03_Losses_Regularization_Evaluation

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1. Regularization

1.1. Stabilization

1.1.1. Background

Take Linear Regression as Example: $\widehat{w} = \left(X^T X\right)^{-1} X^T Y$, if:

- we try to use many dimensions features but only have few observations
- the train data is not "good" (does not present true distribution)

Then some eigenvalues of X may be very small, which means in the inverse, some features will have very large eigenvalues, which means

- the given feature dominates the regression
- new observation of different sample will lead to very large fluctuation on the w, which means, **unstable**

1.1.2. Solution

An idea is: keep the eigenvalues away from 0

$$\widehat{w} = \left(X^T X + \lambda I\right)^{-1} X^T Y$$

- The new w will perform poorer on train data

- But it has high possibility perform better on true data

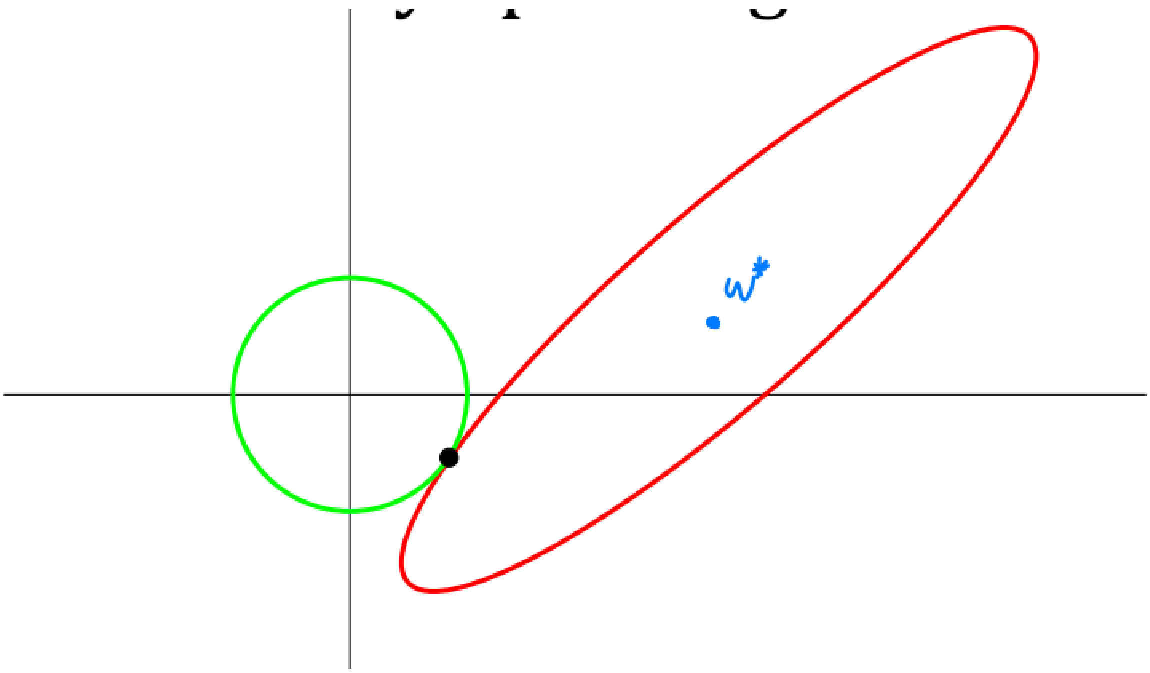
The above equation is equal to:

$$\min_w \sum_{i=1}^{N} \left(x_i^T w - y_i\right)^2 + \lambda \|w\|^2$$

Or the second format:

$$\begin{aligned} &\min_w \sum_{i=1}^{N} \left(f\left(x_i, w\right) - y_i\right)^2 \\ &\text{s.t. } \|w\|^2 \leq \tau \end{aligned}$$

1.1.3. Geometry



1.2. General Approach to regularization

$$\min_w \sum_{i=1}^{N} \ell\left(f\left(x_i, w\right), y_i\right) + R(f) \tag{1}$$

