Data Mining 2

Topic 04 : Hyperparameter Tuning

Lecture 01 : Introduction to Hyperparameters

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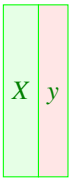
Outline

- Using (skilearn) pipelines
- Learning vs Validation curves

Outline

The Problem



Model Cost Function: $C(X;\theta)$

- To date our model training has focused on optimising the model parameters, but a model can have additional parameters (called hyperparameters) whose values can have significant impact on the performance of the model.
- Usually cannot estimate the hyperparameters as part of the learning step because:
  - Hyperparameters play a quantifiable different role — think, degree of polynomial vs polynomial coefficients.
  - If not continuous — think L_1 vs L_2 option — then can't be used in gradient optimisation methods.
  - Greatly increase the complexity of the learning process.

$\Rightarrow$ Need a separate step to determine optimal values for the hyperparameters.

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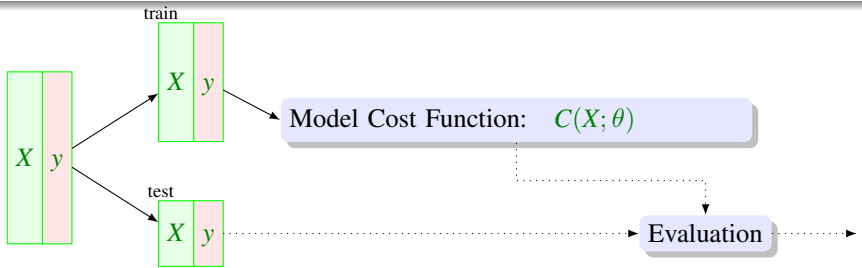

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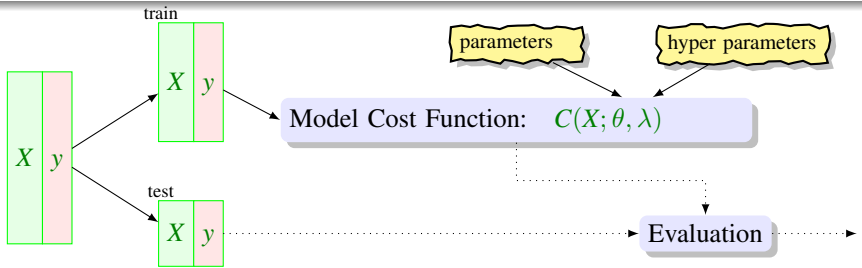

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Parameters vs Hyperparameters

Parameters

- Weights/coefficients/numbers learnt during the training process.
- Automatically estimated.
- Examples:
  - coefficients in a linear / logistic regression.
  - support vectors in a support vector machine.
  - weights in an artificial neural network.

Hyperparameters

- 'Knobs'/'dials'/'switches' used to control the training process.
- Manually specified/set.
- Often used in processes to help estimate model parameters.
- Often set using heuristics.
- Examples:
  - Model selection
  - Feature selection
  - Size/depth of neural networks

Advances in machine learning techniques result in hyperparameters becoming parameters as algorithms improve and computational power increases.

Example — Ridge/Lasso Regression

Both regression methods introduce a new hyperparameter*, λ, that controls the importance of a penalty term:

Ridge Cost function

$$C(X;\theta,\lambda) = \left\|(\theta_0 + \theta_1\vec{x}_1 + \cdots + \theta_n\vec{x}_n) - \vec{y}\right\|_2^2 + \lambda\left\|\theta\right\|_2^2$$

- Performs L_2 regularisation, i.e., adds penalty equivalent to square of the magnitude of coefficients.
- Larger values of λ helps overfitting and effects of multi-collinearity in X.

Lasso Cost function

$$C(X;\theta,\lambda) = \left\|(\theta_0 + \theta_1\vec{x}_1 + \cdots + \theta_n\vec{x}_n) - \vec{y}\right\|_2^2 + \lambda\left\|\theta\right\|_1$$

- Performs L_1 regularisation, i.e., adds penalty equivalent to absolute value of the magnitude of coefficients.
- Also addresses overfitting, but in addition tends to encourage coefficients to become zero rather than near-zero $\implies$ simpler models (feature selection).

*α in sklearn documentation.

