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

1 Introduction

1.1. Parameters vs Hyperparameters	4
2. Model Building using a Pipeline	7
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2.2. Standard Model Building	11
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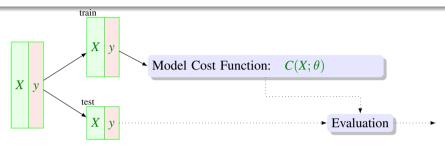
The Problem



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

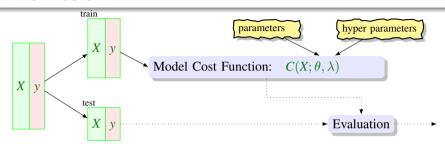
- To date our model training has focused on optimising the model parameters, but a model can have additional parameters (called hyperparameters) whose values can have significant impact on the performance of the model.
- Usually cannot estimate the hyperparameters as part of the learning step because:
 - 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.
- ⇒ Need a separate step to determine optimal values for the hyperparameters

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- ⇒ Need a separate step to determine optimal values for the 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

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

- 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

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

- Performs L₁ 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).

 $[\]alpha$ 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

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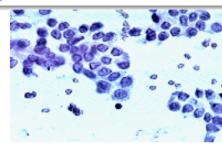
Wisconsin Dataset — Breast Cancer (WDBC)[†]

Outline

- 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',
        'fractal_dimension_worst'l
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 .
(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
 ⇒ need normalising.
- 30 numerical features, some of which expect to be correlated
 ⇒ use PCA.

• Extract feature matrix and target column.

```
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.

```
print (y[:20])

from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
y = le.fit_transform(y)

print (le.transform(["M","B"]))
print (y[:20])
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WDBC — Prepare Data

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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 v=v train cv=10 n iobs=-1)
print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f % (np.mean(scores),np.std(scores)))
```

• Cross validation is easily parallelised — use option n_iobs=-1 for all cores.

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                                                   0.97777778 0.97777778 0.95555556 0.933333331
                                                  CV accuracy: 0.974 + /- 0.019
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from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.linear model import LogisticRegression
pipeline = Pipeline([
   ('scl', StandardScaler()),
   ('clf', LogisticRegression(solver='lbfgs'))
1)
scores = cross_val_score(estimator=pipeline.
   X=X_train, y=y_train, cv=10, n_jobs=-1)
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- 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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from sklearn.preprocessing import StandardScaler
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pipeline = Pipeline([
    ('scl', StandardScaler()),
    ('clf', LogisticRegression(solver='lbfgs'))
1)
                                                    CV accuracy scores: [0.97826087 0.97826087 0.97826087 0.95652174 1.
scores = cross_val_score(estimator=pipeline,
    X=X_train, v=v_train, cv=10, n_jobs=-1)
                                                    0.9777778 0.9777778 0.9555556 0.933333331
                                                    CV accuracy: 0.974 + /- 0.019
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.

```
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'))
1)
scores = cross val score(estimator=pipeline.
   X=X train. v=v train. cv=10. n iobs=-1)
print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

- 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

```
from sklearn.pipeline import Pipeline
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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

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear model import LogisticRegression
                                     CV accuracy scores: [0.93478261 0.91304348 0.97826087 0.89130435 0.97826087 0.95555556
pipeline = Pipeline([
                                      0.95555556 0.93333333 0.97777778 0.91111111
    ('scl', StandardScaler()),
                                     CV accuracy: 0.943 +/- 0.030
    ('pca', PCA(n_components=2)),
    ('clf', LogisticRegression(solver='lbfgs'))
1)
scores = cross val score(estimator=pipeline.
    X=X train. v=v train. cv=10. n iobs=-1)
print('CV accuracy scores: %s' % scores)
print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
```

- 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 . . .

- 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%?) ...

```
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_))
```

Digression ... PCA

- What would be a good choice for the number of principal components?
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print(np.cumsum(pca.explained_variance_ratio_))
                                                   [0.43502782 0.63002788 0.72784307 0.79270717 0.84524094 0.88636894
                                                   0.90872484 0.92520437 0.93900488 0.95105751 0.98162316 0.97045804
                                                   0.97818188 0.98349877 0.986399
                                                                             \Rightarrow 10 components 4552 0 99892219
```

0 99461913 0 99565834 0 996656

0.99941849 0.99969478 0.99992059 0.99997136 0.99999594 1.

- 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%?) ...

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.

0 99941849 0 99969478 0 99992059 0 99997136 0 99999594 1

However shouldn't the overriding metric be based on how much the model accuracy is affected?

Digression ... PCA

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
pipe lr = Pipeline([
                                          CV accuracy scores: [1.
                                                                0.97826087 0.97826087 0.93478261 0.97826087 1.
    ('scl', StandardScaler()),
                                           0.9777778 0.95555556 0.95555556 0.97777781
                                          CV accuracy: 0.974 + /- 0.019
    ('pca', PCA(n_components=10)),
    ('clf', LogisticRegression(solver='lbfgs'))
1)
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)))
```

• 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 $(L_1 \text{ vs } L_2)$ 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've could verify this by generating the correlation matrix ...

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• How important should be the penalty be?

_

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- 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.

