

Loss Functions and Regularization

David I. Inouye

Outline

- ▶ Loss functions
 - ▶ Regression losses
 - ▶ Classification losses
- ▶ Regularization
 - ▶ “Implicit regularization” by changing k in KNN
 - ▶ L2 regularization
 - ▶ L1 regularization and feature selection
- ▶ Caveat: Very brief introduction to these concepts
 - ▶ If you want to learn more, take ECE50024 Machine Learning I

Many machine learning methods minimize the average loss (a.k.a. risk minimization)

- ▶ Remember linear regression objective:

$$\theta^* = \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^n (y_i - f_{\theta}(\mathbf{x}_i))^2$$

- ▶ We can rewrite this as:

$$\theta^* = \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_{\theta}(\mathbf{x}_i))$$

- ▶ where $\ell(y, \hat{y}) = (y - \hat{y})^2$ is the loss function
- ▶ Many supervised ML can be written as above

Many supervised ML can be written minimizing the average loss

- ▶ Ordinary least squares uses **squared loss**:

$$\ell(y, \hat{y}) = (y - \hat{y})^2$$

- ▶ Logistic regression uses **logistic loss**

$$\ell(y, \hat{p} \in [0,1]) = -y \log \hat{p} - (1 - y) \log(1 - \hat{p})$$

$$\ell(y, \hat{z} \in \mathbb{R}) = -y \log \sigma(\hat{z}) - (1 - y) \log(1 - \sigma(\hat{z}))$$

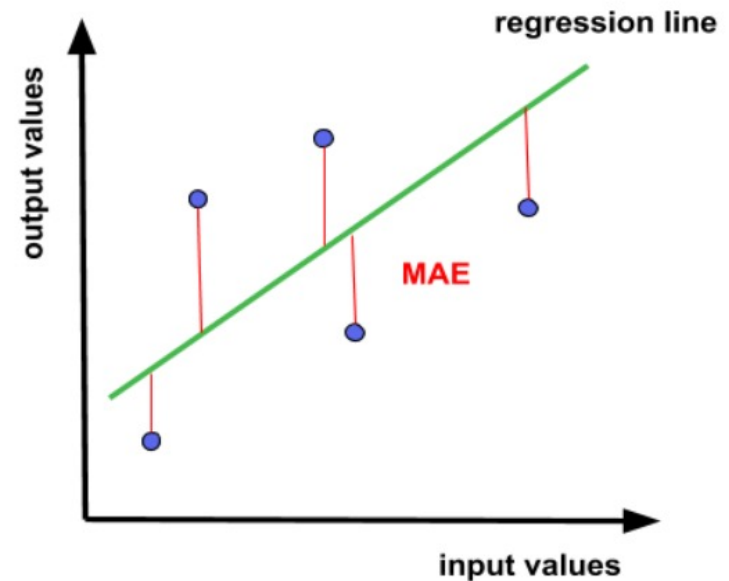
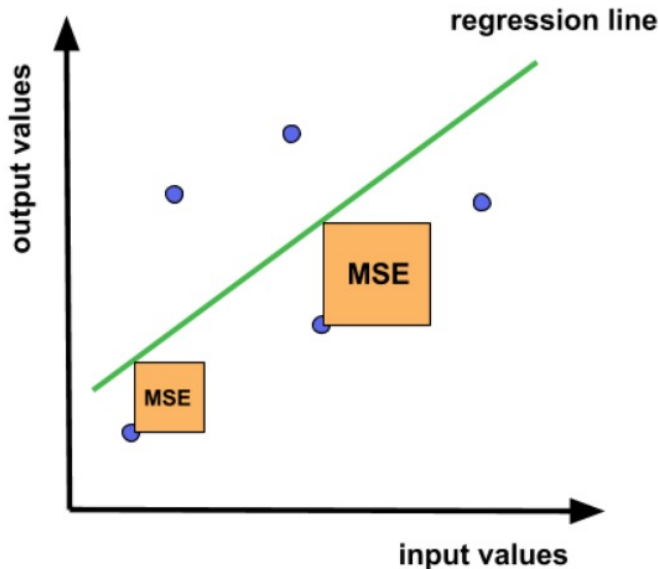
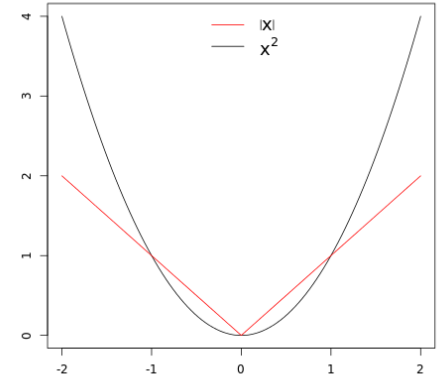
- ▶ Classification error is known as **0-1 loss**

$$\ell(y, \hat{y}) = \begin{cases} 0, & \text{if } y = \hat{y} \\ 1, & \text{otherwise} \end{cases}$$