Example — SVM, (RBF) Kernel

The Radial Basis Function (RBF) kernel has two parameters:

- γ controls how far the influence of a single training example reaches.
  - Low values meaning 'far' and high values meaning 'close'.
  - Can be seen as the inverse of the radius of influence of samples selected by the model as support vectors.
  - If too small, then model is too constrained and cannot capture the complexity or 'shape' of the data.
- C controls the trade off of correct classification of training examples against maximisation of the decision function's margin.
  - For larger values of C, a smaller margin will be accepted if the decision function is better at classifying all training points correctly.
  - A lower C will encourage a larger margin, therefore a simpler decision function, at the cost of training accuracy.
  - In other words C behaves as a regularisation parameter in the SVM.

See interactive demo of effects of parameters (good but uses $1/\sigma$ instead of γ):

Support Vector Machine in Javascript

and SKLearn documentation RBF SVM Parameters

Outline

Wisconsin Dataset — Breast Cancer (WDBC)[†]

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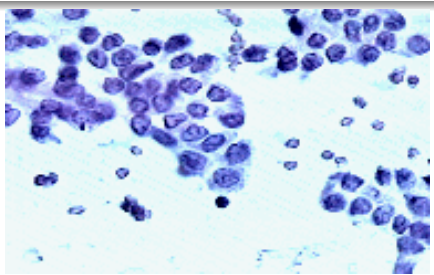

- Aims to predict breast cancer diagnosis based on Fine Needle Aspiration (FNA).
- Resulting classifier using on these nine features successfully diagnosed 97% of new cases.

Construction

- FNA's were done on a total of 569 patients, samples were stained to help differentiate distinguished cell nuclei
- Samples were classified as cancer-based through biopsy and historical confirmation. Non-cancer samples were confirmed by biopsy or follow ups.
- Users then chose areas of the FNA with minimal overlap between nuclei; they then took scans utilising a digital camera.
- `Xcyt` was used to create approximate boundaries, which would then used a process called snakes which converged to give the exact nuclei boundary.
- Once the boundaries for the nuclei were set, calculations were made (of mean, standard error, and max) resulting in 3×10 features.

[*] Machine Learning for Cancer Diagnosis and Prognosis.

WDBC — Load Data

```
UCI = "https://archive.ics.uci.edu/ml/machine-learning-databases/"
DATA_URL = f"{UCI}/breast-cancer-wisconsin/wdbc.data"
DATA_LOCAL = "data/wdbc.data"
SEED = 42

names = ['id_number', 'diagnosis', 'radius_mean',
         'texture_mean', 'perimeter_mean', 'area_mean',
         'smoothness_mean', 'compactness_mean', 'concavity_mean',
         'concave_points_mean', 'symmetry_mean',
         'fractal_dimension_mean', 'radius_se', 'texture_se',
         'perimeter_se', 'area_se', 'smoothness_se',
         'compactness_se', 'concavity_se', 'concave_points_se',
         'symmetry_se', 'fractal_dimension_se',
         'radius_worst', 'texture_worst', 'perimeter_worst',
         'area_worst', 'smoothness_worst',
         'compactness_worst', 'concavity_worst',
         'concave_points_worst', 'symmetry_worst',
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df = pd.read_csv(DATA_URL,header=None, names=names)
df.head(10)
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	id_number	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave_points_mean	.
0	842302	M	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.30010	0.14710	.
1	842517	M	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.08690	0.07017	.
2	84300903	M	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.19740	0.12790	.
3	84348301	M	11.42	20.38	77.58	386.1	0.14250	0.28390	0.24140	0.10520	.
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.19800	0.10430	.
5	843786	M	12.45	15.70	82.57	477.1	0.12780	0.17000	0.15780	0.08089	.
6	844359	M	18.25	19.98	119.60	1040.0	0.09463	0.10900	0.11270	0.07400	.
7	84458202	M	13.71	20.83	90.20	577.9	0.11890	0.16450	0.09366	0.05985	.
8	844981	M	13.00	21.82	87.50	519.8	0.12730	0.19320	0.18590	0.09353	.
9	84501001	M	12.46	24.04	83.97	475.9	0.11860	0.23960	0.22730	0.08543	.

10 rows × 32 columns

