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).

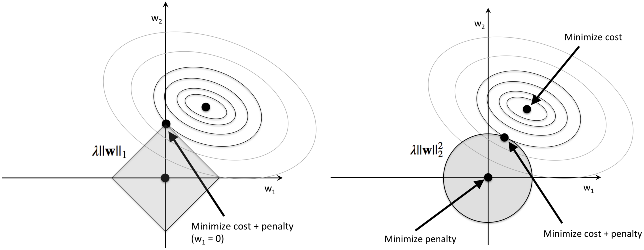
L-2 Regularization

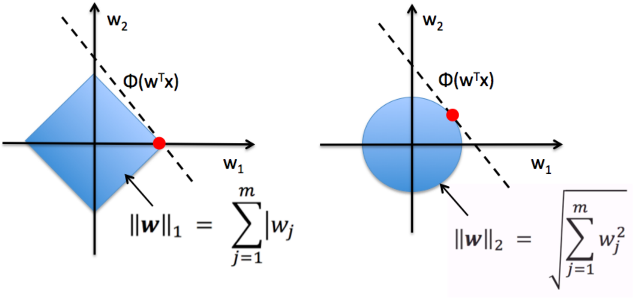
- $R(\boldsymbol{w}) = ||\boldsymbol{w}||_2^2 = \sum_j w_j^2$
- N-sphere boundary (e.g., circle or sphere). Easy to solve the minimum.

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).

$$E\Big(y - \hat{f}(x)\Big)^2 = \mathsf{Bias}(\hat{f}(x))^2 + \mathsf{Var}(\hat{f}(x)) + \mathsf{Var}(\varepsilon)$$

$$\text{where,} \quad y = f(x) + \varepsilon \quad \text{(true pattern)}$$

- By *a given 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

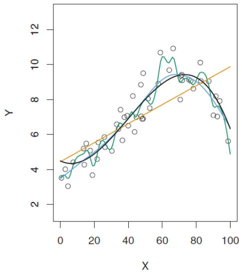
Bias

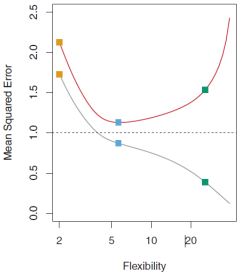
- Error from $\hat{f}$ not correctly representing the true f (e.g. linear regression on non-linear data).
- A model has **high bias** when $\hat{f}$ overly simply f (under-fitting), i.e., the used parameters are too few.

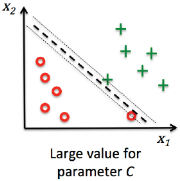
Variance

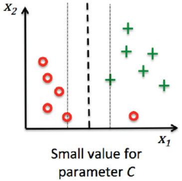
- Error from variability or sensitivity (vs consistency) of the trained model $\hat{f}$ against the selection of training dataset.
- A model has **high variance** when the model is too flexible (overfitting), i.e., there are too many parameters, e.g. KNN with $K = 1$, high-order polynomial regression,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

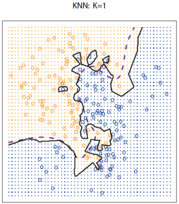
Bias and Variance (examples)

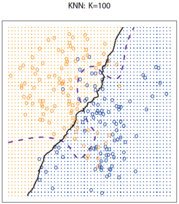


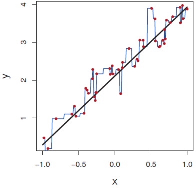


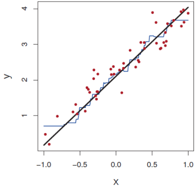








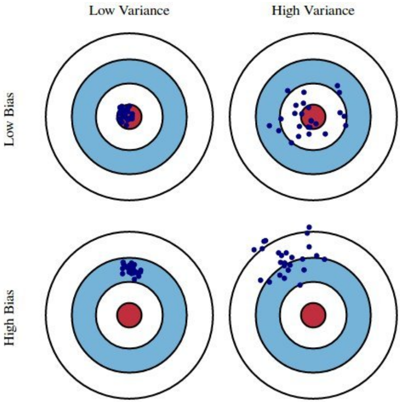




- Grey line: Bias vs the number of parameters
- Red line: MSE measured with the true f (black line).

