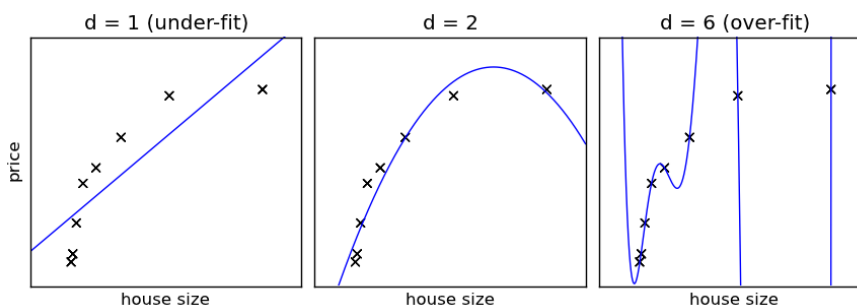
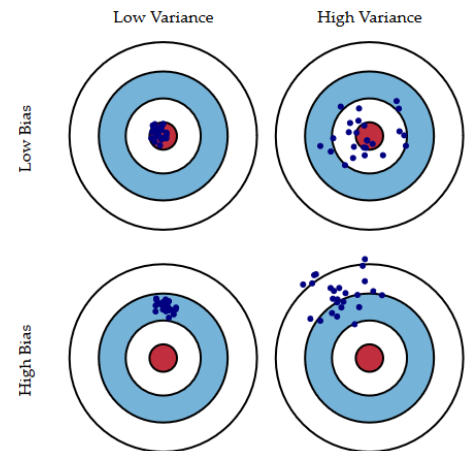


Material Summary: Model Training and Improvement

1. Regularization

1.1 Bias-Variance Tradeoff

- When we fit models, we have two main sources of errors
 - Bias** – how far are the predicted from the actual values
 - Variance** – variability of prediction for a certain data point
- Illustration – shooter aimed at a bullseye target
 - High bias – the aim is shifted away from the center
 - High variance – the points are more "spread out"
- When we fit several models, they perform differently
 - Some are not complex enough (don't describe data well enough)
 - Underfitting** (high bias)
 - Some may describe the data "too well" and **fail to generalize** when **new** data points are introduced
 - Overfitting** (high variance)
- Optimal model: tradeoff between underfitting and overfitting
 - Usually, underfitting is easy to spot
 - Poor performance w.r.t. some metric
 - Overfitting is more complicated
 - Many methods exist to prevent overfitting



1.2 Regularization

- Method for finding a good bias-variance tradeoff
 - Filter out noise from data
 - Handle highly correlated features
- L2** regularization – "second norm" (Euclidean):

$$\lambda ||w||_2^2 \equiv \lambda \sum_{j=1}^n w_j^2$$

- λ – regularization parameter
- Shrinks all model weights by the same value

- L1** regularization – "first norm":

$$\lambda ||w||_1 \equiv \lambda \sum_{j=1}^n |w_j|$$

- Sets some coefficients to 0: feature selection
- In the ideal case, we can use both L1 and L2
- Usage: add the regularization term to the cost function
 - $\lambda > 0$, larger \Rightarrow stronger regularization

1.3 Linear Regression with Regularization

- Ridge regression** – L2

- Cost function:

$$J(w) = \frac{1}{2n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2 + \lambda \|w\|_2^2$$

```
from sklearn.linear_model import Ridge
model = Ridge(alpha = 0.01)
```

- **LASSO (Least Absolute Shrinkage and Selection Operator) – L1**

- Cost function:

$$J(w) = \frac{1}{2n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2 + \lambda \|w\|_1$$

```
from sklearn.linear_model import Lasso
model = Lasso(alpha = 0.01)
```

- Elastic Net

- Has both regularization terms

```
from sklearn.linear_model import ElasticNet
model = ElasticNet(alpha = 1.0, l1_ratio = 0.5)
```