```
df = pd.read_csv(DATA_URL,header=None, names=names)
df.head(10)
```

WDBC — View Data

See EDA of Breast Cancer Dataset for EDA of this dataset.

	count	mean	std	min	25%	50%	75%	max
id_number	569.0	3.037183e+07	1.250206e+08	8670.000000	869218.000000	906024.000000	8.813129e+06	9.113205e+08
radius_mean	569.0	1.412729e+01	3.524049e+00	6.981000	11.700000	13.370000	1.578000e+01	2.811000e+01
texture_mean	569.0	1.928965e+01	4.301036e+00	9.710000	16.170000	18.840000	2.180000e+01	3.928000e+01
perimeter_mean	569.0	9.196903e+01	2.429898e+01	43.790000	75.170000	86.240000	1.041000e+02	1.885000e+02
area_mean	569.0	6.548891e+02	3.519141e+02	143.500000	420.300000	551.100000	7.827000e+02	2.501000e+03
smoothness_mean	569.0	9.636028e-02	1.406413e-02	0.052630	0.086370	0.095870	1.053000e-01	1.634000e-01
compactness_mean	569.0	1.043410e-01	5.281276e-02	0.019380	0.064920	0.092630	1.304000e-01	3.454000e-01
concavity_mean	569.0	8.879932e-02	7.971981e-02	0.000000	0.029560	0.061540	1.307000e-01	4.268000e-01
concave_points_mean	569.0	4.891915e-02	3.880284e-02	0.000000	0.020310	0.033500	7.400000e-02	2.012000e-01
symmetry_mean	569.0	1.811619e-01	2.741428e-02	0.106000	0.161900	0.179200	1.957000e-01	3.040000e-01
fractal_dimension_mean	569.0	6.279761e-02	7.060363e-03	0.049960	0.057700	0.061540	6.612000e-02	9.744000e-02
radius_se	569.0	4.051721e-01	2.773127e-01	0.111500	0.232400	0.324200	4.789000e-01	2.873000e+00
texture_se	569.0	1.216853e+00	5.516484e-01	0.360200	0.833900	1.108000	1.474000e+00	4.885000e+00
perimeter_se	569.0	2.866059e+00	2.021855e+00	0.757000	1.606000	2.287000	3.357000e+00	2.198000e+01
area_se	569.0	4.033708e+01	4.549101e+01	6.802000	17.850000	24.530000	4.519000e+01	5.422000e+02
smoothness_se	569.0	7.040979e-03	3.002518e-03	0.001713	0.005169	0.006380	8.146000e-03	3.113000e-02
compactness_se	569.0	2.547814e-02	1.790818e-02	0.002252	0.013080	0.020450	3.245000e-02	1.354000e-01
concavity_se	569.0	3.189372e-02	3.018606e-02	0.000000	0.015090	0.025890	4.205000e-02	3.960000e-01
concave_points_se	569.0	1.179614e-02	6.170285e-03	0.000000	0.007638	0.010930	1.471000e-02	5.279000e-02
symmetry_se	569.0	2.054230e-02	8.266372e-03	0.007882	0.015160	0.018730	2.348000e-02	7.895000e-02
fractal_dimension_se	569.0	3.794904e-03	2.646071e-03	0.000895	0.002248	0.003187	4.558000e-03	2.984000e-02
radius_worst	569.0	1.626919e+01	4.833242e+00	7.930000	13.010000	14.970000	1.879000e+01	3.604000e+01
texture_worst	569.0	2.567722e+01	6.146258e+00	12.020000	21.080000	25.410000	2.972000e+01	4.954000e+01
perimeter_worst	569.0	1.072612e+02	3.360254e+01	50.410000	84.110000	97.660000	1.254000e+02	2.512000e+02
area_worst	569.0	8.805831e+02	5.693570e+02	185.200000	515.300000	686.500000	1.084000e+03	4.254000e+03

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- no missing values
- big differences in mean/std
  $\Rightarrow$ need normalising.
- 30 numerical features, some of which expect to be correlated
  $\Rightarrow$ use PCA.

WDBC — Prepare Data

- Extract feature matrix and target column.

3
```
X = df.iloc[:, 2:].values
y = df.diagnosis.values
```

- Encode (categorical) target column.

  Could do our own mapping (see Churn). No big deal either way.

4
```
print (y[:20])

from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
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[1 0]
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]
```

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from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.20, random_state=SEED)

from sklearn.preprocessing import StandardScaler
ss = StandardScaler()
X_train_scaled = ss.fit_transform(X_train)
X_test_scaled = ss.transform(X_test)

from sklearn.linear_model import LogisticRegression
clf = LogisticRegression(solver='lbfgs')

from sklearn.model_selection import cross_val_score
scores = cross_val_score(estimator=clf,
    X=X_train_scaled, y=y_train, cv=10, n_jobs=-1)

print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),np.std(scores)))
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- Cross validation is easily parallelised — use option `n_jobs=-1` for all cores.

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```
CV accuracy scores: [0.97826087 0.97826087 0.97826087 0.95652174 1.
1.
 0.97777778 0.97777778 0.95555556 0.93333333]
CV accuracy: 0.974 +/- 0.019
```