Example: Absolute error is less sensitive to outliers but is harder to optimize

- ▶ Absolute error loss is:

$$\ell(y, \hat{y}) = |y - \hat{y}|$$



Example: The hinge loss is used for learning support vector machine (SVM) classifiers

► Hinge loss is defined as:

$$\ell(y, \hat{z}) = \max\{0, 1 - y\hat{z}\}$$

(Note: $y \in \{-1, 1\}$)

$$\ell(y, \hat{z}) = \begin{cases} \begin{cases} 1 - \hat{z}, & \hat{z} \leq 1 \\ 0, & \hat{z} > 1 \end{cases} & y = 1 \\ \begin{cases} 1 + \hat{z}, & \hat{z} \geq -1 \\ 0, & \hat{z} < -1 \end{cases} & y = -1 \end{cases}$$

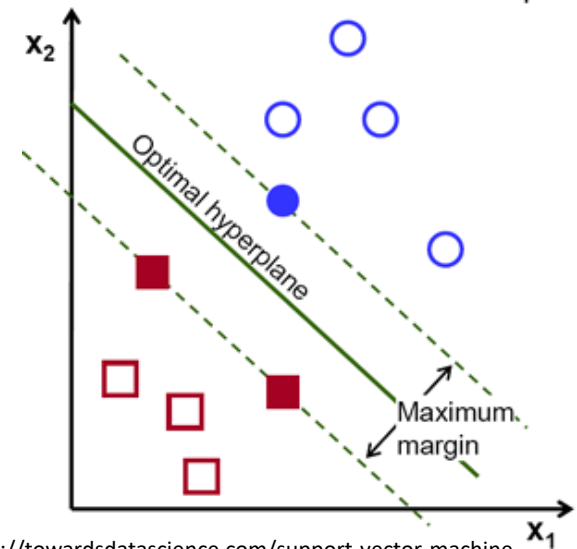
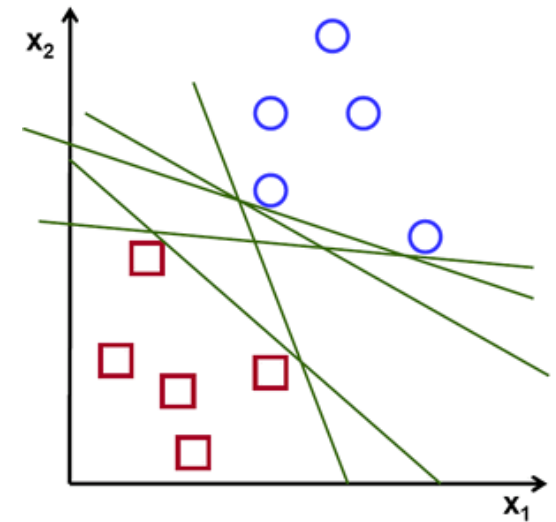
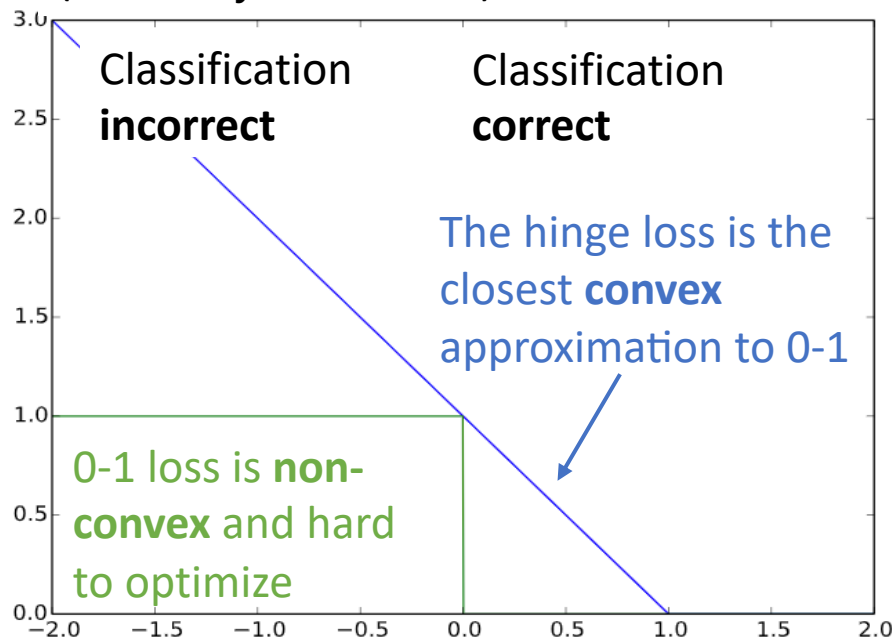
Example: The hinge loss is used for learning support vector machine (SVM) classifiers

