Cross-Validation and Hyper-parameter Search

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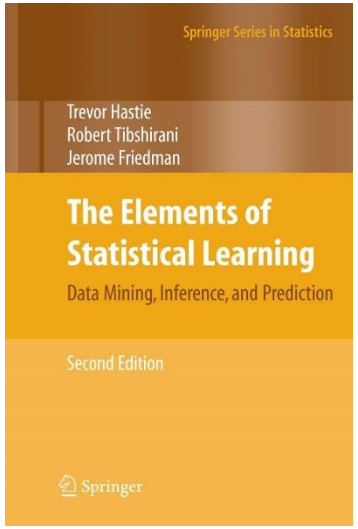
Outline

- How to Validate Models?
    - Holdout Validation
    - K-Fold Cross-Validation
    - Other Variants

- Hyper-parameter Search Methods
    - Grid Search
    - Random Search
    - Optuna

Hastie *et al.* (2008)
The Elements of Statistical Learning.
2nd Ed. Springer.



Bishop (2006)
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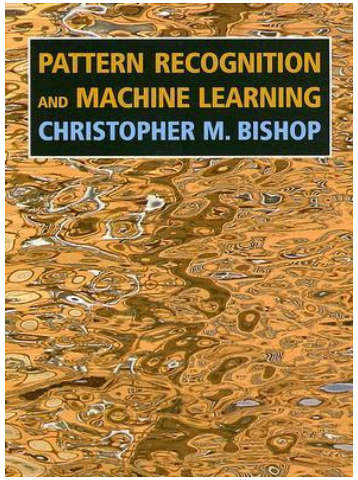
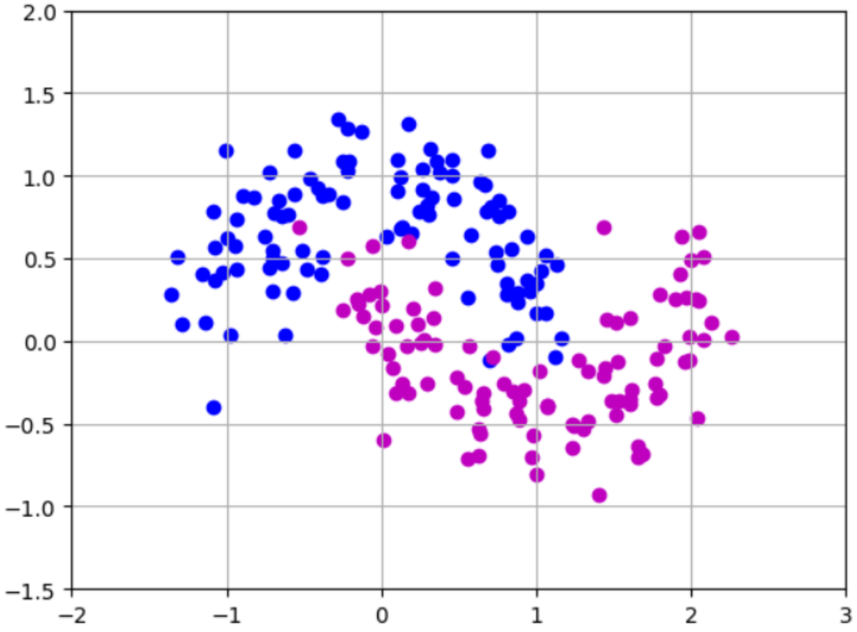


Why validate our models?

Example 1: Two Moons Data Set

Given the following binary classification data set, fit an SVM classifier with $C = 20$ and default kernel in Scikit-learn.



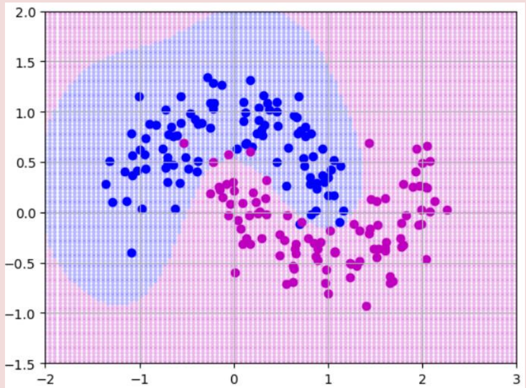
SVM without Validation

- All data points were used to train the SVM. No data points are left to test if the SVM would work well in practice!

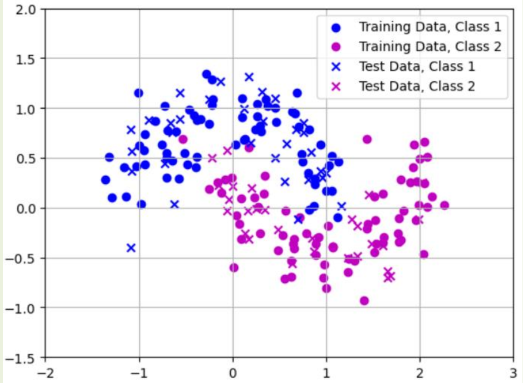
97.0%
Accuracy

99	1
5	95

Confusion matrix



SVM with Validation



- Prior to analysis, the data was split:
  - **70% Training, 30% Testing**

- Reported accuracies:

97.8%
Training accuracy

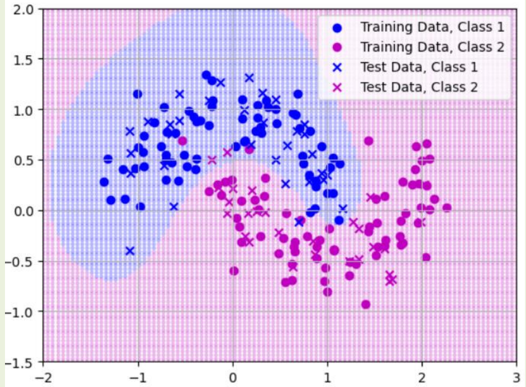
93.3%
Test accuracy

67	1
2	70

Training confusion matrix

30	2
2	26

Test confusion matrix



Model Validation

What we did here is called Holdout Validation.