- Split into train/test subsets … normalise … and train.
- Cross validation is easily parallelised — use option `n_jobs=-1` for all cores.

WDBC — Using a Pipeline I

```
12 from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression

pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('clf', LogisticRegression(solver='lbfgs'))
])

scores = cross_val_score(estimator=pipeline,
    X=X_train, y=y_train, cv=10, n_jobs=-1)

print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),np.std(scores)))
```

- A pipeline is a sequence (list) of models (scaler/filters/classifiers/...) which is passed to `cross_val_score` instead of classifier as in previous slide.
- Pipes can ensure that operations (transformations, new features added) on train dataset are also applied to test/validation dataset.

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```
CV accuracy scores: [0.97826087 0.97826087 0.97826087 0.95652174 1.
1.
 0.97777778 0.97777778 0.95555556 0.93333333]
CV accuracy: 0.974 +/- 0.019
```

- A pipeline is a sequence (list) of models (scaler/filters/classifiers/...) which is passed to `cross_val_score` instead of classifier as in previous slide.
- Pipes can ensure that operations (transformations, new features added) on train dataset are also applied to test/validation dataset.

WDBC — Using a Pipeline II

```
15 from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression

pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('pca', PCA(n_components=2)),
    ('clf', LogisticRegression(solver='lbfgs'))
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print('CV accuracy scores: %s' % scores)
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```

- Inserting more steps into pipeline is trivial — here PCA with 2 principal components.
- OK, model is much simpler but I have lost some accuracy . . . perhaps I was too aggressive in picking 2 . . .

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```

```
CV accuracy scores: [0.93478261 0.91304348 0.97826087 0.89130435 0.97826087 0.95555556
 0.95555556 0.93333333 0.97777778 0.91111111]
CV accuracy: 0.943 +/- 0.030
```

- Inserting more steps into pipeline is trivial — here PCA with 2 principal components.
- OK, model is much simpler but I have lost some accuracy . . . perhaps I was too aggressive in picking 2 . . .

Digression . . . PCA

- What would be a good choice for the number of principal components?
- Or, more importantly, what metric could we use to determine this?

We could use PCA **specific information** that reports on the amount of variation in the components . . . to date we have used the arbitrary limit of explaining 95% of the variation . . . (but why 95%?) . . .

```
18
from sklearn.preprocessing import StandardScaler
ss = StandardScaler()
X_train_scaled = ss.fit_transform(X_train)
X_test_scaled = ss.transform(X_test)

pca = PCA(n_components=30)
X_train_scaled_pca = pca.fit_transform(X_train_scaled)
print(np.cumsum(pca.explained_variance_ratio_))
```

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```

```
[0.43502782 0.63002788 0.72784307 0.79270717 0.84524094 0.88636894
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 0.97818188 0.98349877 0.986399   16898 0.9929821
 0.99461913 0.99565834 0.996656   4552 0.99892219
 0.99941849 0.99969478 0.99992059 0.99997136 0.99999594 1. ]
```

⇒ 10 components

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 0.99941849 0.99969478 0.99992059 0.99997136 0.99999594 1. ]
```

⇒ 10 components (0.95105751 ≈ 16898, 0.99565834 ≈ 4552, 0.99892219)

OK, this works (as with 10 components the classifier accuracy is back > 0.97 (next slide)) and is easy since we are using PCA specific metrics.
However shouldn't the overriding metric be based on how much the model accuracy is affected?

Digression . . . PCA

