Machine Learning for Finance (FIN 570) Hyperparameter Tuning: Bias-Variance Tradeoff, Cross-Validation, and Evaluation Metric

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Regularization L-1 vs L-2

Give a penalty for complexity or overfitting. The cost function to minimize:

$$J(\boldsymbol{w}) = J_0(\boldsymbol{w}) + \lambda\, R(\boldsymbol{w}) \quad (= C\, J_0(\boldsymbol{w}) + R(\boldsymbol{w})),$$

where $J_0(\boldsymbol{w})$ is the un-regularized cost function, e.g., log-likelihood (logistic), RSS (linear) or slack variable sum (SVM).

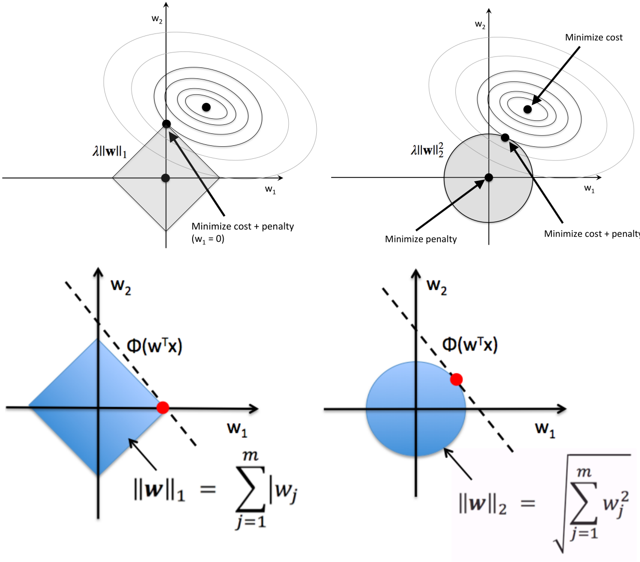
L-2 Regularization

- $R(\boldsymbol{w}) = \|\boldsymbol{w}\|_2^2 = \sum_j w_j^2$
- N-sphere boundary (e.g., circle or sphere). Easy to locate the minimum.

L-1 Regularization

- $R(\boldsymbol{w}) = \|\boldsymbol{w}\|_1 = \sum_j |w_j|$
- 'Diamond' boundary: leads to sparse vector (many zero components)
- Effectively works as feature selection

Regularization L-1 vs L-2



Measuring quality of ML method

Given a ML method, we want to minimize the mean squared error (MSE) on **test data set** (expected test MSE).

$$E\Big(y - \hat{f}(x)\Big)^2 = \text{Bias}(\hat{f}(x))^2 + \text{Var}(\hat{f}(x)) + \text{Var}(\varepsilon),$$
$$\text{where} \quad y = f(x) + \varepsilon \quad \text{(true pattern)}$$

- By "given a ML method", we mean that model (LR, SVM, etc) and hyper-parameter (C, γ, reduced dimension k for PCA/LDA, etc) are fixed. However fitted model parameters (i.e., $\hat{f}$) can change over training set.
- The expectation is made over repeatedly selecting different training vs test dataset. Therefore, the expectation is over $\hat{f}$ as well as x.
- We need to minimize Bias$(\hat{f}(x))^2$ and Var$(\hat{f}(x))$ together while Var(ε) is fundamentally irreducible.

Bias and Variance

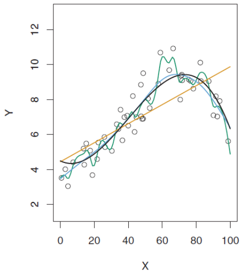
Bias

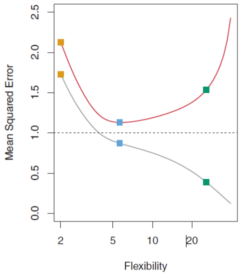
- Error from $\hat{f}$ not correctly representing the true f (e.g. linear regression on non-linear data).
- A model has **high bias** when $\hat{f}$ overly simply f (under-fitting), i.e., the used parameters are too few.

