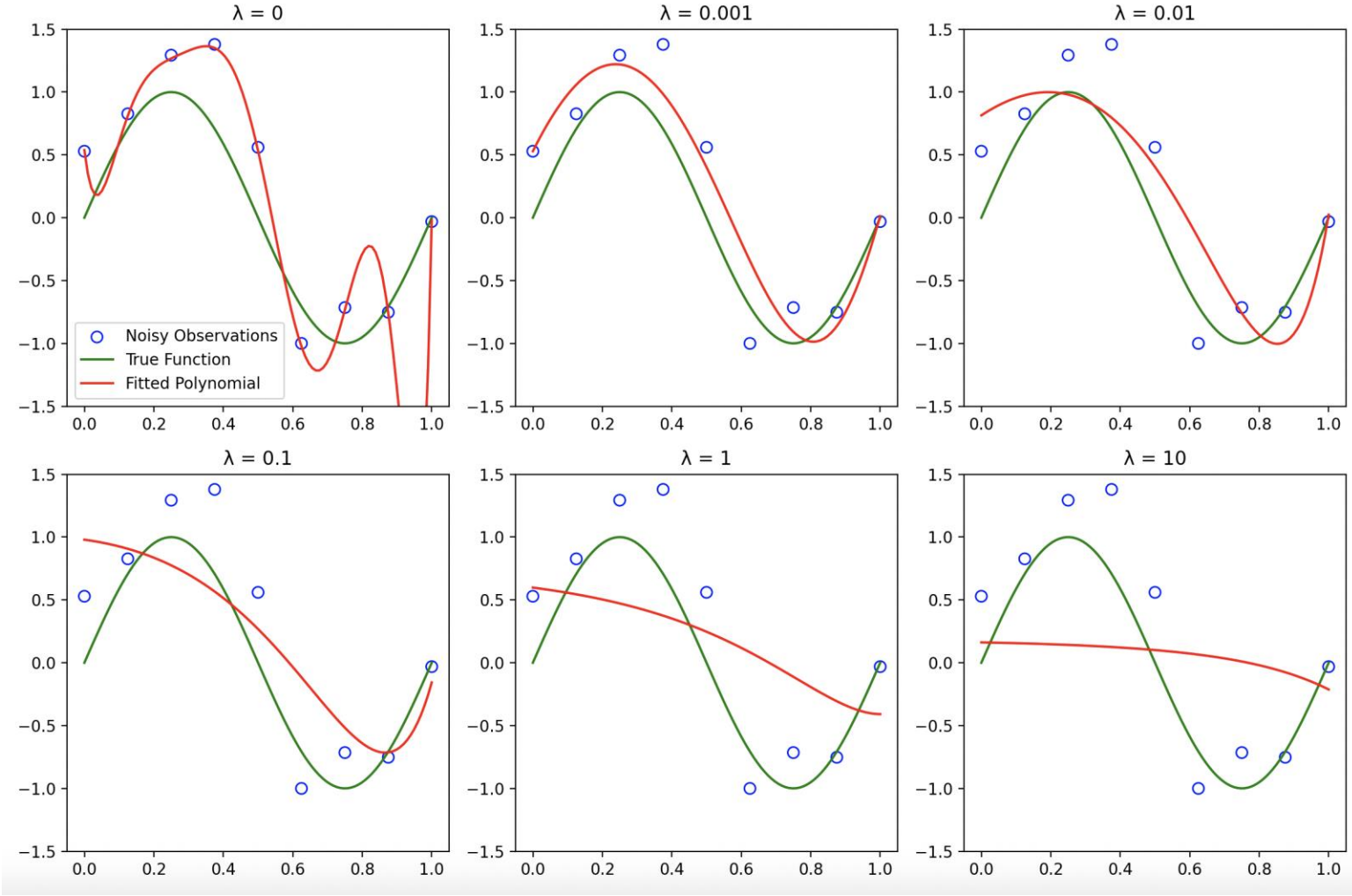
- p-norm regularized least square

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \|X\theta - y\|_2^2 + \lambda \|\theta\|_p^p$$