```
22 from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
pipe_lr = Pipeline([
    ('scl', StandardScaler()),
    ('pca', PCA(n_components=10)),
    ('clf', LogisticRegression(solver='lbfgs'))
])

from sklearn.model_selection import KFold, cross_val_score
scores = cross_val_score(estimator=pipe_lr, X=X_train, y=y_train, cv=10, n_jobs=-1)

print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),np.std(scores)))
```

```
CV accuracy scores: [1.        0.97826087 0.97826087 0.93478261 0.97826087 1.
 0.97777778 0.95555556 0.95555556 0.97777778]
CV accuracy: 0.974 +/- 0.019
```

- With 10 components the accuracy is 97.4%.

Recap of where we are

We have a dataset where:

- Clean dataset with no missing values, but have 30 numerical (continuous) features with reasonable expectation of multi-collinearity issues[‡].
- Given the dimension of 30, it seems reasonable to apply PCA, but how many principal components should we pick?

  `n_components`
- Given the suspected multi-collinearity, the regularisation in the logistic regression is important.
  - What type of penalty (L_1 vs L_2) should we use?

    `penalty`
  - How important should be the penalty be?

    `C`

We want a general procedure to determine optimal values of these hyperparameters:

- First approach is to generate **validation curves** which will look at each parameter in turn.
- Then we will look at more automatic techniques — grid and random searches.

[‡]Issues are there, ~~we~~ you could verify this by generating the correlation matrix ...

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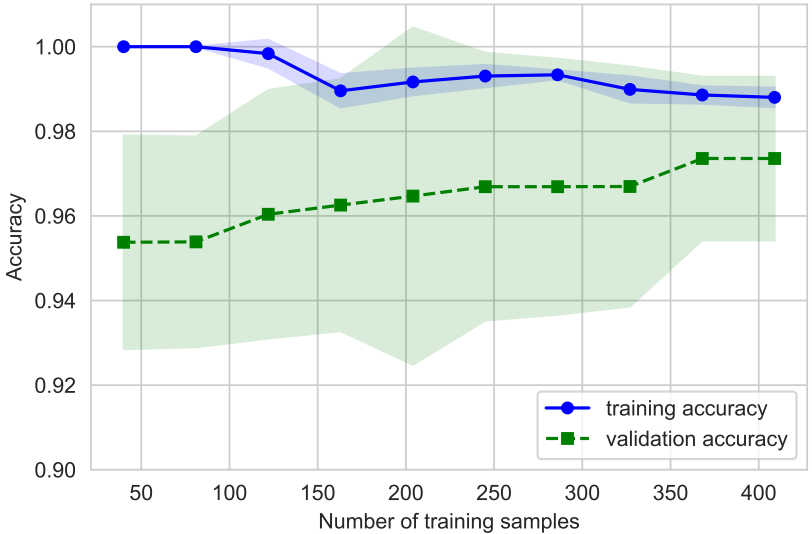
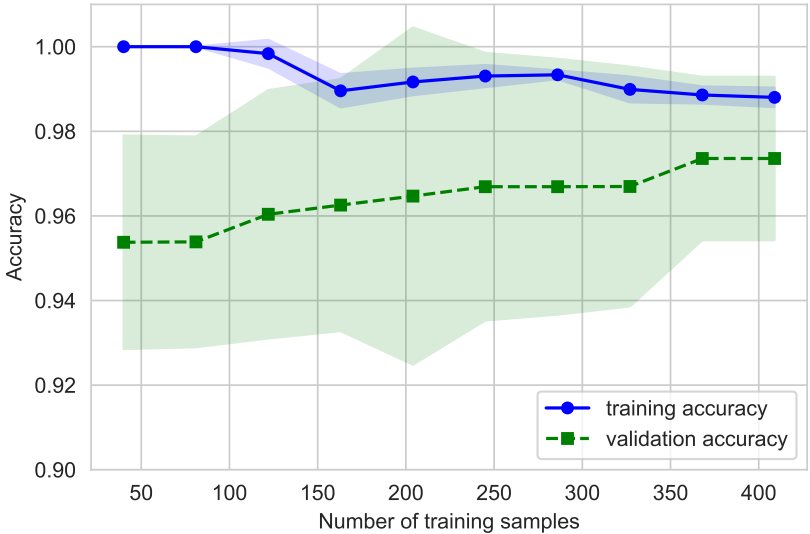
Outline

Learning Curve



Learning Curve



The learning curve shows how the model metrics change as the number of training samples increase (or over line).

- An under-fit model would have a flat/decreasing training accuracy.
- An over-fit model tends to have a validation accuracy that decreases to a point and begins increasing again.
- The learning curve is a tool for finding out if an estimator would benefit from more data, or if the model is too simple (under-fit/biased).

Learning Curve via Pipelines

We pass the pipeline to the `learning_curve` function and specify values for the `train_sizes` ...