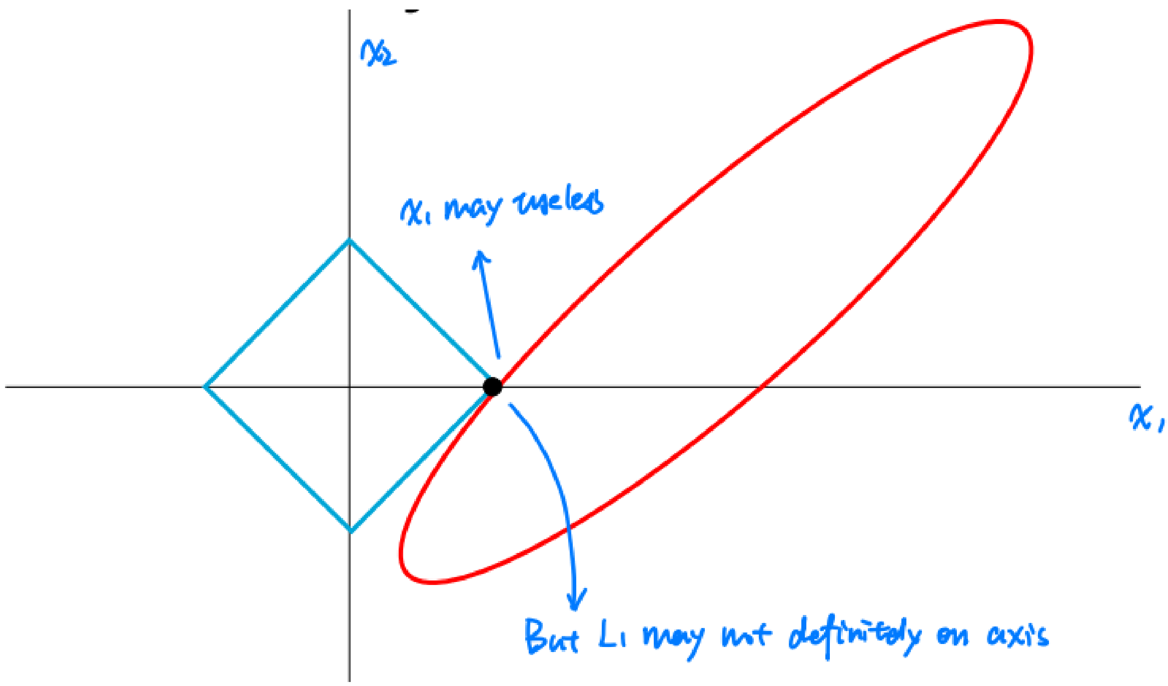
1.3. Sparsity Regularization

- <u>*Sparsity*</u>: make some w_i to zero
  - To some extend means **simplify the model** (lower down the overfitting)

1.3.1. Model

$$\begin{aligned} & \min_w \sum_{i=1}^N \left(f\left(x_i, w\right)-y_i\right)^2 \\ & \text{s.t. } \|w\|_1 \leq \tau \end{aligned} \tag{2}$$

1.3.2. Geometry



2. Bias-Variance

2.1. Bias-Variance Decomposition

Assume we have a given format of classification/regression function: f

- optimal prediction $f^*(x)$ (may not belong to $\mathbb{F}$)
- estimate based on some given data $\hat{f}(x) \in \mathbb{F}$

$$\begin{aligned} & \mathbb{E}\left[\left(f^*-\hat{f}\right)^2\right] \\ = & \mathbb{E}\left[\left(f^*-\mathbb{E} \hat{f}\right)^2\right]+\mathbb{E}\left[(\mathbb{E} \hat{f}-\hat{f})^2\right] \\ = & \text{ bias }^2+\text{ variance } \end{aligned} \tag{3}$$

Understanding

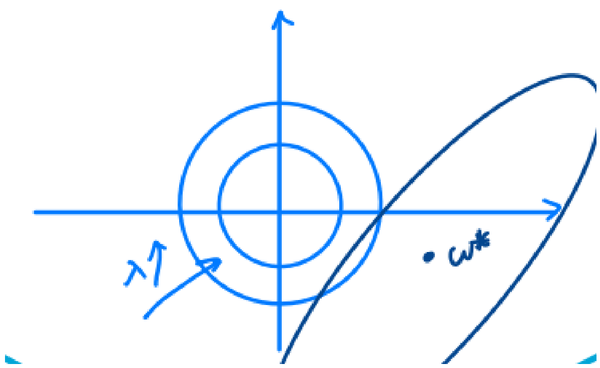
- bias is something like "inherent error" between model assumption and real optimal function