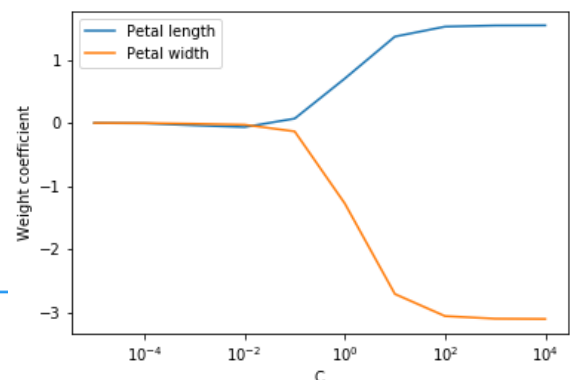
1.4 Logistic Regression with Regularization

- The LogisticRegression class in scikit-learn accepts a regularization parameter C
 - Added to the cost function, L2-type
 - $C = \frac{1}{\lambda}$ (by convention)
- Increasing C \Rightarrow weaker regularization
 - The algorithm follows the data more closely
- Decreasing C \Rightarrow stronger regularization
 - The algorithm "doesn't care too much about the data"
- How to choose a value?
 - We'll talk about this later, stay **tuned**...

1.5 Visualizing Regularization Parameters

- Perform a logistic regression on the [Iris](#) dataset with several values of C
 - Display the weights
 - Observe how decreased C leads to weight shrinking

```
iris = load_iris()
attributes, labels = iris.data[:, [2, 3]], iris.target
weights, params = [], []
for c in np.arange(-5, 5):
    model = LogisticRegression(C = 10.0 ** c)
    model.fit(attributes, labels)
    weights.append(model.coef_[1]) # Display only the second class
    params.append(10.0 ** c)
weights = np.array(weights)
plt.plot(params, weights[:, 0], label = "Petal length")
plt.plot(params, weights[:, 1], label = "Petal width")
plt.xlabel("C")
plt.ylabel("Weight coefficient")
plt.xscale("log")
plt.legend()
plt.show()
```



2. Model Testing

2.1 Training and Testing Sets

- One of the most important rules in machine learning is
 - NEVER test the model with the data you trained it on!**
 - The model may "cheat" and learn the answers instead of finding structure in the data
- Since we usually have one dataset, it's useful to "hold out" some of the data for testing
 - E.g., **70%** of the data is for training and **30%** – for testing
 - We need to take **randomized samples**
 - In cases of classification, we need [stratified](#) samples
- scikit-learn has a convenient method for this

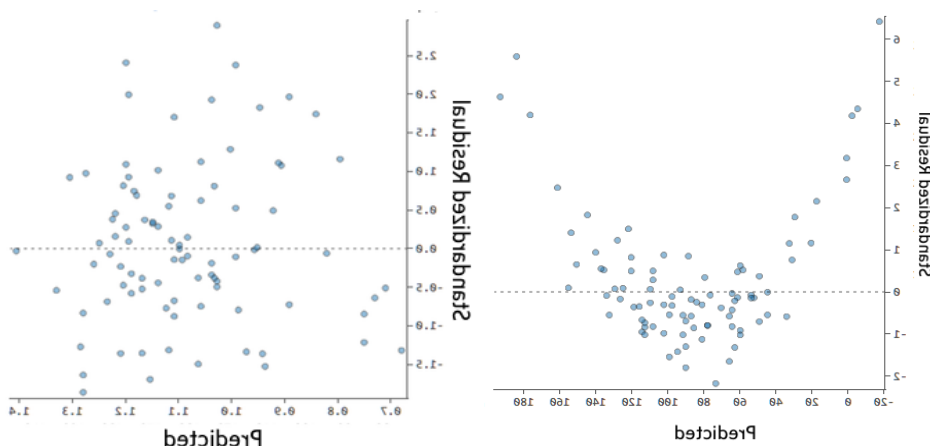
```
from sklearn.model_selection import train_test_split
attr_train, attr_test, l_train, l_test = train_test_split(attributes, labels, train_size = 0.7)
```