```
23 from sklearn.model_selection import learning_curve
   pipeline = Pipeline([
       ('scl', StandardScaler()),
       ('clf', LogisticRegression(solver='lbfgs'))
   ])
   train_sizes, train_scores, test_scores = learning_curve(estimator=pipeline,
       X=X_train, y=y_train,
       train_sizes=np.linspace(0.1, 1.0, 10),
       cv=10,
       n_jobs=1)
```

Then compute statistics from the generated scores ...

```
24 train_mean = np.mean(train_scores, axis=1)
   train_std = np.std(train_scores, axis=1)
   test_mean = np.mean(test_scores, axis=1)
   test_std = np.std(test_scores, axis=1)
```

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test_mean = np.mean(test_scores, axis=1)
test_std = np.std(test_scores, axis=1)
```

Learning Curve via Pipelines II

Finally, we generate the actual learning curve using the usual plot and pimping code.

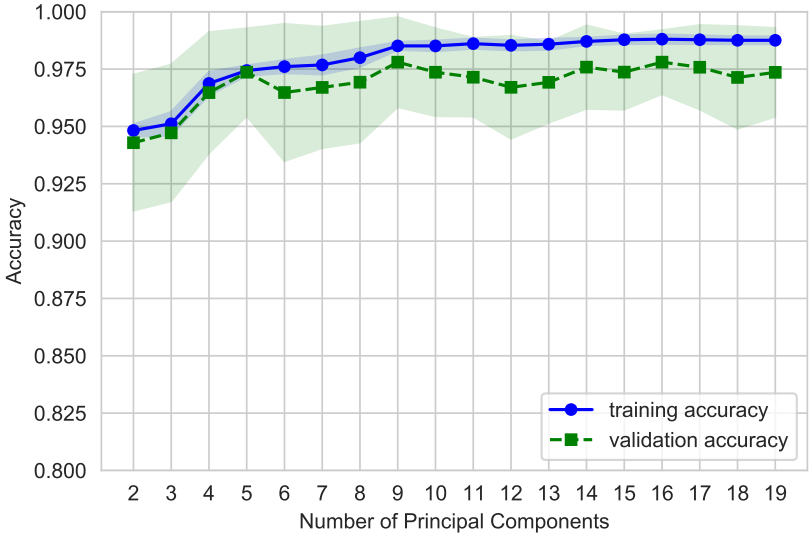
```
27 plt.plot(train_sizes, train_mean, color='blue', marker='o',
       markersize=5, label='training accuracy')
   plt.fill_between(train_sizes, train_mean + train_std, train_mean - train_std,
       alpha=0.15, color='blue')

   plt.plot(train_sizes, test_mean, color='green', linestyle='--', marker='s',
       markersize=5, label='validation accuracy')
   plt.fill_between(train_sizes, test_mean + test_std, test_mean - test_std,
       alpha=0.15, color='green')

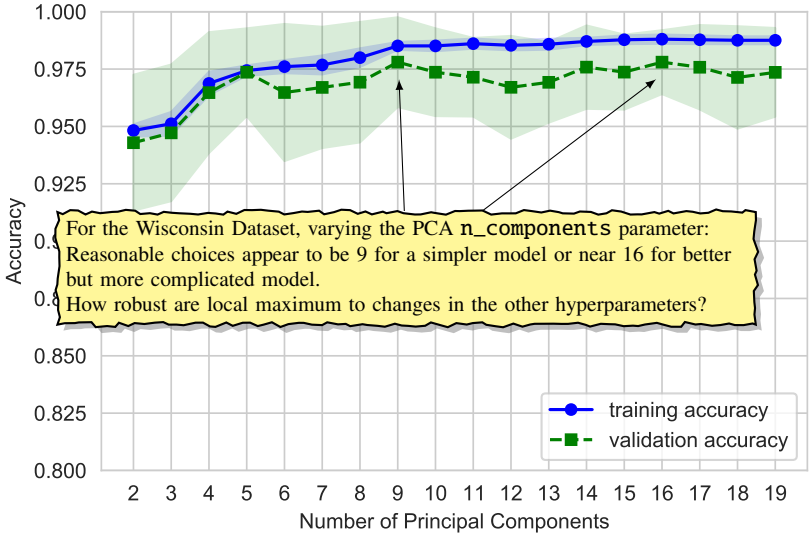
   plt.xlabel('Number of training samples')
   plt.ylabel('Accuracy')
   plt.legend(loc='lower right')
   plt.ylim(0.9, 1.01)

   plt.savefig("LC.pdf", bbox_inches="tight")
   plt.show()
```

Validation Curve — PCA, `n_components`



Validation Curve — PCA, `n_components`



The Validation Curve shows the sensitivity between model's accuracy with change in some (hyper-)parameter of the model.