SVM with Validation

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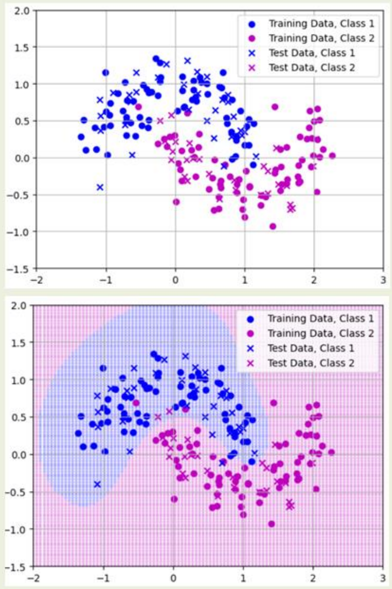
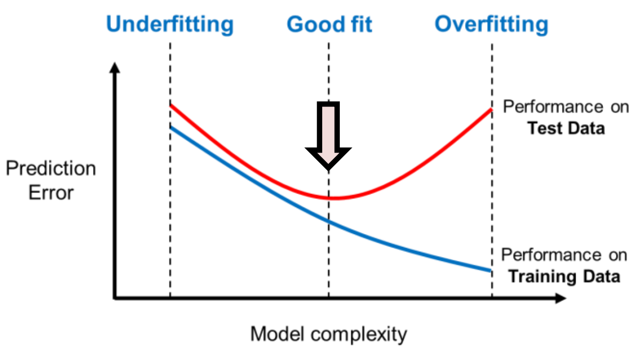
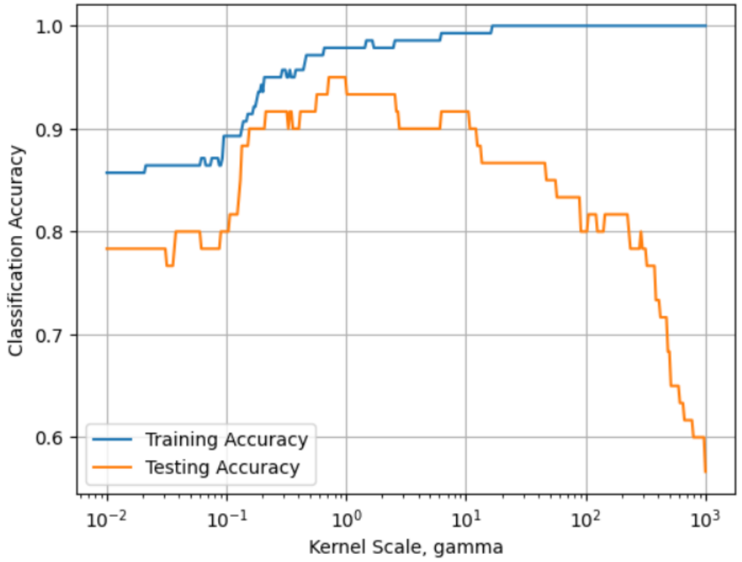
Test confusion matrix



Holdout Validation

- Split data set into Training and Testing.
- Split can be 70%-30%, 60%-40%, or 85%-15%.
- Test data are “held out” from the training phase.
- Avoid data leakage! Test data should be independent from training data.
- We can investigate the testing accuracy while varying a hyper-parameter in the model:
  - In our example, here are the SVM training and testing accuracies at varying values of the *RBF kernel scale*, all others being constant.
  - We can see the regions where SVM underfits and overfits.





Model Validation

Holdout Validation

- Train the model 1 time, validate it 1 time.
- Validation score is the score for the test data.

Train (70%)	Test (30%)

K-fold Cross-Validation

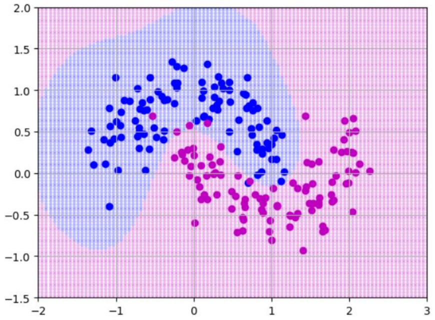
- Train the model K times, validate it K times.
- Overall cross-validation score is the average of K results.
- Data set is used more wisely than holdout.

				Test
			Test	
		Test		
	Test			
Test				

5-fold

Example 1: Two Moons Data Set

- No need to explicitly split the data in the code.
- We only need to specify the no. of splits, K.



5-fold Test Accuracies

100%
95%
95%
92.5%
97.5%

5-fold Cross-validation Score

96%

± 0.029

10-fold Cross-validation Score

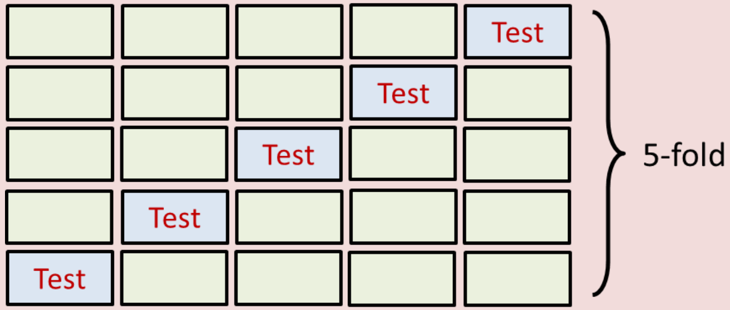
96%

± 0.032

Model Validation

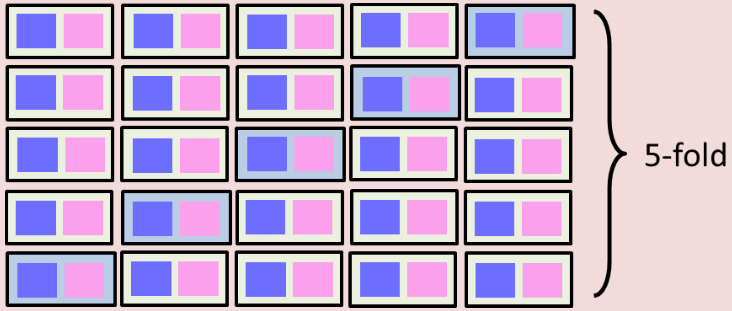
K-fold Cross-Validation

- Train the model K times, validate it K times.
- Overall cross-validation score is the average of K results.
- Data set is used more wisely than Holdout.

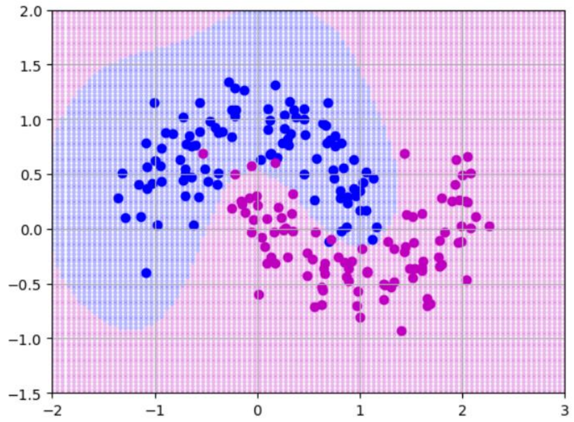


Stratified K-fold Cross-Validation

- Same as K-fold cross-validation but the percentage of samples from each class is *preserved*.