► Hinge loss is defined as:

$$\ell(y, \hat{z}) = \max\{0, 1 - y\hat{z}\}$$

(Note: $y \in \{-1, 1\}$)

(Assume $y = 1$ below)



<https://towardsdatascience.com/support-vector-machine-introduction-to-machine-learning-algorithms-934a444fca47>

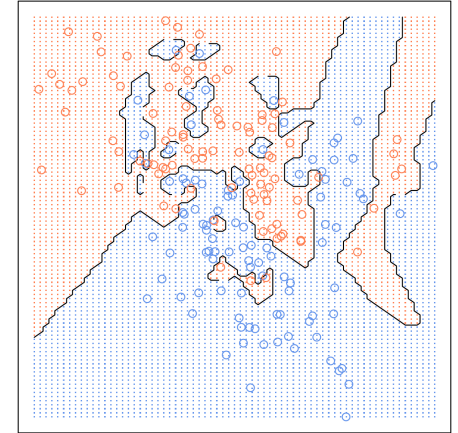
Regularization is a common method to improve *generalization* by reducing the complexity of a model

▶ k in KNN can be seen as an *implicit* regularization technique

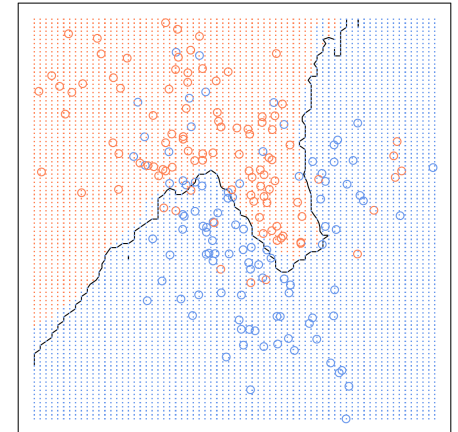
▶ We can use *explicit* regularization for parametric models by adding a regularizer $R(\theta)$

$$\min_{\theta} \sum_i \ell(y_i, f_{\theta}(x_i)) + \lambda R(\theta)$$

1-nearest neighbours



20-nearest neighbours



<https://kevinzakka.github.io/2016/07/13/k-nearest-neighbor/>

Brief aside: 1D polynomial regression can be computed by creating polynomial “pseudo” features