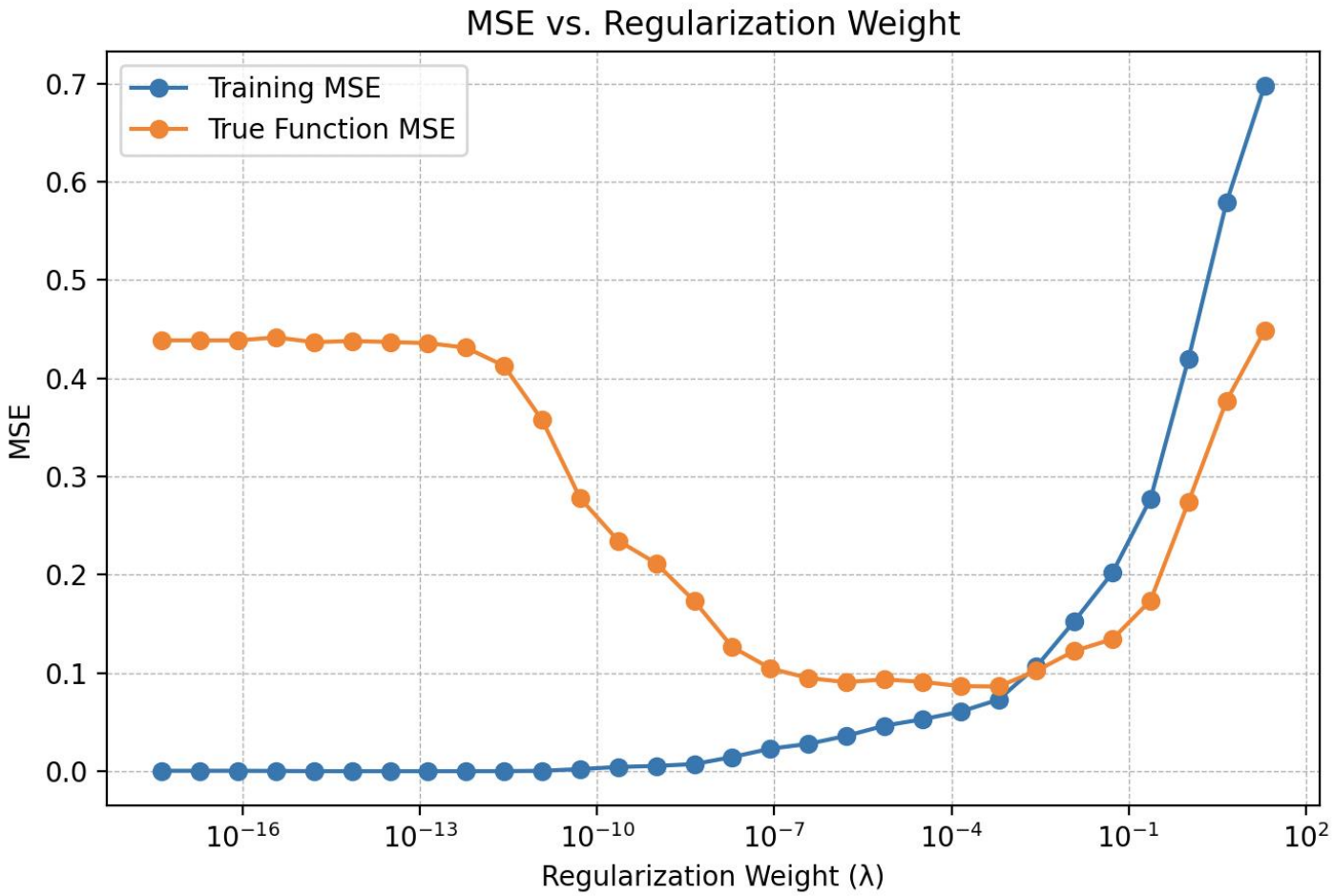
  - when p=2, this is called “Ridge Regression”
  - when p=1, this is called “Lasso”

- Direct solver for Ridge Regression in HW2.

Fitted curve as L-2 regularization weight increases



The mean square errors as we adjust the L2 regularization weight



- Discussion:
  - Why training error increases with regularization weight?
  - Why is test error in a U-shaped curve?