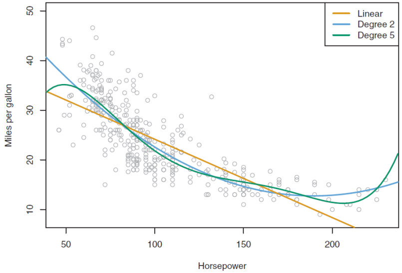
Bias-Variance Tradeoff

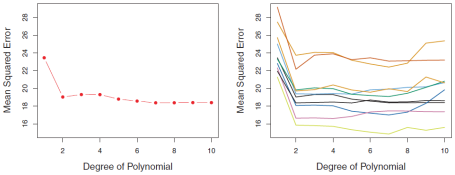
- It is hard to reduce both bias and variance.
- As the model flexibility increase, bias decreases but variance increases. It is important to find a right trade-off.
- Bias-variance tradeoff is one of the most important theme in ML (and other fields!).
- In real problems, the true pattern f is unknown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



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

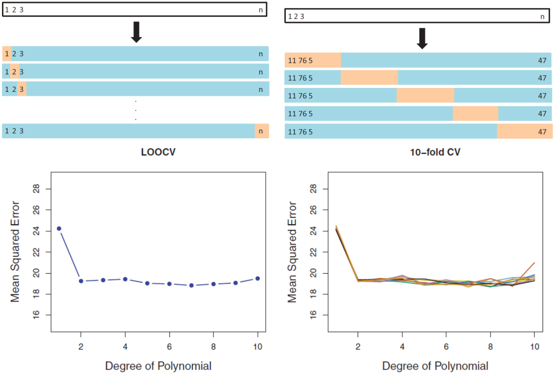
- Divide observations into a **training set** and a **validation (hold-out) set**.
- Fit model on the training set and measure error on the validation set.
- Error rate is highly variable (sensitive to division) and over-estimated than the true test error rate as the model is trained on fewer observations.
- 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.



Evaluation Metrics

Confusion Matrix

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

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

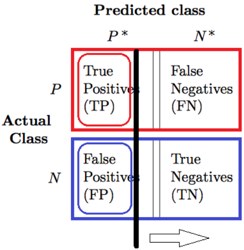
- Accuracy (ACC) $= \dfrac{\text{TP} + \text{TN}}{\text{ALL}} = \dfrac{40 + 910}{1000} = 95\%$
- Error (ERR) $= 1 - \text{ACC} = \dfrac{\text{FP} + \text{FN}}{\text{ALL}} = \dfrac{10 + 40}{1000} = 5\%$
- However, accuracy/error may be misleading!

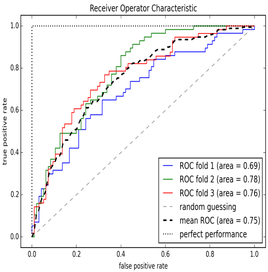
Evaluation Metrics

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

- Precision (PRE) $= \dfrac{\text{TP}}{P^*} = \dfrac{\text{TP}}{\text{TP}+\text{FP}} = \dfrac{40}{50} = 80\%$
  Case: Spam mail filter (minimize FP)
- Recall (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 (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: graph of (FPR, TPR) for varying classification threshold of the binary classification.
- Area Under Curve (AUC) give an overall accuracy of a classifier, summarizing over all possible threshold
- The diagonal line is from random-guessing: ROC AUC $=$ 0.5
  A model with lower AUC than 0.5 is worthless.
- A perfect classifier (Γ-shaped lines): ROC AUC $=$ 1.