- regression is the sensitivity of the given assumption regarding to dataset

2.2. Bias-Variance Tradeoff and Regularization

larger λ

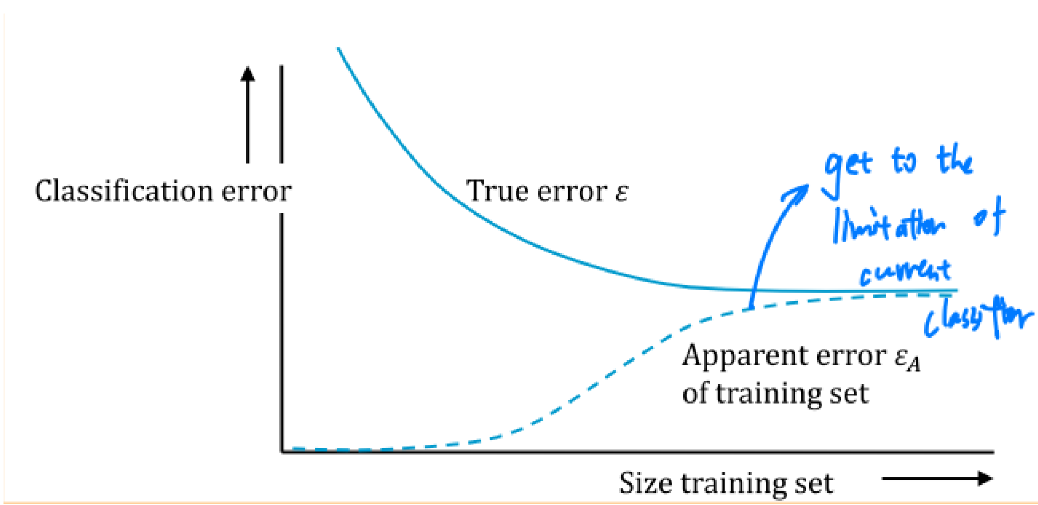
- larger bias: go away from original information from the dataset
- smaller variance: because above, dataset fluctuation is not so important