Example 1: Two Moons Data Set



Results for an SVM classifier with $C = 20$ and default kernel in Scikit-learn:

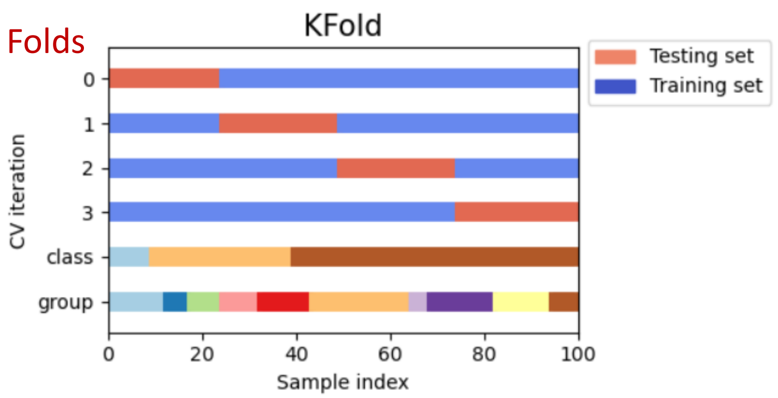
5-fold Cross-validation Score	10-fold Cross-validation Score	5-fold Stratified Cross-validation Score
96% ± 0.029	**96%** ± 0.032	**96.5%** ± 0.029

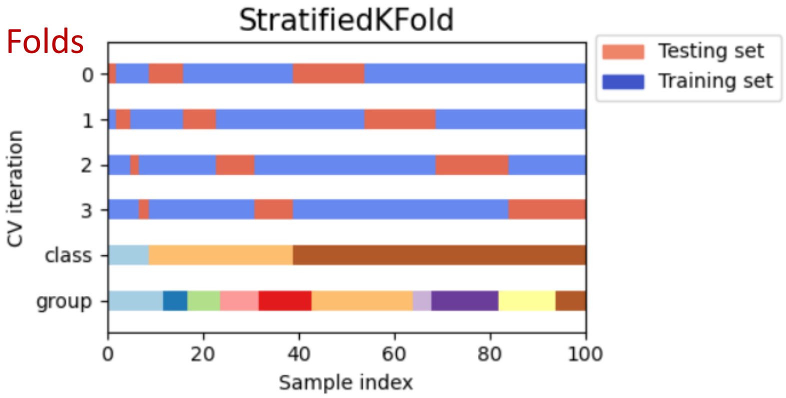
Model Validation

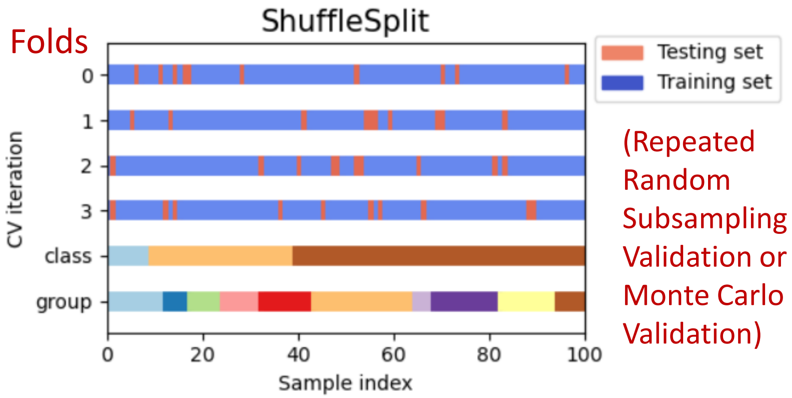
An example of “grouped” data is when medical samples are taken multiple times from one patient: Samples from one patient is one group.

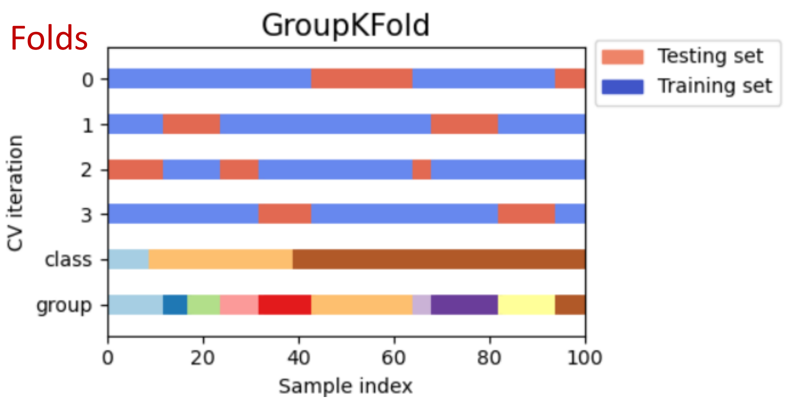
Other Kinds of Validation Schemes

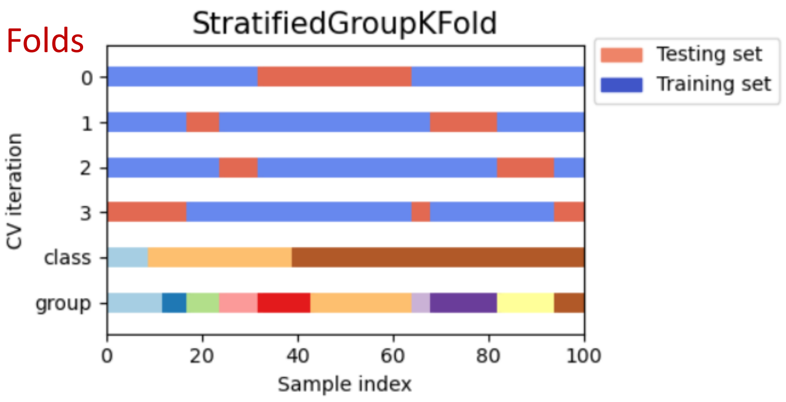
Say we have 100 randomly generated input datapoints, with 3 classes split unevenly across datapoints, and 10 “groups” split unevenly across datapoints. Different validation schemes utilize group and class info differently.

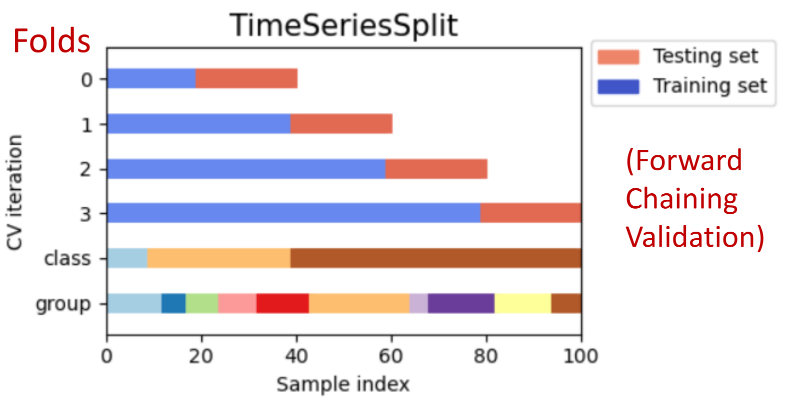




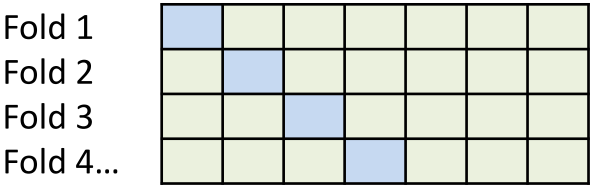






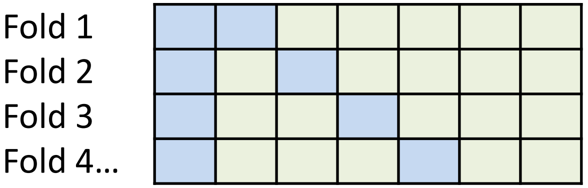


Model Validation: Other Variants



Leave-one-out Cross-Validation (LOOCV)

- Same as **N**-fold cross-validation, where **N** is the number of samples.
- In each fold, **test data size is always 1**.
- **Total number of folds is always N**.