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Outline

3. Learning and Validation Curves

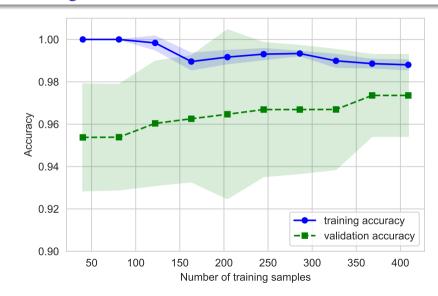
3.1. Learning Curves

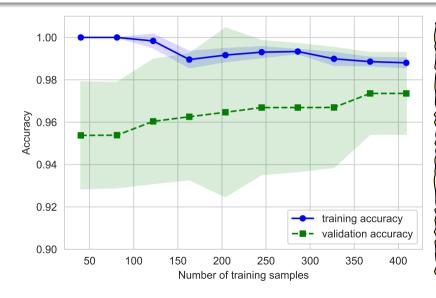
3.2. Validation Curves

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2. Model Building using a Pipeline	7
2.1. Wisconsin Dataset — Breast Cancer	8
2.2. Standard Model Building	11
2.3. Model Building using a Pipeline	13

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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 ...

```
from sklearn.model_selection import learning_curve
pipeline = Pipeline([
   ('scl', StandardScaler()).
   ('clf', LogisticRegression(solver='lbfgs'))
1)
train sizes, train scores, test scores = learning curve(estimator=pipeline,
   X=X_train. v=v_train.
   train_sizes=np.linspace(0.1, 1.0, 10),
   cv=10.
   n_iobs=1)
```

Learning Curve via Pipelines

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

```
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 . . .

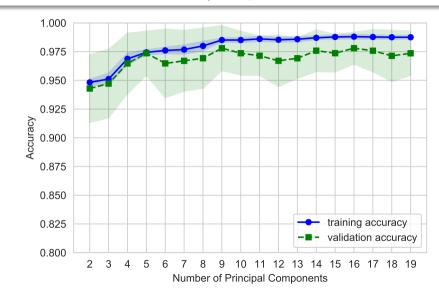
```
train_mean = np.mean(train_scores, axis=1)
train_std = np.std(train_scores, axis=1)
test_mean = np.mean(test_scores, axis=1)
test_std = np.std(test_scores, axis=1)
```

Learning Curve via Pipelines

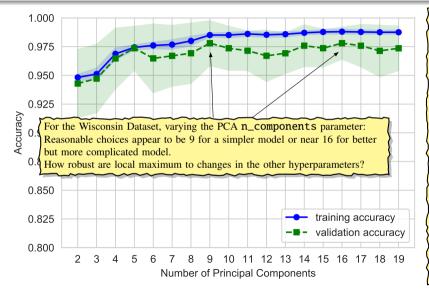
Finally, we generate the actual learning curve using the usual plot and pimping code.

```
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.vlabel('Accuracy')
plt.legend(loc='lower right')
plt.vlim(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

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

```
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'))
1)
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 ...

```
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

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

```
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'))
1)
from sklearn.model_selection import validation_curve
param_range = range(2.20)
train_scores, test_scores = validation_curve(
                                                                    Parameter name is concatenation of
   estimator=pipeline, X=X_train, y=y_train, cv=10,
                                                                    pipeline step name, pca, and the
   param name='pca n components', param range=param range)
                                                                    parameter name n_components
```

Then compute statistics from the generated scores ...

```
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)
                                                                                            23 of 28
```

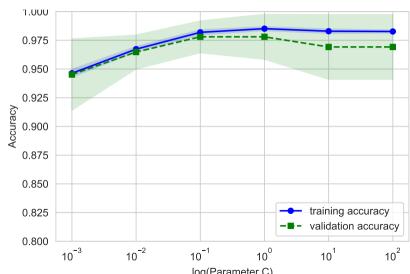
Validation Curve — PCA, n components

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

```
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.vlabel('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()
```

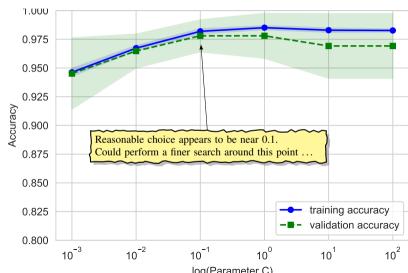
Validation Curve — LogisticRegression, c

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



Validation Curve — LogisticRegression, c

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



Validation Curve — LogisticRegression, c

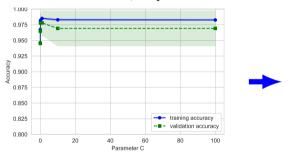
Code is near identical to that we used for modifying the n_components of the pca step:

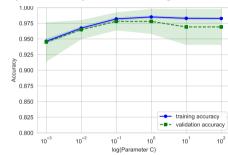
```
pipeline = Pipeline([
   ('scl', StandardScaler()),
   ('pca', PCA(n_components=9)),
   ('clf', LogisticRegression(solver='liblinear', penalty='l2'))
1)
from sklearn.model selection import validation curve
param\_range = [0.001, 0.01, 0.1, 1.0, 10.0, 100.0]
train_scores, test_scores = validation_curve(estimator=pipeline.
   X=X_train.v=v_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 — Logistic Regression, 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.

- 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.