2.2 Evaluating Model Performance

- Once we train the model, we use the test data to score it
 - Using one of the scoring metrics
- Scoring metrics
 - Regression: usually coefficient of determination R^2 – proportion of variance predictable from the independent variables
 - Other: mean squared error, mean absolute error, explained variance
 - Classification: usually accuracy (how many items have been properly classified)
 - Other: precision, recall, F1
- For more metrics, look at the [docs](#)
- The output from scoring tells us how good the model is

2.3 Evaluating Regression

- No fixed rules, use your intuition and knowledge about the data
- Several guidelines
 - One metric is [usually not enough](#)
 - For example, mean squared error and coefficient of determination
 - Also useful: mean absolute error and mean squared error
 - Create a residual plot ($O - E$: observed minus estimated)
 - There should be no visible structure
 - If there is some structure in the residuals, the model fails to explain something
 - Create a histogram of the residuals
 - Most residuals should be "sufficiently close" to zero
 - There should be no observable structure



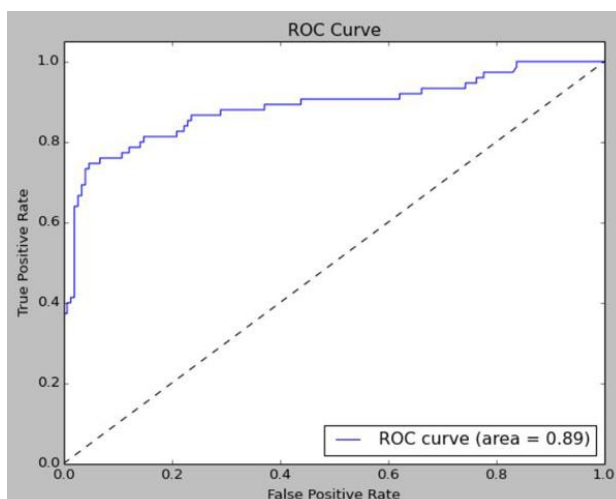
2.4 Evaluating Classification

- Confusion matrix (error matrix)
 - Shows predicted vs. actual classes
 - Simplest case: 2-class classifier
 - Can be extended
 - FP \equiv Type I error, FN \equiv Type II error
- Metrics: numbers derived from the confusion matrix
 - Accuracy (number of correctly classified samples): $A = \frac{TP+TN}{TP+TN+FP+FN}$
 - If detecting anomalies, accuracy can be misleading
 - Precision (how many selected samples are relevant): $P = \frac{TP}{TP+FP}$
 - Recall (how many relevant samples are selected): $R = \frac{TP}{TP+FN}$
 - F1-score: $\frac{2TP}{2TP+FP+FN} = 2 \frac{R \cdot P}{R+P}$
 - Many more metrics exist (useful for specific cases)

	p' (Predicted)	n' (Predicted)
p (Actual)	True Positive	False Negative
n (Actual)	False Positive	True Negative