- Two curves are present in a validation curve — one for the training set score and one for the cross-validation score.
- Ideally validation score and the training score look as similar as possible.
- A validation curve is used to evaluate an existing model based on hyper-parameters and is not used to tune a model. This is because, if we tune the model according to the validation score, the model may be biased towards the specific data against which the model is tuned; thereby, not being a good estimate of the generalisation of the model.

Validation Curve — PCA, n_components II

We pass the pipeline and (hyper-)parameter info to the validation_curve function, ...

```
28 from sklearn.pipeline import Pipeline
   from sklearn.preprocessing import StandardScaler
   from sklearn.decomposition import PCA
   from sklearn.linear_model import LogisticRegression
   pipeline = Pipeline([
       ('scl', StandardScaler()),
       ('pca', PCA(n_components=10)),
       ('clf', LogisticRegression(solver='liblinear', penalty='l2'))
   ])

   from sklearn.model_selection import validation_curve
   param_range = range(2,20)
   train_scores, test_scores = validation_curve(
       estimator=pipeline, X=X_train, y=y_train, cv=10,
       param_name='pca__n_components', param_range=param_range)
```

Parameter name is concatenation of pipeline step name, pca, and the parameter name n_components.

Then compute statistics from the generated scores ...

```
29 train_mean = np.mean(train_scores, axis=1)
   train_std = np.std(train_scores, axis=1)
   test_mean = np.mean(test_scores, axis=1)
   test_std = np.std(test_scores, axis=1)
```

Validation Curve — PCA, n_components II

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30
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train_mean = np.mean(train_scores, axis=1)
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test_std = np.std(test_scores, axis=1)
```
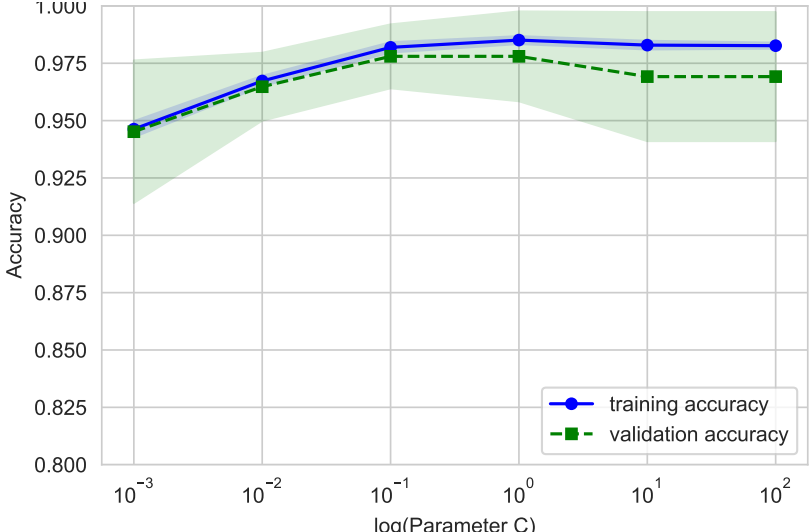

Validation Curve — PCA, n_components III

Finally, we generate the actual learning curve using the usual plot and pimping code.

```
32
plt.plot(param_range, train_mean, color='blue', marker='o', markersize=5,
    label='training accuracy')
plt.fill_between(param_range, train_mean + train_std, train_mean - train_std,
    alpha=0.15, color='blue')

plt.plot(param_range, test_mean, color='green', marker='s', markersize=5,
    linestyle='--', label='validation accuracy')
plt.fill_between(param_range, test_mean + test_std, test_mean - test_std,
    alpha=0.15, color='green')

plt.xlabel('Number of Principal Components')
plt.ylabel('Accuracy')
plt.xticks(range(2,20))
plt.legend(loc='lower right')
plt.ylim(0.8, 1.0)