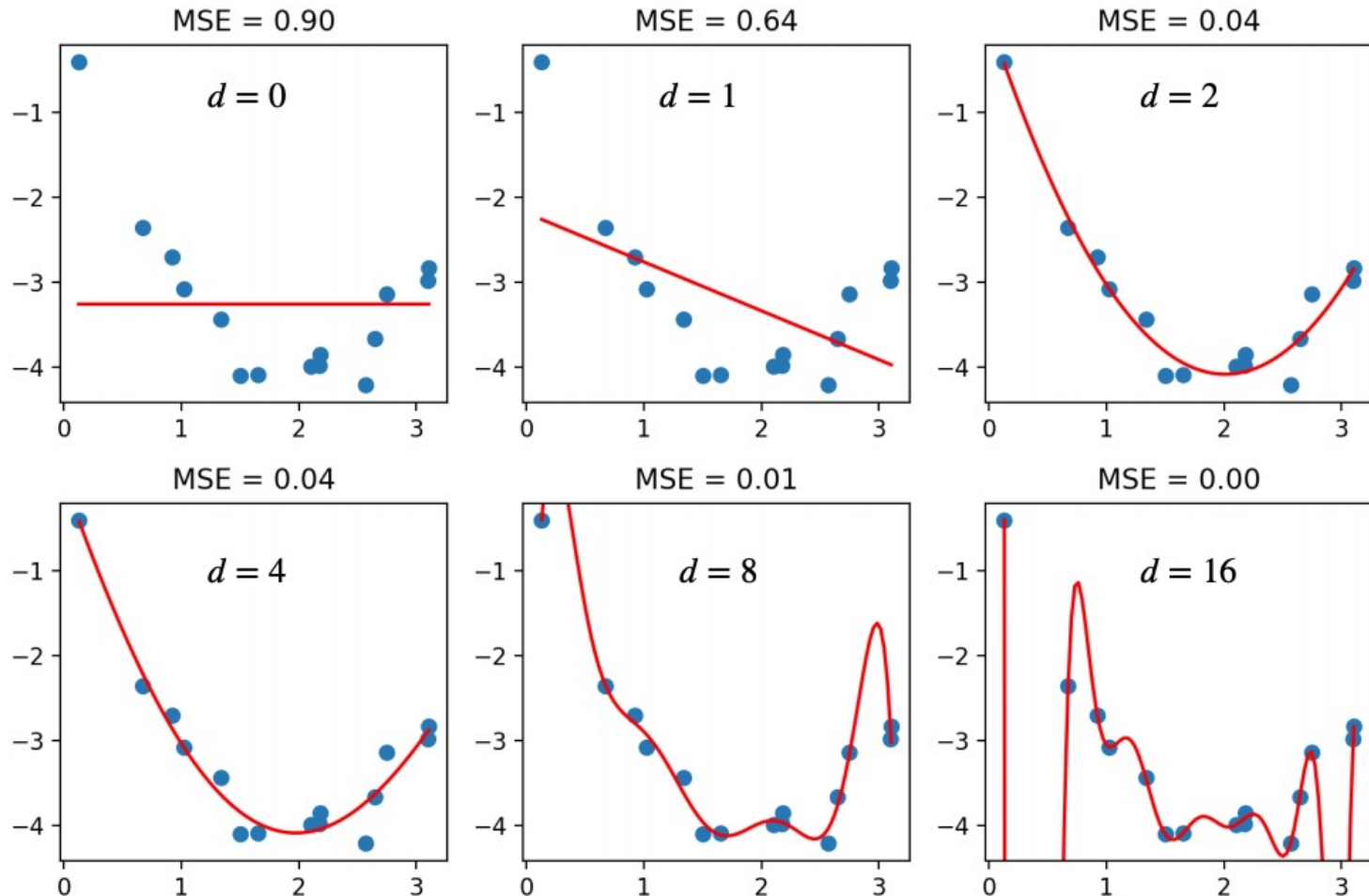
- ▶ Suppose we have 1D input data, i.e., $X \in \mathcal{R}^{n \times 1}$
- ▶ We can create pseudo polynomial features, e.g.

$$X' = \begin{bmatrix} x_1 & x_1^2 & x_1^3 \\ x_2 & x_2^2 & x_2^3 \\ x_3 & x_3^2 & x_3^3 \end{bmatrix} \in \mathcal{R}^{n \times 3}$$

- ▶ Linear regression can then be used to fit a polynomial model

$$y_i = \theta_1 x_i + \theta_2 (x_i^2) + \theta_3 (x_i^3) \dots$$

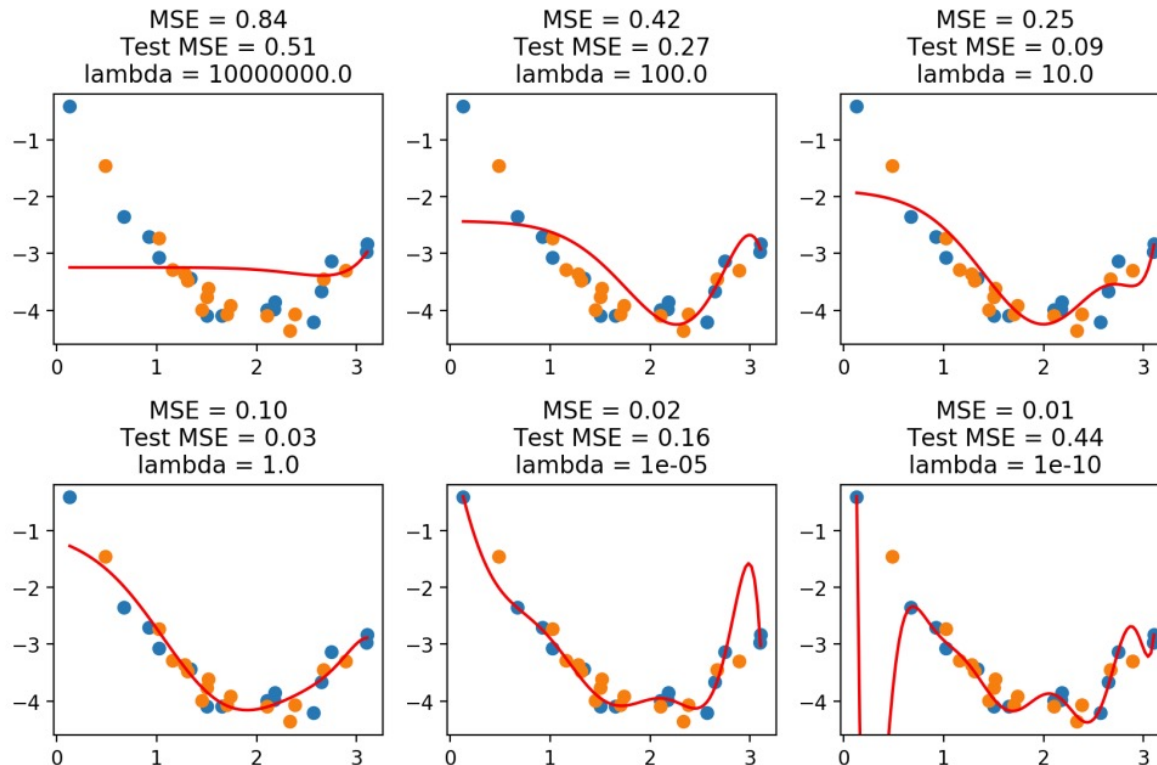
Brief aside: 1D polynomial regression can be computed by creating polynomial “pseudo” features