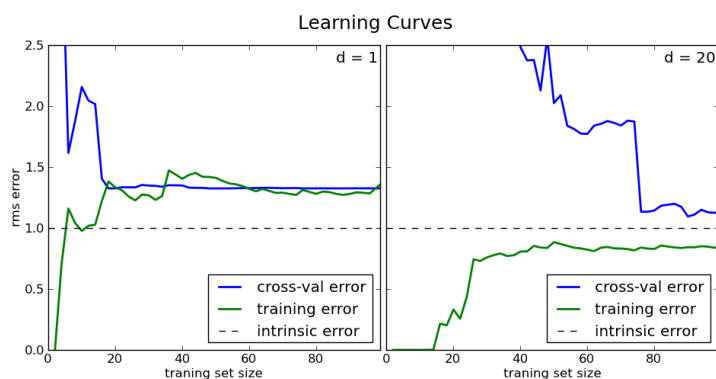
2.5 Receiver Operating Characteristic

- Limited to 2-class classification
 - We can use "1 vs. all" for more classes
- A plot of true positive rate vs. false positive rate
 - A "bisector line" represents truly random guessing
 - Any curve above the line is better than random
 - Closer to the upper left corner = better
 - Below the line: still better than random, we have to reverse the classifier output
- Area under the curve (AUC): closer to 1 = better
- [Example](#) in scikit-learn



2.6 Learning and Validation Curves

- Plots which allow us to diagnose bias and variance problems
 - Some metric (e.g., accuracy) vs. a model parameter (e.g., sample size)
 - Plot two curves – for the training and validation data
- High bias – accuracy for training and validation is too low
 - Solution: add more model features, decrease regularization
- High variance – large gap between the two curves
 - Solution: remove model features (preprocessing / feature selection/ feature engineering, etc.), increase regularization
- [Tutorial](#) (scikit-learn)



2.7 Cross-Validation

- Most algorithms improve their parameters based on the test scores
 - This means knowledge of test data may "leak" into the algorithm and overfit the data
- Solution: cross-validation
 - Split all data into k groups (folds) – usually $k = 10$
 - More samples = fewer folds
 - Using a KFold splitter
 - Each time train with $k - 1$ folds and test with the other fold

```
from sklearn.model_selection import StratifiedKFold, cross_val_score  
  
k_fold = StratifiedKFold(n_splits = 5)
```

```
scores = cross_val_score(model, attributes, labels, cv = k_fold)
```

2.8 Improved Technique

- Test / train set → faster
- Cross-validation → more accurate
- Best performance (but even slower): combine the methods
 - Leave out some of the data for testing at the beginning (e.g. 30%)
 - Perform cross-validation on the other 70%
 - Fine-tune the model and / or select one of many models based on the best cross-validation score
 - Run the best model on the other 30%
 - We selected the best model based on the training data ⇒ we have some bias
 - One model will always have the highest score, even if it's by chance
 - This truly out-of-sample method removes (some of) the bias
 - Model selection: choose the best performing model

2.9 Hyperparameter Tuning

- Techniques for choosing the best model hyperparameters
 - Such as regularization

- Most widely used: grid search
 - "Brute-force": specify parameters; run models with all possible parameter combinations; choose the best model
- Randomized search – each setting is sampled randomly from a parameter range
 - Faster but not guaranteed to produce the best results

```
from sklearn.model_selection import GridSearchCV

tuned_params = [{"C": [0.001, 0.01, 0.1, 1, 10, 100, 1000],
                  "penalty": ["l1", "l2"]}]
grid = GridSearchCV(LogisticRegression(), tuned_params)
grid.fit(attr_train, l_train)
print(grid.best_params_) # Estimator: grid.best_estimator_
```

2.10 Making the Best of Our Models

- Usually, we don't know right away which algorithm will perform best
- We select several algorithm types
 - Fine-tune their parameters using grid search (or some other technique)
 - Select the best combination of parameters
- After that, we compare the best algorithms from each type
 - Using the model selection procedure
 - Hold-out (test) set + cross-validation set
 - Select the best performing model type on the cross-validation set
 - Test it on the "hold-out" set
- Improvements: perform test / train split on the hyperparameter tuning step; use different performance scores

3. Manipulating Features

3.1 Guidelines for Manipulating Features

- Main ideas
 - **Reduce** the number of features (\Rightarrow simpler model)
 - Keep **relevant** information only
- Feature selection
 - Removing irrelevant features
 - Regularization does a good job at this
 - Other methods: dimensionality reduction
 - We'll talk about this later in the course
- Feature engineering
 - Producing new, meaningful features
 - Requires a lot of work and domain knowledge