Leave-P-out Cross-Validation (LPOCV)

- Also similar with K-fold cross-validation.
- In each fold, **test data size is always P**.
- **Total number of folds is always Combination(N, P)**, since all possible ways to take P samples from N are exhausted.
- Difference between LPOCV and K-fold CV with K=N-P:
  LPOCV may create *overlapping* test data sets, but K-fold CV ensures that test data in each fold do not overlap.

Results for an SVM classifier with $C = 20$ and default kernel in Scikit-learn:

5-fold Cross-validation Score	10-fold Cross-validation Score	5-fold Stratified Cross-validation Score	LOOCV Score	L-2-OCV Score	Monte Carlo Validation Score
96%	**96%**	**96.5%**	**96%**	**96%**	**96%**
± 0.029	± 0.032	± 0.029	± 0.196	± 0.139	± 0.029

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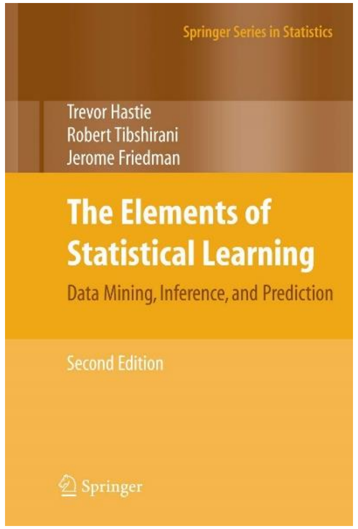

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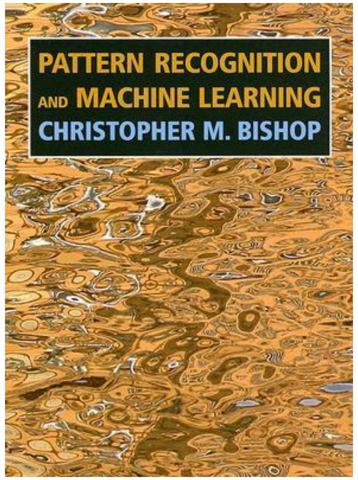


Hyper-parameter Tuning

<u>Model Parameters</u>

The knobs in the model that are tuned upon exposure to training data. (e.g. $\boldsymbol{w}, \boldsymbol{b}$)

<u>Hyper-parameters</u>

The knobs in the model that are tuned **prior** to exposure to training data. (e.g. λ, l)

- Often, hyper-parameters are just tuned manually based on user experience (e.g. heuristics).
- Different hyper-parameter settings can give different models.
- Their values control the training behavior itself.

Examples

	Model Parameters	Hyper-Parameters
Linear Regression	Weights, w	Regularization parameter, λ Type of regularization
Logistic Regression	Weights, w	Regularization parameter, λ Type of regularization Solver
Locally Weighted Regression	Weights, w	Weighting function, ω Bandwidth, τ
Support Vector Classifier	Dual variables, α Bias, b	Kernel type Kernel scale Box constraint Multi-class strategy

Hyper-parameter Tuning

<u>Model Parameters</u>

The knobs in the model that are tuned upon exposure to training data. (e.g. $\boldsymbol{w}, \boldsymbol{b}$)

<u>Hyper-parameters</u>

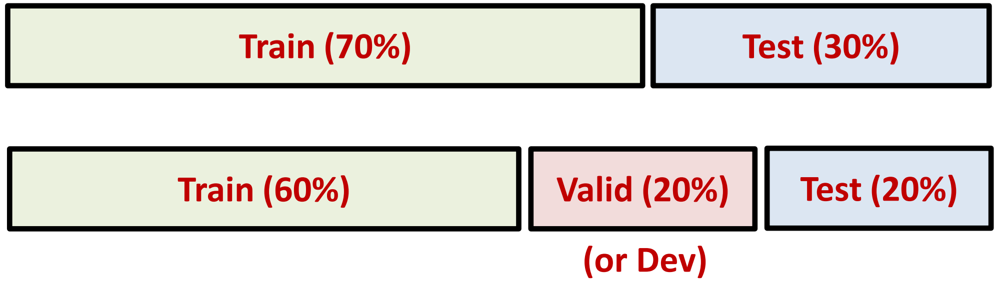
The knobs in the model that are tuned **prior** to exposure to training data. (e.g. λ, l)

To perform hyper-parameter tuning, we now need a **validation data set** aside from the training and test data sets.

Holdout Validation: *Revisited*

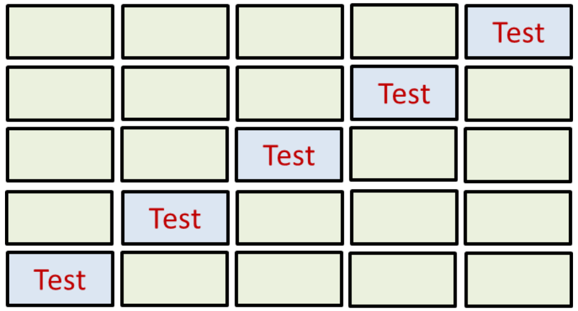
If we wish to **validate** a single model:

If we wish to **tune** a model's hyper-parameters:

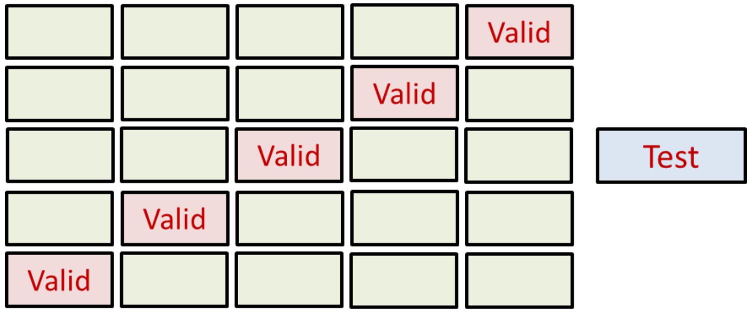


K-fold Cross-Validation: *Revisited*

If we wish to **validate** a single model:

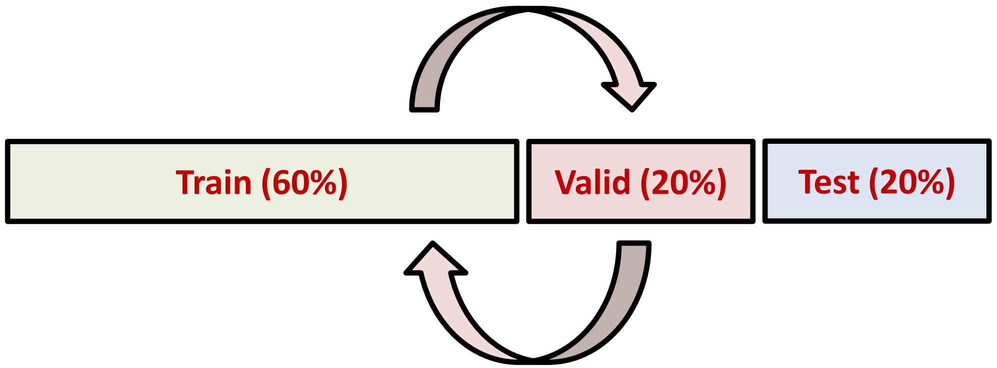


If we wish to **tune** a model's hyper-parameters:

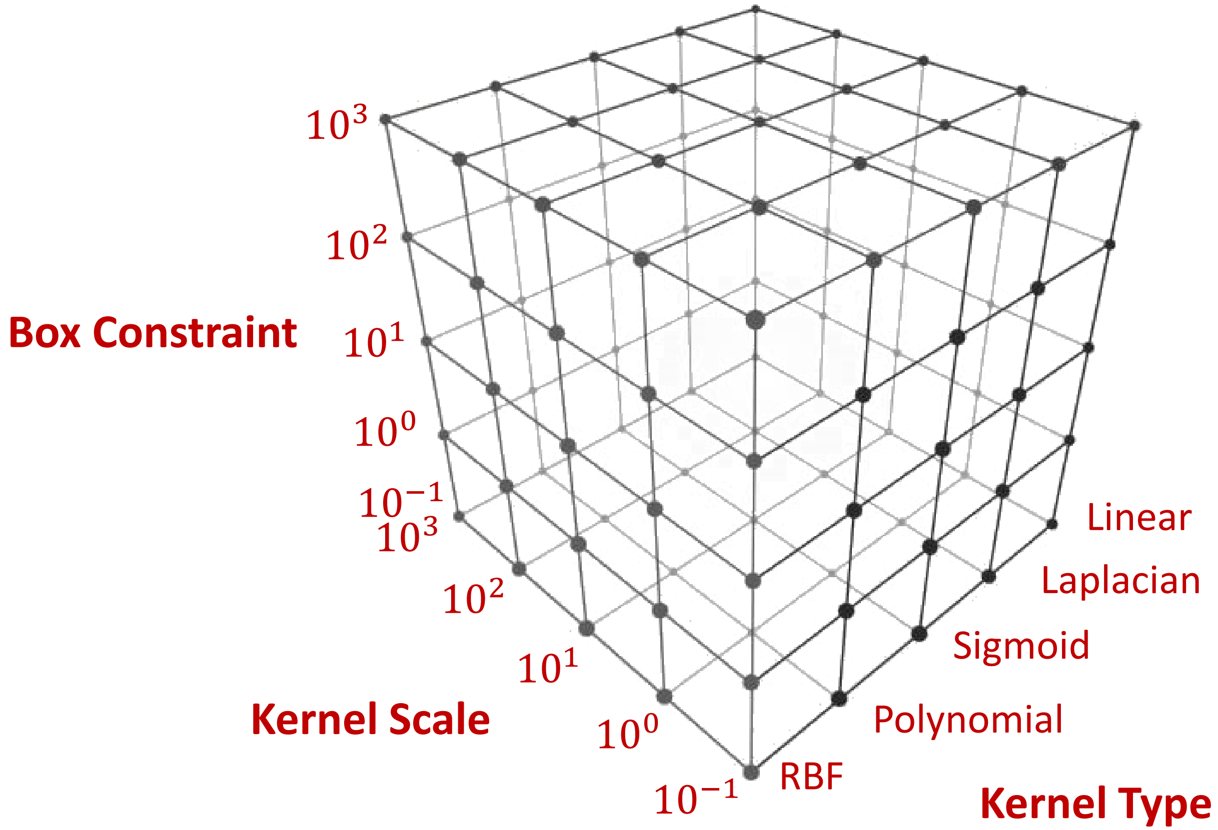


Hyper-parameter Tuning: Grid Search

1. Define a hyper-parameter grid.
2. For each hyper-parameter combination,
   a. Train a candidate model using training data.
   b. Compute its performance on the validation data.
3. Report the hyper-parameter combination with the *highest score* on validation data.
4. Make one final validation on test data.

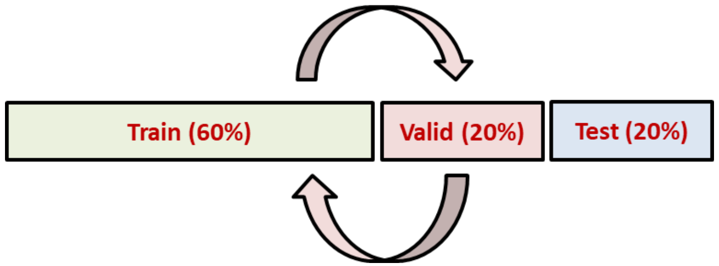


For example, in the Support Vector Classifier:



Hyper-parameter Tuning: Random Search

- Random Search acknowledges that some hyper-parameters are unimportant to investigate.
- Instead of checking the entire grid of candidate parameters, searching randomly inside the search space is more efficient (Bergstra and Bengio, 2012).
- Search range can be a distribution rather than just a list of values as in Grid Search.
- Only need to specify how many times (n_iter) we sample the search space.