Ridge Regression: A squared norm regularizer encourages small parameter values

- ▶ Ridge regression is defined as:

$$\min_{\theta} \|\mathbf{y} - X\theta\|_2^2 + \lambda \|\theta\|_2^2$$

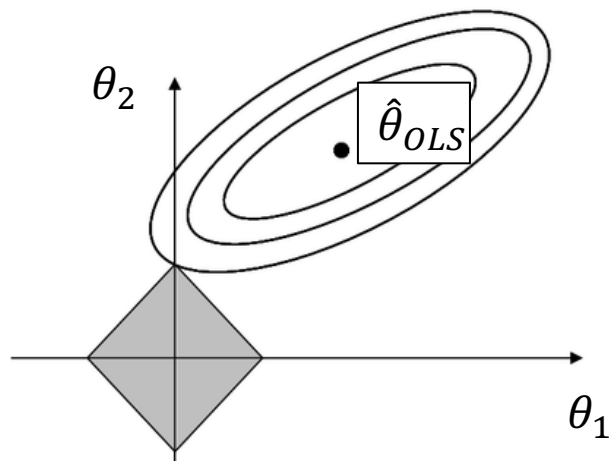
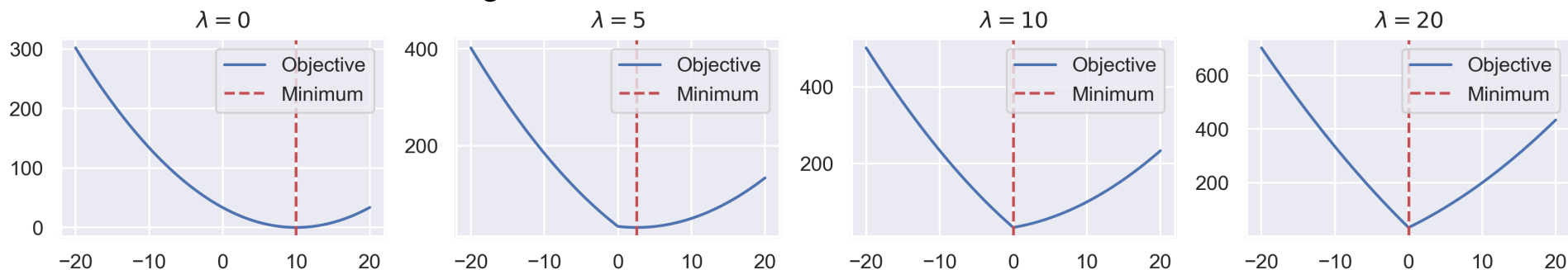


Regularizing the parameters of 1D polynomial regression helps to improve test MSE if chosen appropriately.

Lasso Regression: An L_1 norm regularizer encourages sparsity in the parameters (i.e., zeros)

- ▶ Lasso regression is defined as:

$$\min_{\theta} \|\mathbf{y} - X\theta\|_2^2 + \lambda \|\theta\|_1$$



Because lasso encourages **exact zeros**, lasso can be used for feature selection.

$$\begin{aligned} f_{\theta}(x) &= \theta_1 x_1 + \theta_2 x_2 \\ &= (0)x_1 + \theta_2 x_2 \\ &= \theta_2 x_2 \end{aligned}$$