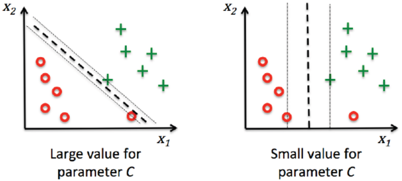
Variance

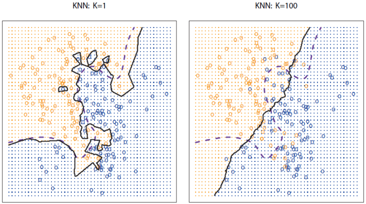
- Error from variability or sensitivity (vs consistency) of the trained model $\hat{f}$ against the selection of training dataset.
- A model has **high variance** when the model is too flexible (overfitting), i.e., there are too many parameters, e.g. KNN with $K = 1$, high-order polynomial regression, SVM/LR with large C (small λ), decision tree with many leaves, etc.

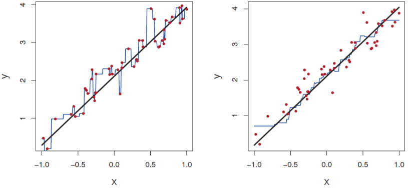
Bias and Variance (examples)







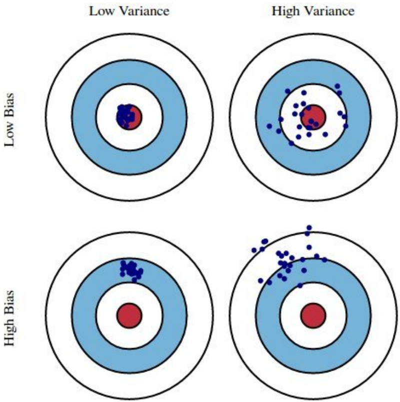




- Grey line: Bias vs the number of parameters
- Red line: MSE measured with the true f (black line).

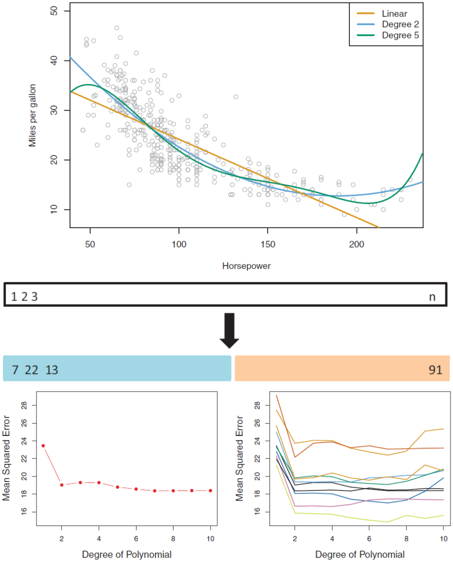
Bias-Variance Trade-off

- It is hard to reduce bias and variance simultaneously (but easy to have high bias and variance simultaneously).
- As model flexibility increases, bias decreases but variance increases. It is important to find a right trade-off.
- Bias-variance trade-off is one of the most important theme in ML (and other fields!).
- In real problems, the true pattern $f(x)$ is unknown and the dataset size is limited. How can we efficiently measure the expected test MSE?



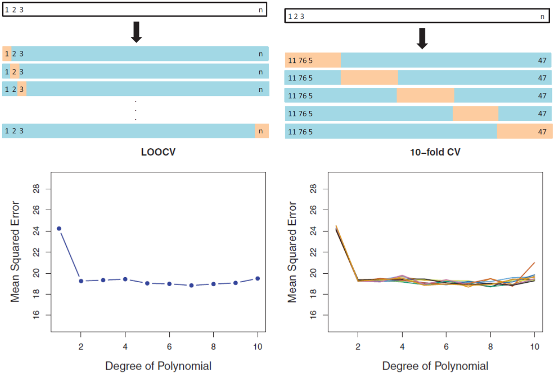
Cross-Validation(CV): Validation Set (Hold-out set)

- Divide observations into a **training set** and a **validation (hold-out) set**.
- Fit model on the training set and measure error on the validation set.
- Error rate is highly variable (sensitive to division) and over-estimated than the true test error rate as the model is trained on fewer observations.
- Training set is further divided into **training** and **validation** sets. Validation set is used for model selection and hyper-parameter funning.