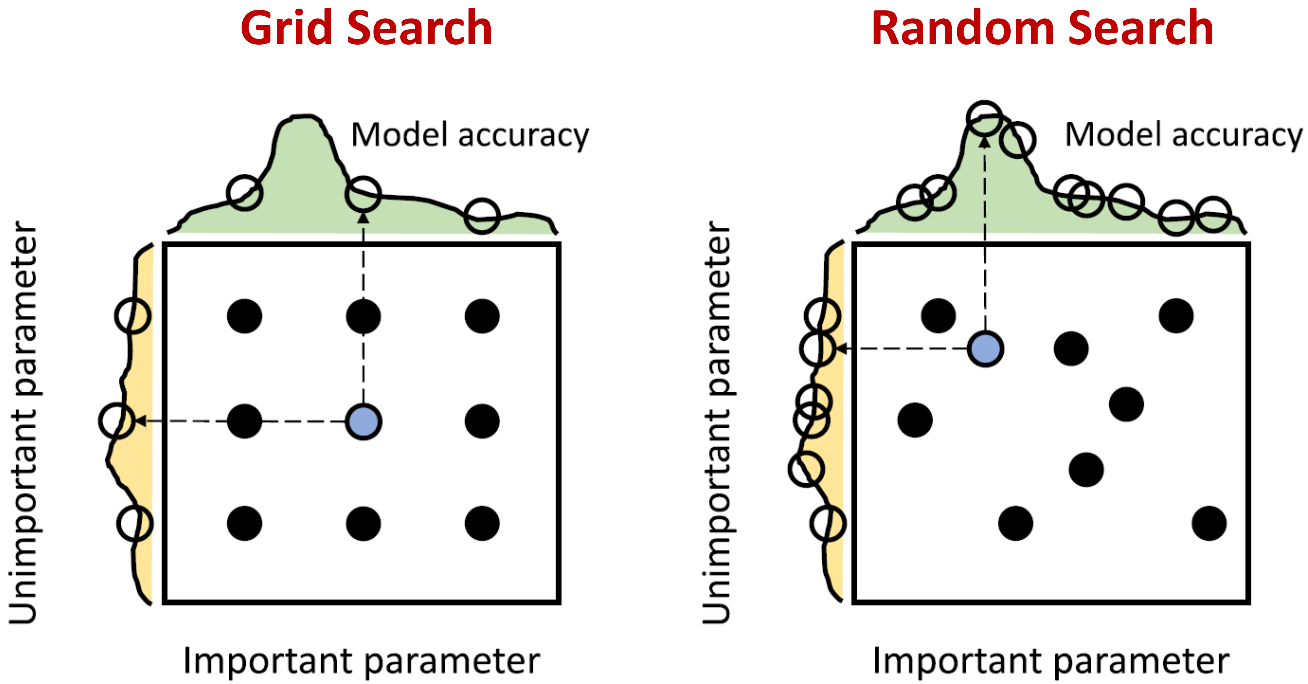


Figure from Pilario et al., (2021). A Kernel Design Approach to Improve Kernel Subspace Identification. IEEE Trans. On Industrial Electronics. 68(7): 6171-6180.

Hyper-parameter Tuning

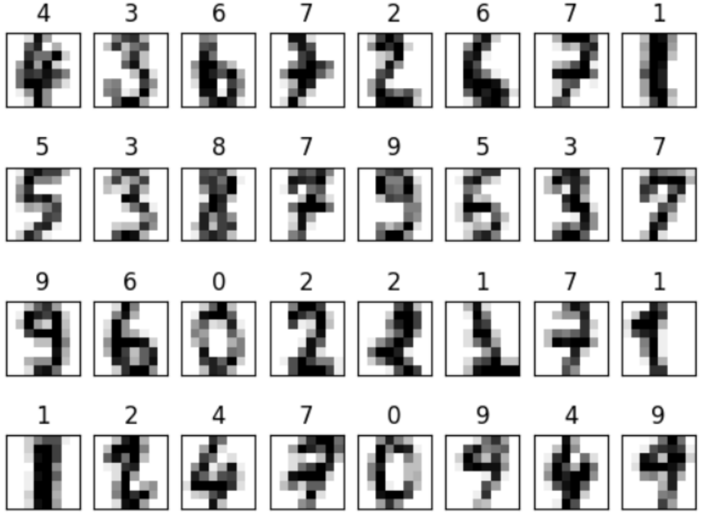
Example 2: 8x8 Handwritten Digit Recognition

Source: https://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits

- Each datapoint is an 8x8 image of a digit.
- Available in scikit-learn datasets as "load_digits."
- Other details:
  - Classes: 10 (0, 1, 2, 3, 4, 5, 6, 7, 8, 9)
  - Samples per class: ~180
  - Total no. of samples: 1797
  - Dimensionality: 64
  - Feature values: 0 to 16

Tune an SVM with the following hyper-parameter value grid candidates:

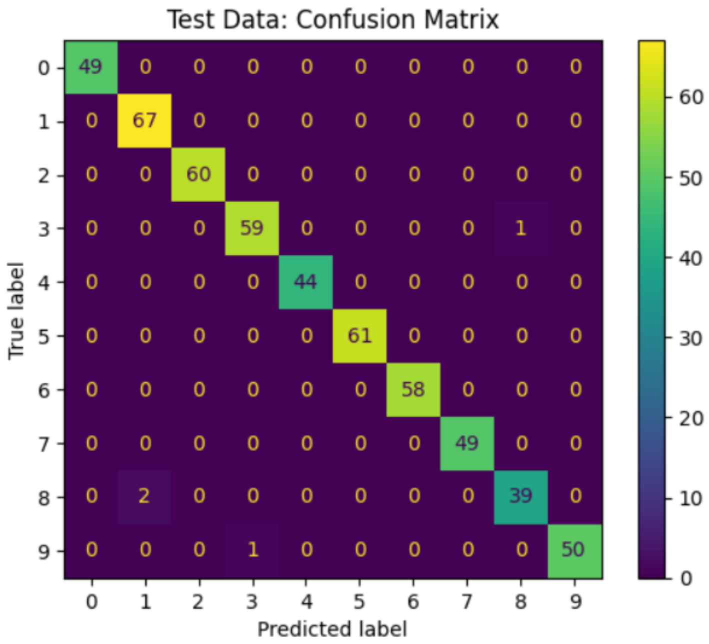
C: $10^{-1}, 10^{0}, 10^{1}, 10^{2}, 10^{3}$
Gamma: $10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}$
Kernel: RBF, Poly, Linear, Sigmoid



Grid Search Results

Best SVM:
C = 1
Gamma = 0.001
Kernel = RBF

Accuracy: 0.99
No. of Trials: 100
Runtime: 60.83 sec



Note: GridSearchCV uses the following defaults:

- Score is based on Stratified 5-fold cross-validation.
- For classification, the performance metric being optimized is the accuracy score.
- The multi-class strategy is one-vs-rest.