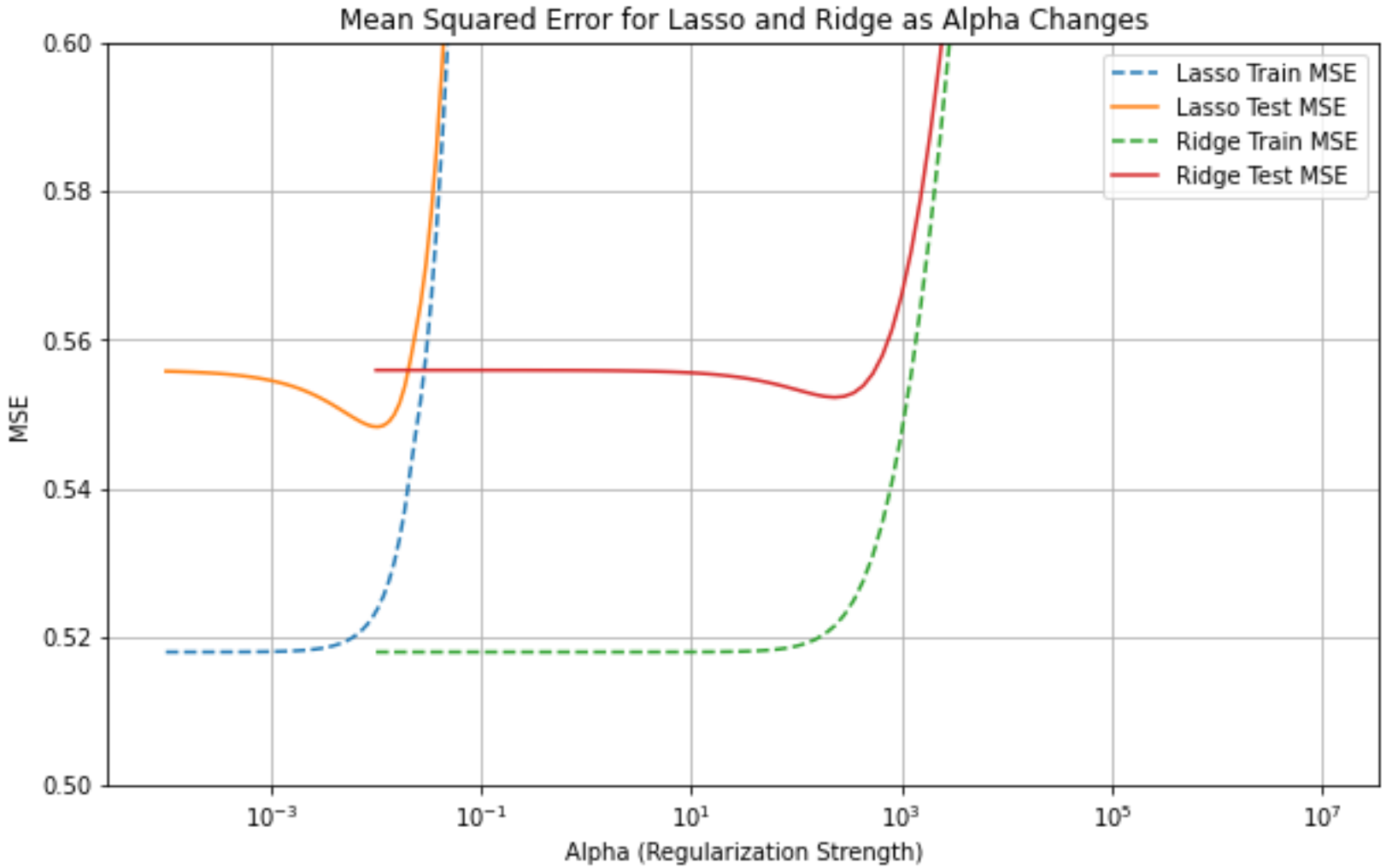
Case study: Housing price dataset

- Example data

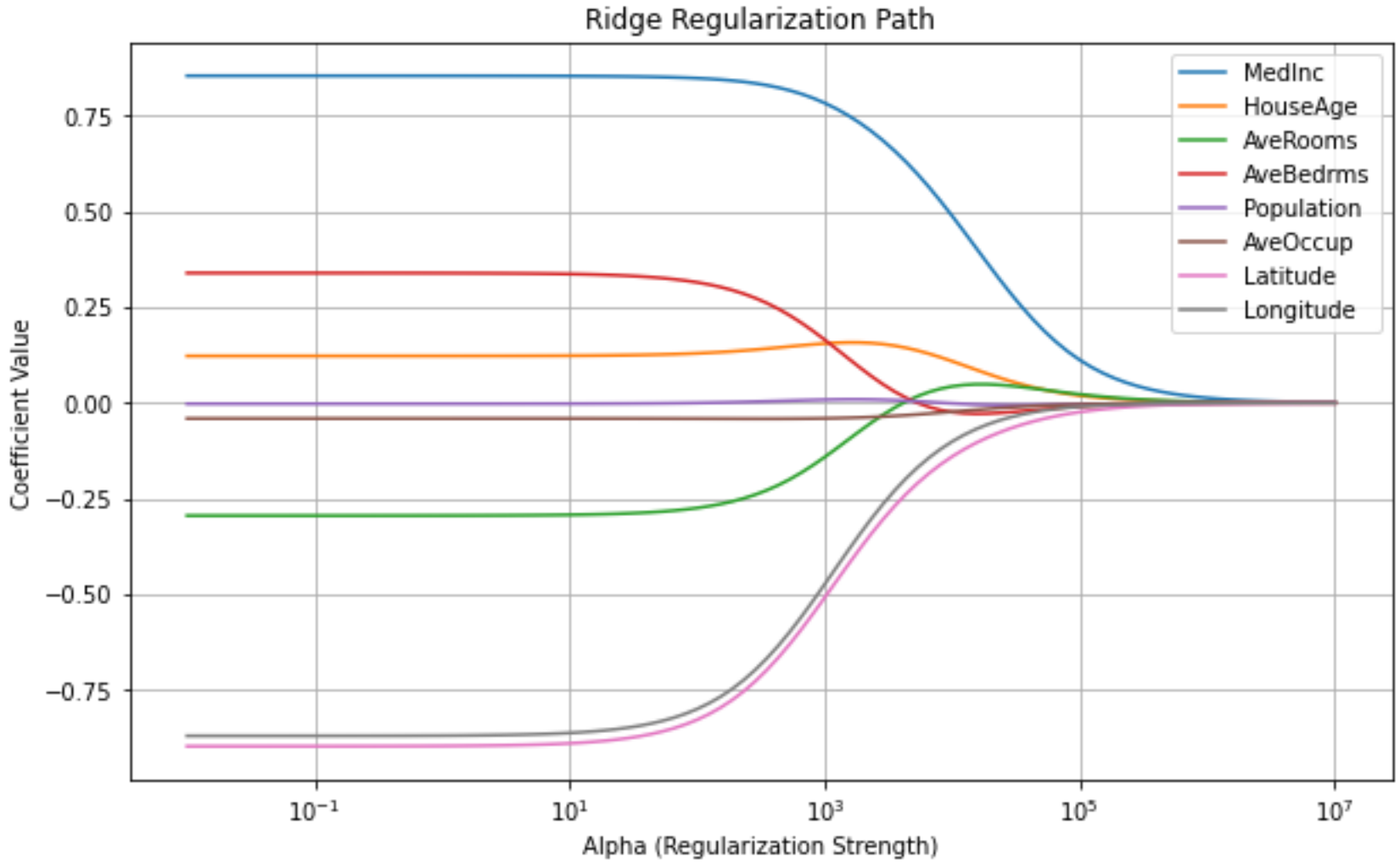
	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	Longitude	Target
0	8.3252	41.0	6.984127	1.023810	322.0	2.555556	37.88	-122.23	4.526
1	8.3014	21.0	6.238137	0.971880	2401.0	2.109842	37.86	-122.22	3.585
2	7.2574	52.0	8.288136	1.073446	496.0	2.802260	37.85	-122.24	3.521
3	5.6431	52.0	5.817352	1.073059	558.0	2.547945	37.85	-122.25	3.413
4	3.8462	52.0	6.281853	1.081081	565.0	2.181467	37.85	-122.25	3.422

- Questions one can ask:
  - How well can one use the 8 features to predict house price (i.e., Target)?
  - Which feature is more predictive with house price?
  - What is the effect of regularization?

The MSE vs regularization weight



The “Regularization path” for L2-regularization



How to interpret the fitted coefficients?

- The “sign” indicates positive or negative correlation with the label
- The “magnitude” indicates how strongly correlated.

Summary

- Linear regression
  - Solving the Least Square problem {with GD, SGD and direct solver}
- Regularization
  - Controls the parameter complexity of the fitted function
  - Prevents overfitting!
  - Different regularization: L-2 (most popular) and L-1
- Case study: Predict Housing Price
  - Effect of regularization on training test and test error
  - Regularization path (Effect of regularization on coefficients)

Midterm course project presentations

- Each group has 4 min
  - 4 min limit is strictly enforced to ensure all groups can present
- Contents:
  - Background, Problem setup, Challenges, Current progress, Plans
- Clarity:
  - Figure (most preferred), tables, bullet points, words, sentences (least preferred)
  - Figure: x-axis and y-axis need to be defined
  - Table: row and column need to be defined