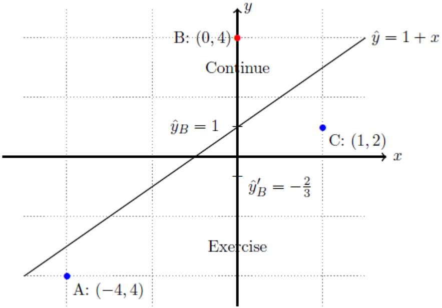


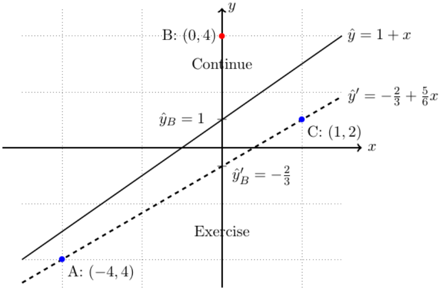
Cross-Validation: Leave-One-Out (LOOCV) and k-Fold CV

- LOOCV: train model with one sample left out and measure the error on the sample. Error is close to the true test rate but computation is heavy (train n times).
- k-fold CV: divide the samples into k (typically 5 or 10) folds. Train model on $k-1$ **training** folds and measure error on the remaining **test** fold.



- LOOCV can be computed analytically in linear regression.
- An example with 3 data points:





LOOCV in linear regression (2/3)

The multivariate regression $Y \sim X\beta$:

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{H}\boldsymbol{y}, \quad \text{where} \quad \boldsymbol{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y},\ \boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T$$

$$\boldsymbol{y} = \begin{bmatrix} \vdots \\ y_j \\ \vdots \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} \vdots \\ -\boldsymbol{x}_j- \\ \vdots \end{bmatrix} \begin{matrix} (M \times N) \\ (M \ll N) \end{matrix}, \qquad \begin{matrix} \boldsymbol{x}_j : j\text{-th row vector of } \boldsymbol{X} \\ y_j : j\text{-th value of } \boldsymbol{y} \end{matrix}$$

Let $\boldsymbol{X}_{\text{-}j}$ and $\boldsymbol{y}_{\text{-}j}$ be $\boldsymbol{X}$ and $\boldsymbol{y}$ with j-th row removed, respectively.
To compute the regression coefficients $\boldsymbol{\beta}_{\text{-}j}$ from $\boldsymbol{X}_{\text{-}j}$ and $\boldsymbol{y}_{\text{-}j}$, we use

$$\boldsymbol{X}_{\text{-}j}^T\boldsymbol{X}_{\text{-}j} = \boldsymbol{X}^T\boldsymbol{X} - \boldsymbol{x}_j^T\boldsymbol{x}_j, \quad \boldsymbol{X}_{\text{-}j}^T\boldsymbol{y}_{\text{-}j} = \boldsymbol{X}^T\boldsymbol{y} - \boldsymbol{x}_j^T y_j,$$

and the Sherman-Morrison formula, (intuition: $\frac{1}{X-\varepsilon} \approx \frac{1}{X} + \frac{\varepsilon}{X^2}$)

$$(\boldsymbol{X}_{\text{-}j}^T\boldsymbol{X}_{\text{-}j})^{-1} = (\boldsymbol{X}^T\boldsymbol{X})^{-1} + \frac{(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{x}_j^T\boldsymbol{x}_j(\boldsymbol{X}^T\boldsymbol{X})^{-1}}{1-h_j},$$

where $\boldsymbol{h}$ be the diagonal vector of the hat matrix $\boldsymbol{H}$:

$$\boldsymbol{h} = \text{diag}\left(\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\right) \quad \text{or} \quad h_j = \boldsymbol{x}_j(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{x}_j^T$$

LOOCV in linear regression (3/3)

- The regression coefficients $\hat{\boldsymbol{\beta}}_{\text{-}j}$ (the j-th sample removed) is

$$\begin{aligned}\hat{\boldsymbol{\beta}}_{\text{-}j} &= (\boldsymbol{X}_{\text{-}j}^T \boldsymbol{X}_{\text{-}j})^{-1} \boldsymbol{X}_{\text{-}j}^T \boldsymbol{y}_{\text{-}j} \\ &= \left((\boldsymbol{X}^T \boldsymbol{X})^{-1} + \frac{(\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x}_j^T \boldsymbol{x}_j (\boldsymbol{X}^T \boldsymbol{X})^{-1}}{1 - h_j} \right) (\boldsymbol{X}^T \boldsymbol{y} - \boldsymbol{x}_j^T y_j) \\ &= \hat{\boldsymbol{\beta}} - (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x}_j^T \frac{e_j}{1 - h_j} \quad \text{for the prediction error } \boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}.\end{aligned}$$