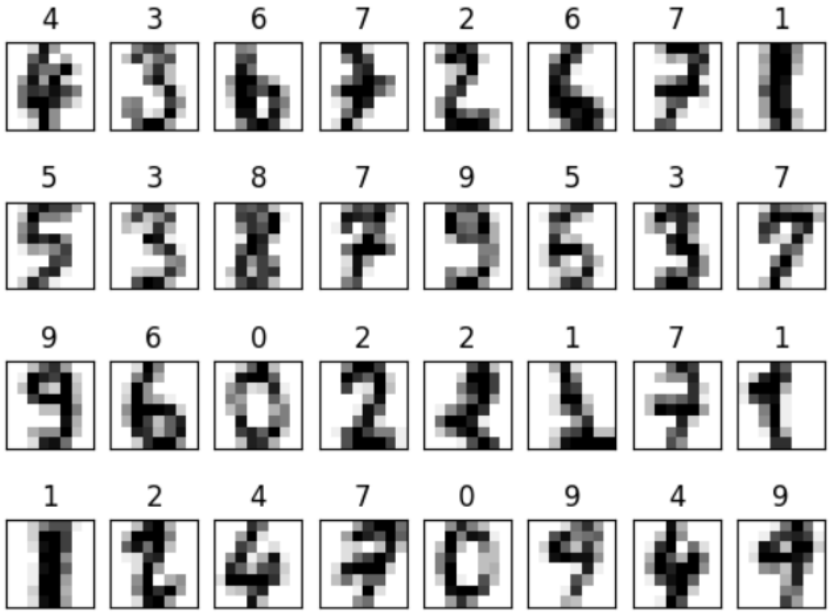
Hyper-parameter Tuning

Example 2: 8x8 Handwritten Digit Recognition

Source: https://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits

Tune an SVM with the following hyper-parameter value grid candidates:

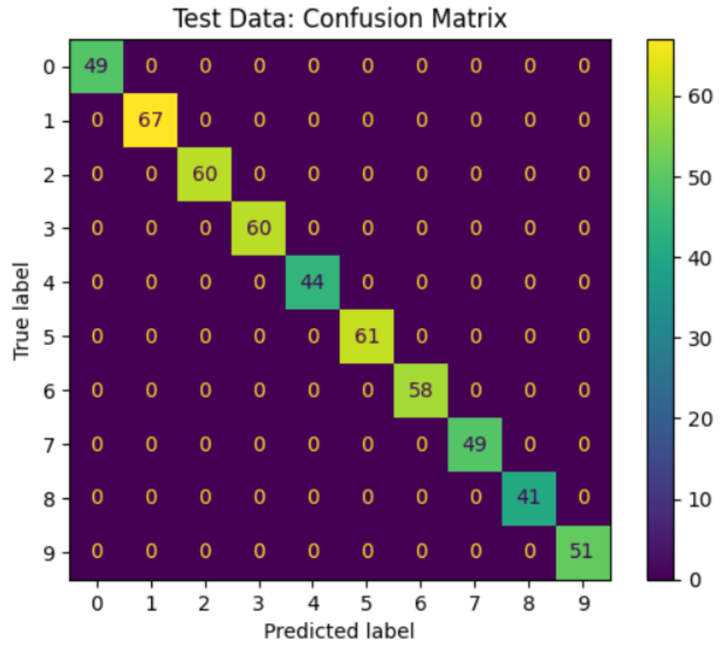
C: Exponential Distribution $(\lambda = 100)$
Gamma: Exponential Distribution $(\lambda = 0.1)$
Kernel: RBF, Poly, Linear, Sigmoid



Random Search Results

Best SVM:
C = 105.31
Gamma = 0.00068
Kernel = RBF

Accuracy: 1.00
No. of Trials: 20
Runtime: 23.90 sec



Random Search proves to be more efficient than Grid Search in this example.

Hyper-parameter Tuning: Optuna

OPTUNA

Optuna: A hyperparameter optimization framework

Akiba et al., (2019) Optuna: A Next-generation Hyperparameter Optimization Framework. https://arxiv.org/pdf/1907.10902.pdf

Optuna has modern functionalities as follows:

Lightweight, versatile, and platform agnostic architecture

- Handle a wide variety of tasks with a simple installation that has few requirements.

Pythonic search spaces

- Define search spaces using familiar Python syntax including conditionals and loops.

Efficient optimization algorithms

- Adopt state-of-the-art algorithms for sampling hyperparameters and efficiently pruning unpromising trials.

Easy parallelization

- Scale studies to tens or hundreds of workers with little or no changes to the code.

Quick visualization

- Inspect optimization histories from a variety of plotting functions.

- Grid Search implemented in `GridSampler`
- Random Search implemented in `RandomSampler`
- Tree-structured Parzen Estimator algorithm implemented in `TPESampler`
- CMA-ES based algorithm implemented in `CmaEsSampler`
- Algorithm to enable partial fixed parameters implemented in `PartialFixedSampler`
- Nondominated Sorting Genetic Algorithm II implemented in `NSGAIISampler`
- A Quasi Monte Carlo sampling algorithm implemented in `QMCSampler`

The default sampler is `TPESampler`.

Main algorithm:

TPE (Tree-structured Parzen Estimator)

- A variant of Bayesian Optimization

Hyper-parameter Tuning: Optuna

Main algorithm:

TPE (Tree-structured Parzen Estimator)

- A variant of Bayesian Optimization

Advantages:

- BO is sample-efficient. It is suited for black-box objective functions that are *expensive* to evaluate.
- BO is gradient-free. It does not need to calculate gradients of the objective function.
- BO can easily control the trade-off between exploration and exploitation.
- In particular, the **Tree-structured Parzen Estimator** can optimize both categorical and continuous hyper-parameters, where as GP-EI can only optimize continuous ones.

What is Bayesian Optimization (BO)?

A global optimization method that uses Bayes Theorem to sequentially direct the search for the optimum.

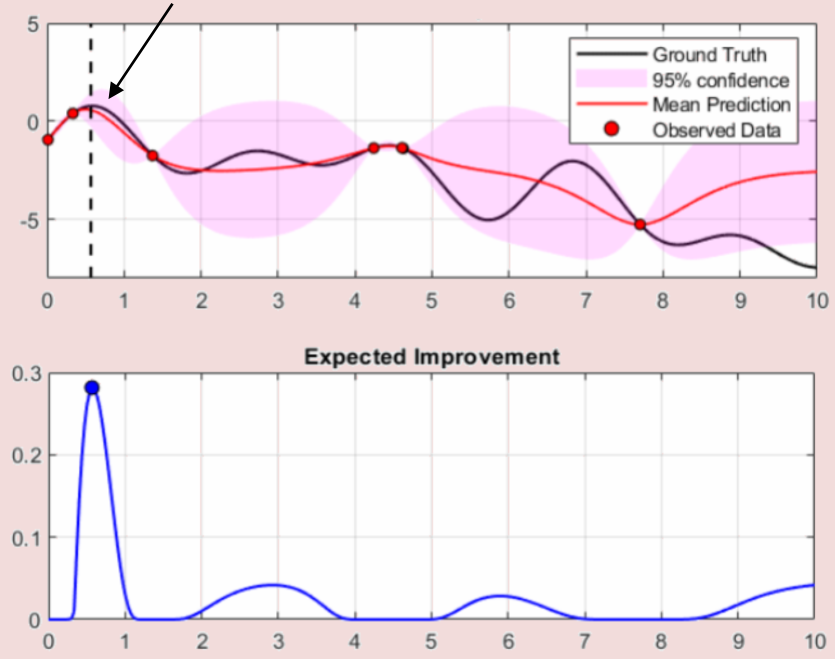
One variant of BO is the GP-EI (Gaussian process, Expected Improvement) scheme.