plt.savefig("VC__pca__n_components.pdf", bbox_inches="tight")
plt.show()
```

Validation Curve — LogisticRegression, c

We can also examine other hyper-parameters in our pipeline — for example, the regulerisation parameter, C:



Validation Curve — LogisticRegression, C

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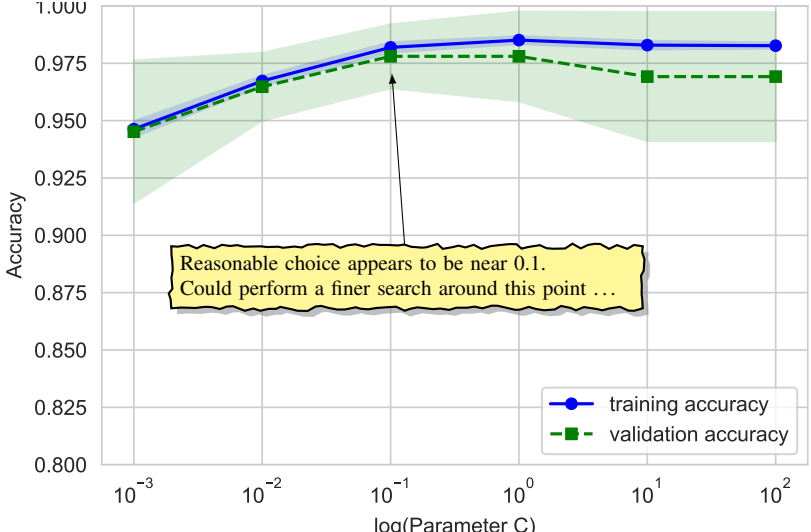


Validation Curve — LogisticRegression, C II

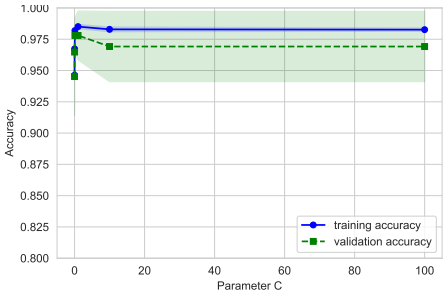
Code is near identical to that we used for modifying the `n_components` of the `pca` step:

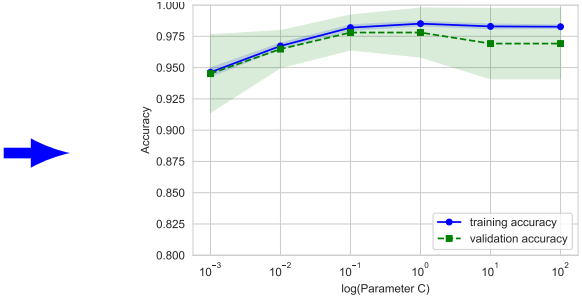
```
33 pipeline = Pipeline([
       ('scl', StandardScaler()),
       ('pca', PCA(n_components=9)),
       ('clf', LogisticRegression(solver='liblinear', penalty='l2'))
   ])

   from sklearn.model_selection import validation_curve
   param_range = [0.001, 0.01, 0.1, 1.0, 10.0, 100.0]
   train_scores, test_scores = validation_curve(estimator=pipeline,
       X=X_train, y=y_train, cv=10,
       param_name='clf__C', param_range=param_range)
```

- Set number of PCA components at 9 based on results to date.
- Range of parameter *C* is large so prefer a geometric (constant factor, not constant difference) sweep. Could use `np.logspace` here.

Validation Curve — LogisticRegression, C

Rest of code is identical (except for obvious label differences) and use of `plt.xscale('log')`





Without `plt.xscale('log')`

The interesting region is compressed and difficult to read.

With `plt.xscale('log')`

Interesting region is readable.

Recap of where we are

- Given a pipeline / model we "can" tune each of the hyperparameters by constructing a validation curve.
- Problems . . . (manual approach is not practical anything but small problems)
  - Can have a huge (100s – 1,000s) number of parameters.
  - A sequence of 1-dimensional searches is not the same as one d-dimensional search — interplay between hyper-parameters.
- Approaches / Techniques . . .
  - Grid Search — Systematic, regular, predetermined deterministic sample of parameter space.
  - Random Search — Non-adaptive, random sample of parameter space.
  - Bayesian Search — Adaptive, random sample of parameter space.