- Moreover, the corrected estimation values $\hat{\boldsymbol{y}}'$ and the new prediction errors $\boldsymbol{e}'$ for all points are obtained in one go as

$$\hat{\boldsymbol{y}}' = \hat{\boldsymbol{y}} - \frac{\boldsymbol{h} \cdot \boldsymbol{e}}{\boldsymbol{1} - \boldsymbol{h}} \quad \text{or} \quad \boldsymbol{e}' = \frac{\boldsymbol{e}}{\boldsymbol{1} - \boldsymbol{h}},$$

  where $\cdot$ and the fraction are the element-wise operations.
- Given that $0 < h_j < 1$, the correction is always in the direction of reducing over-fitting or increasing the prediction error.
- Little extra computation: $\boldsymbol{h}$ is a byproduct of the regression.

$$\boldsymbol{h} = \text{row sum}(\boldsymbol{X} \cdot \boldsymbol{X}(\boldsymbol{X}^T \boldsymbol{X})^{-1}) \Leftarrow \boldsymbol{\beta} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

Evaluation Metrics

Confusion Matrix

Credit card Default		Predicted P^*	Predicted N^*	Total
Actual	P	40	40	80
Actual	N	10	910	920
	Total	50	950	1000

Predicted class

		P^*	N^*
Actual class	P	True positives (TP)	False negatives (FN)
Actual class	N	False positives (FP)	True negatives (TN)

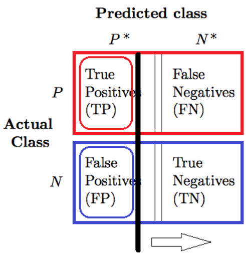
- Accuracy ($\texttt{ACC}$) $= \dfrac{\text{TP}+\text{TN}}{\text{ALL}} = \dfrac{40+910}{1000} = 95\%$
- Error ($\texttt{ERR}$) $= 1 - \text{ACC} = \dfrac{\text{FP}+\text{FN}}{\text{ALL}} = \dfrac{10+40}{1000} = 5\%$
- However, accuracy/error may be misleading!

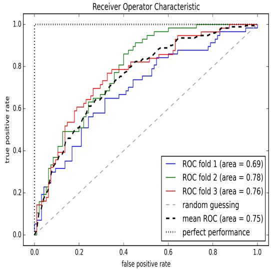
Evaluation Metrics

		Predicted	
		P^*	N^*
Actual	P	TP (40)	FN (40)
	N	FP (10)	TN (910)

- Precision ($\texttt{PRE}$) $= \dfrac{\text{TP}}{P^*} = \dfrac{\text{TP}}{\text{TP}+\text{FP}} = \dfrac{40}{50} = 80\%$
  Case: Spam mail filter (minimize FP)
- Recall ($\texttt{REC}$) $= \dfrac{\text{TP}}{P} = \dfrac{\text{TP}}{\text{TP}+\text{FN}} = \dfrac{40}{80} = 50\%$
  Case: Credit approval, Cancer diagnosis (minimize FN)
- F1-Score ($\texttt{F1}$) $= \dfrac{2\,\text{PRE}\times\text{REC}}{\text{PRE}+\text{REC}} = 61.5\%$ $\quad \left(\dfrac{2}{\text{F1}} = \dfrac{1}{\text{PRE}} + \dfrac{1}{\text{REC}}\right)$
  The harmonic average of PRE and REC to ensure $0 \le \text{F1} \le 1$
  A widely used accuracy for binary classification with imbalanced sample.

Receiver Operator Characteristic (ROC) Curve





- True Positive Rate (TPR=REC) = TP$/P = 50\%$
- False Positive Rate (FPR) = FP$/N = 10/920 = 1.1\%$
- ROC curve is the set of (FPR, TPR) points for different classification binary classification threshold p from 0 to 1.
- Area under the curve (AUC) gives an accuracy of a classifier summarizing over all possible threshold
  - Perfect model: ROC AUC = 1 (Γ-shaped lines)
  - Random guess: ROC AUC = 0.5 ($y = x$ line, TPR=FPR=$1 - p$)
  - A model with ROC AUC < 0.5 is worthless.

Dealing with Class Imbalance

- Class imbalance is common, causing the model biased to the majority class.
- Use alternative metrics (e.g., PRE, REC, F1) in model selection.
- Use `class_weight='balanced'` option in sklearn. If r is the ratio of the minority class,

$$\log L = \sum_i \frac{y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i)}{w_i}, \quad w_i = \begin{cases} 2r & \text{if } y_i = 1 \\ 2(1-r) & \text{if } y_i = 0 \end{cases}$$

- Undersampling: delete majority class samples.
- Oversampling: add copies of minority class samples.
- Synthetic Minority Oversampling Technique (SMOTE): imbalanced-learn package