We'll learn about this in a future lecture.

Example:
In this example, the goal is to find the max value of the **black** curve.

- So far, we tested 6 samples from the black curve.
- A surrogate model (**red** curve) was fitted to these samples.
- The uncertainty of the surrogate model is given as the **pink** shaded area.
- A **blue** curve was generated from the surrogate's outputs, and it tells us where to optimally sample next.

Maximum



Hyper-parameter Tuning

Example 2: 8x8 Handwritten Digit Recognition

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Create a handwritten digit recognizer that optimizes between the best Logistic regression and best SVM model with the following hyper-parameters:

SVM

C: 10^{-1} to 10^{3} (log-scale)

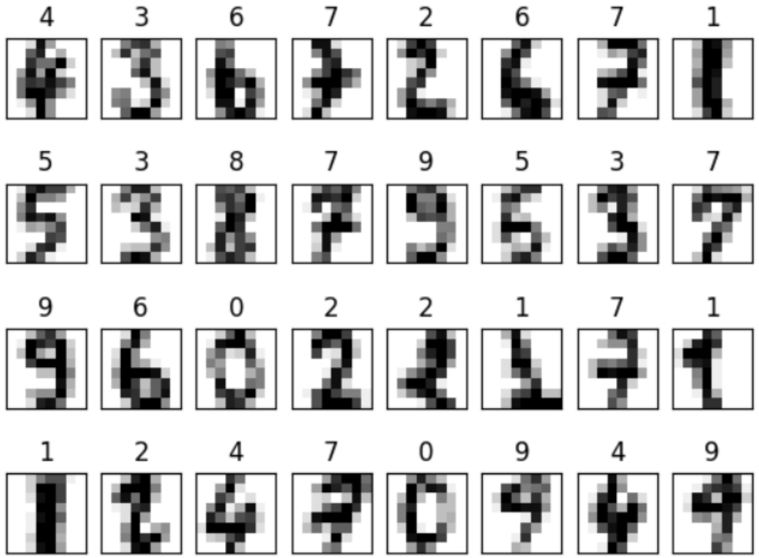
Gamma: 10^{-4} to 10^{1} (log-scale)

Kernel: RBF, Poly, Linear, Sigmoid

Logistic Regression

Penalty: L1, L2

Regularization: 10^{-2} to 10^{2} (log-scale)



Optuna Results

Best Model:

SVM

C = 100.7

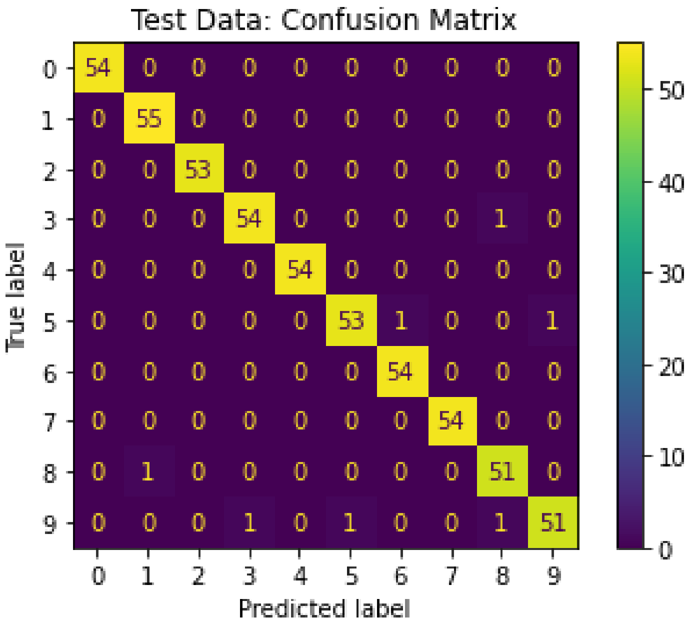
Gamma = 0.0002

Kernel = RBF

Accuracy: 0.987

No. of Trials: 100

Runtime: 41.52 sec



You can add more models and let Optuna find which of them is best, while each of them are also tuned!

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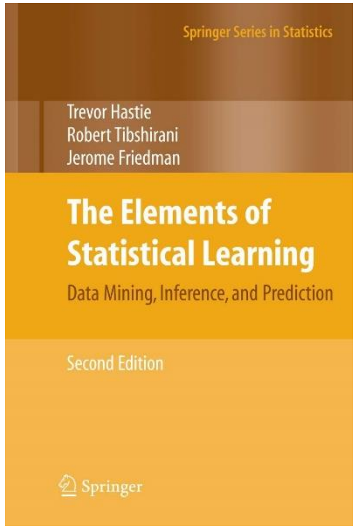

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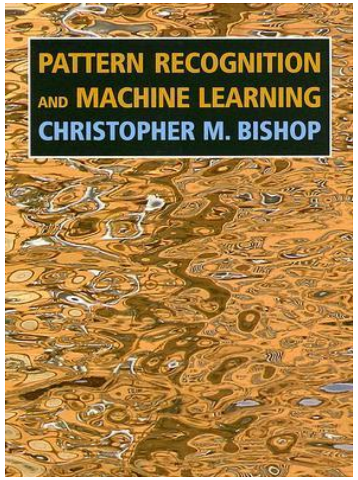

Further Reading

- https://scikit-learn.org/stable/auto_examples/model_selection/plot_cv_indices.html
- https://scikit-learn.org/stable/auto_examples/model_selection/plot_randomized_search.html
- https://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits
- https://www.mygreatlearning.com/blog/gridsearchcv
- https://www.kaggle.com/code/vitalflux/k-fold-cross-validation-example/notebook
- R. Bharat Rao, G. Fung, R. Rosales, On the Dangers of Cross-Validation. An Experimental Evaluation, SIAM 2008.
- Optuna paper: https://arxiv.org/pdf/1907.10902.pdf
- https://neptune.ai/blog/optuna-guide-how-to-monitor-hyper-parameter-optimization-runs
- Hyperopt paper: https://pdfs.semanticscholar.org/d4f4/9717c9adb46137f49606ebbdf17e3598b5a5.pdf
- Frazier, 2018. A Tutorial on Bayesian Optimization: https://arxiv.org/abs/1807.02811
- Hyper-parameter Optimization: https://medium.com/criteo-engineering/hyper-parameter-optimization-algorithms-2fe447525903
- Bergstra, James S., Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. “Algorithms for hyper-parameter optimization.” In *Advances in neural information processing systems*, pp. 2546–2554. 2011.
- Bergstra, James, and Yoshua Bengio. “Random search for hyper-parameter optimization.” *Journal of Machine Learning Research* 13, no. Feb (2012): 281–305.
- Yang, L. and Shami, A. (2020). On hyperparameter optimization of machine learning algorithms: Theory and practice. *Neurocomputing*, 415:295–316. https://www.sciencedirect.com/science/article/pii/S0925231220311693