3. Evaluating Learners

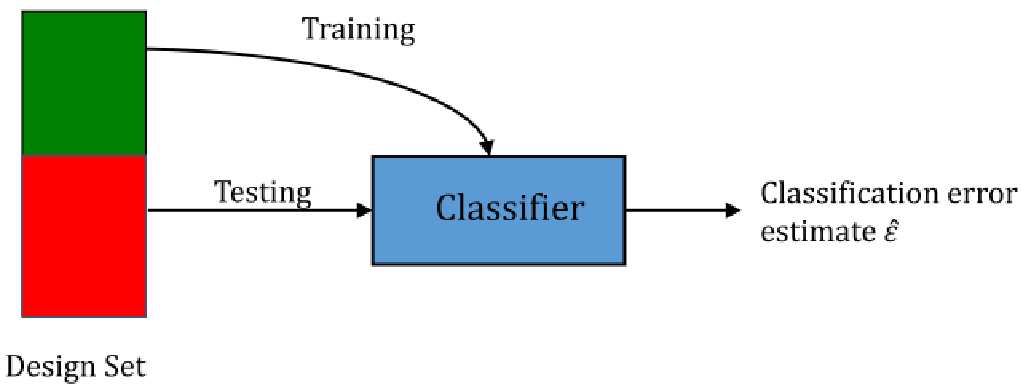
We will use **classifiers** as example

3.1. Errors

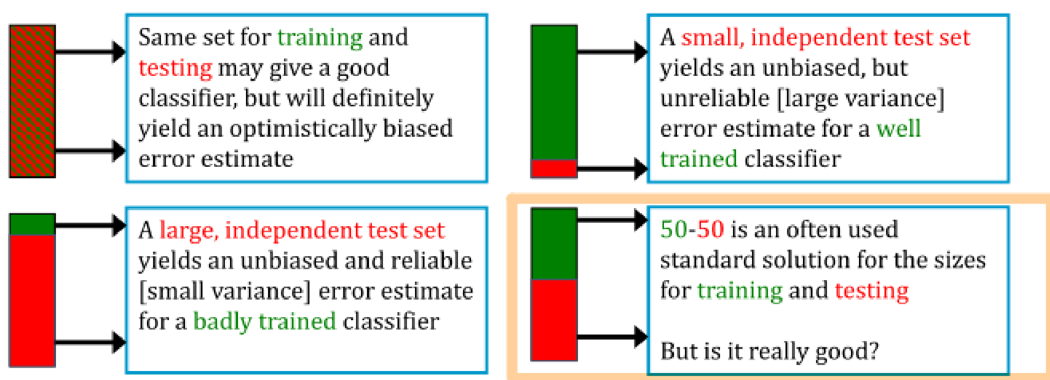


3.1.1. Estimate True Error

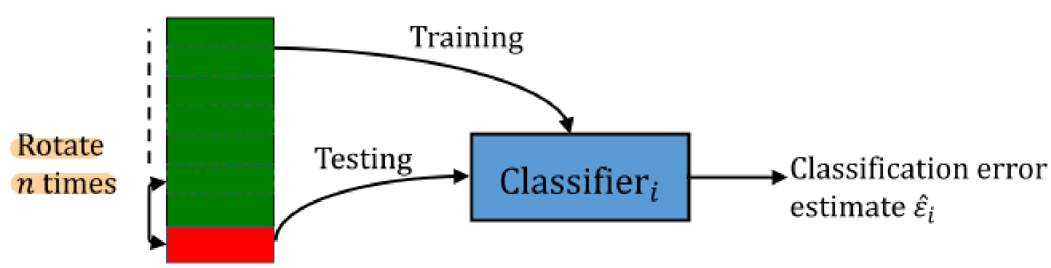
We can estimate *true error* based on test set

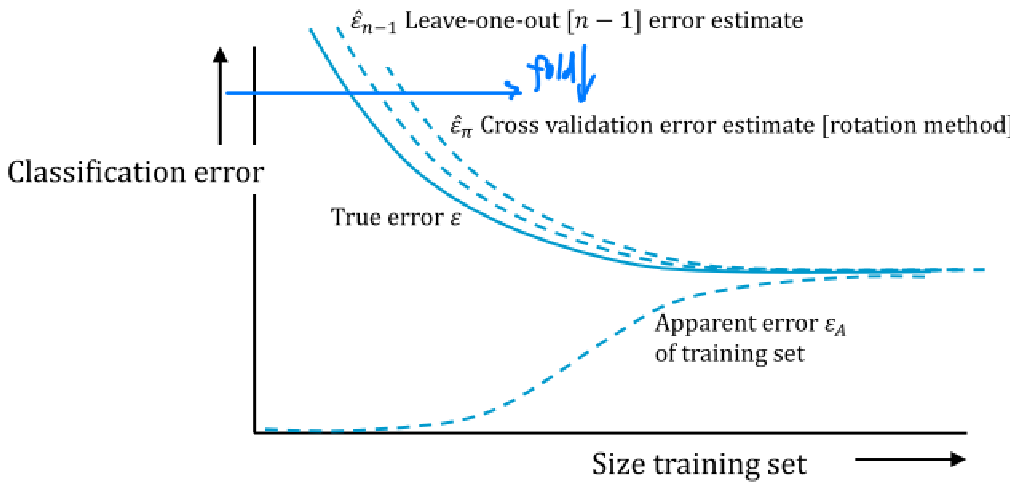


Other training set → other classifier
Other test set → other error estimate

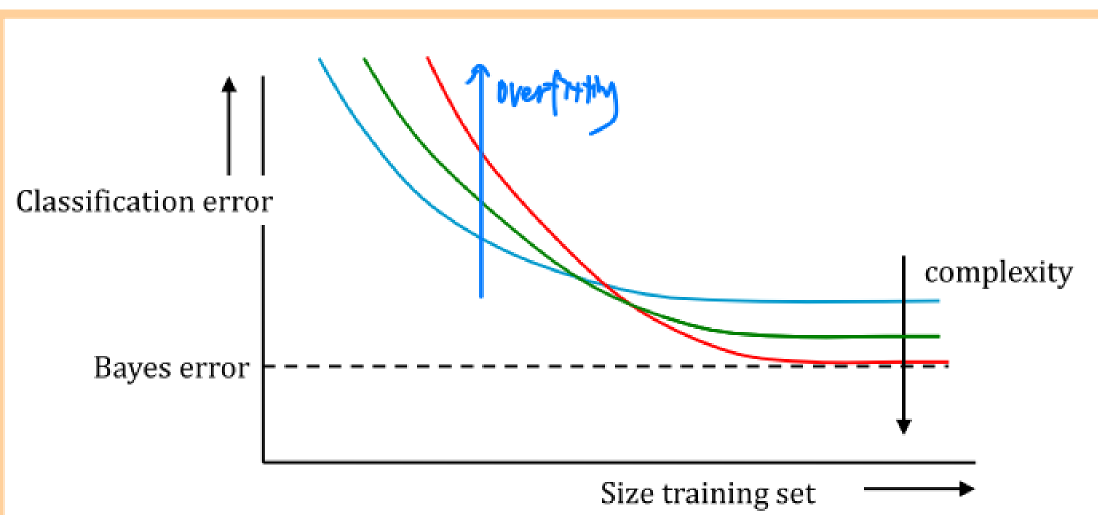


3.1.2. Cross Validation

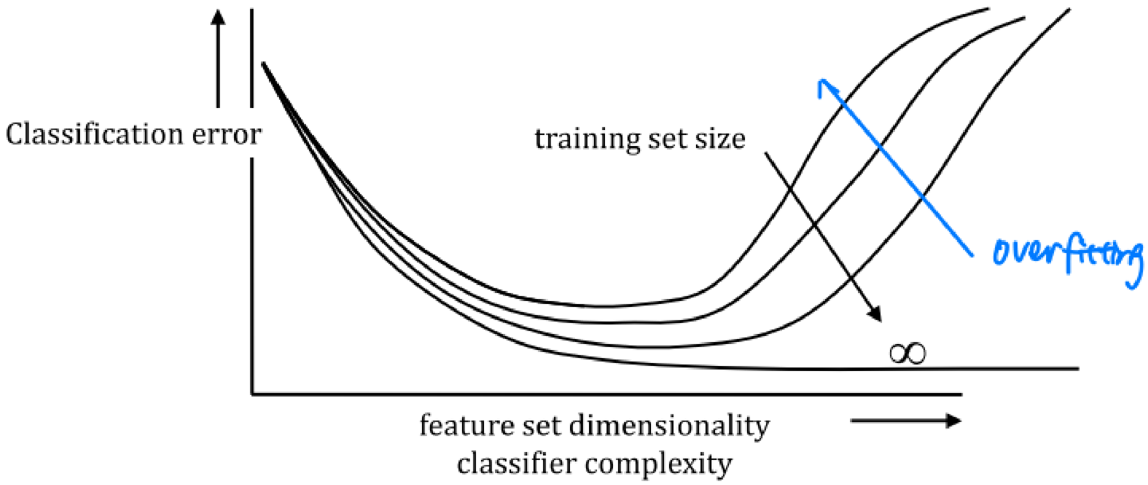




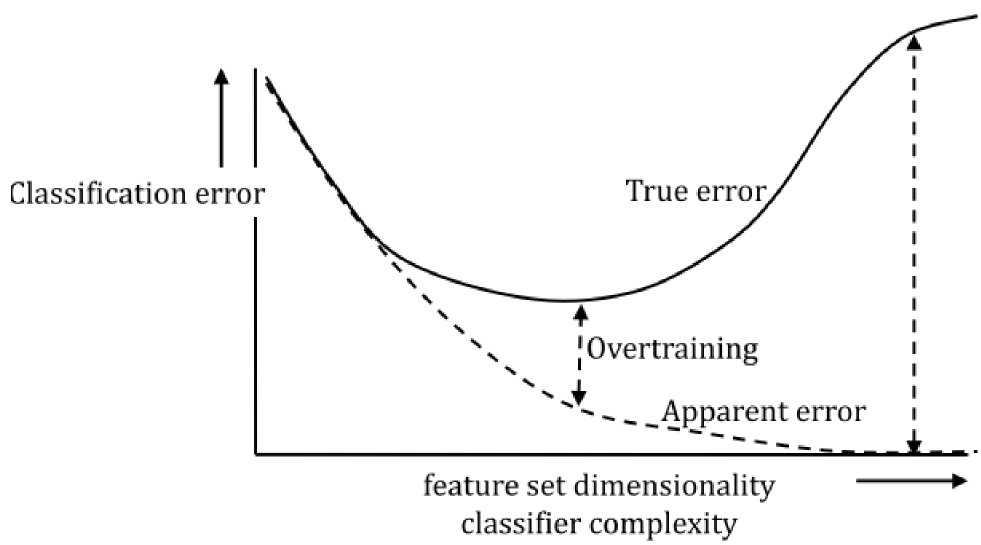
3.2. Learning Curves



3.3. Feature Curves



3.4. Curse of Dimensionality



For a given set, when the complexity is higher, whether the data set is large enough to learn all parameters of the classifier is unknown.

3.5. Confusion Matrices

Provides counts of class-dependent errors : How many object have been classified as A that should have been classified as B?