Predictive Modelling

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Predictive Modelling

- Today we are going to change paradigm and focus on one form of predictive modelling
  - Supervised learning
- "Can I predict a quantity if I know other relevant quantities"
  - Can I predict the weather if know historical data, time of the year, etc?
  - Can I predict if a car will break down given how old it is?
  - Can I predict how many likes a Facebook page will get?

Supervised learning framework

- A teacher provides a label/target for each example in the training set: $\mathcal{X} = \{(\boldsymbol{x}^t, y^t)\}_{t=1}^N$.
- By using the labelled examples, we learn a model ($\hat{f}(x)$) which provides outputs ($\hat{y}$) that are close enough to the observed ones on the training set (y).
- We expect our model outputs to be close to the true process outputs on unseen data.

How good are these predictions?

- Quality of learning
  - Bias - Variance decomposition
  - Measuring the quality of a supervised learning algorithm
  - Getting error estimates on predictions
  - Measuring the performance of our model

Scikit-learn

- Golden trinity of the Scipy ecosystem together with Pandas and Numpy
- This is not a machine learning module, we have more of a "birds-eye" view of the algorithms involved
  - We will see them as objects that have various interesting properties
  - You still need to understand what they do more or less
- You will need to be able to use scikit-learn to create new models
- Essential part of the Data Scientist toolbox

The dataset

The example data we are going to use today come from:

Moro, Sérgio, Paulo Rita, and Bernardo Vala. "Predicting social media performance metrics and evaluation of the impact on brand building: A data mining approach." Journal of Business Research 69.9 (2016): 3341-3351.

The dataset contains 500 publicly available instances.

We are trying to predict the performance of a new post.

Given a list of samples

	Category	Page total likes	Type	Post Month	Post Hour	Post Weekday	Paid
0	2	139441	Photo	12	3	4	0.0
1	2	139441	Status	12	10	3	0.0
2	3	139441	Photo	12	3	3	0.0
3	2	139441	Photo	12	10	2	1.0
4	2	139441	Photo	12	3	2	0.0

	like	share	Total Interactions
0	79.0	17.0	100
1	130.0	29.0	164
2	66.0	14.0	80
3	1572.0	147.0	1777
4	325.0	49.0	393

Loading the data

```
df = pd.read_csv("./dataset_Facebook.csv", delimiter=";")
df.head() # just prints top 5 columns if you are in ipython

features = ["Category",
            "Page total likes",
            "Type",
            "Post Month",
            "Post Hour",
            "Post Weekday",
            "Paid"]


outcomes=  ["Lifetime Post Total Reach",
            "Lifetime Post Total Impressions",
            "Lifetime Engaged Users",
            "Lifetime Post Consumers",
            "Lifetime Post Consumptions",
            "Lifetime Post Impressions by people who have liked your Page",
            "Lifetime Post reach by people who like your Page",
            "Lifetime People who have liked your Page and engaged with your post",
            "comment",
            "like",
            "share",
            "Total Interactions"]
```

Cleaning up

```
df = df.dropna()

outcomes_of_interest = ["Lifetime Post Consumers", "likes"]

#scikit-learn does not accept string-formatted data
df[["Type"]] = df[["Type"]].apply(LabelEncoder().fit_transform)


X_df = df[features].copy()
y_df = df[outcomes_of_interest].copy()

X_df.head()  # shows first 5 rows
```

	Category	Page total likes	Type	Post Month	Post Hour	Post Weekday	Paid
0	2	139441	1	12	3	4	0.0
1	2	139441	2	12	10	3	0.0
2	3	139441	1	12	3	3	0.0
3	2	139441	1	12	10	2	1.0
4	2	139441	1	12	3	2	0.0

Playing with dataframes

- Make sure you make copies of the dataframe if you want to modify it but keep the original
- Otherwise it is just views on the same data
  - You will modify everything
- Note the double "[[column1, column2...]]" notation
  - If you just use [column1] you get back a Series, not a DataFrame
- We used the LabelEncoder to encode the labels
  - but how about decoding?

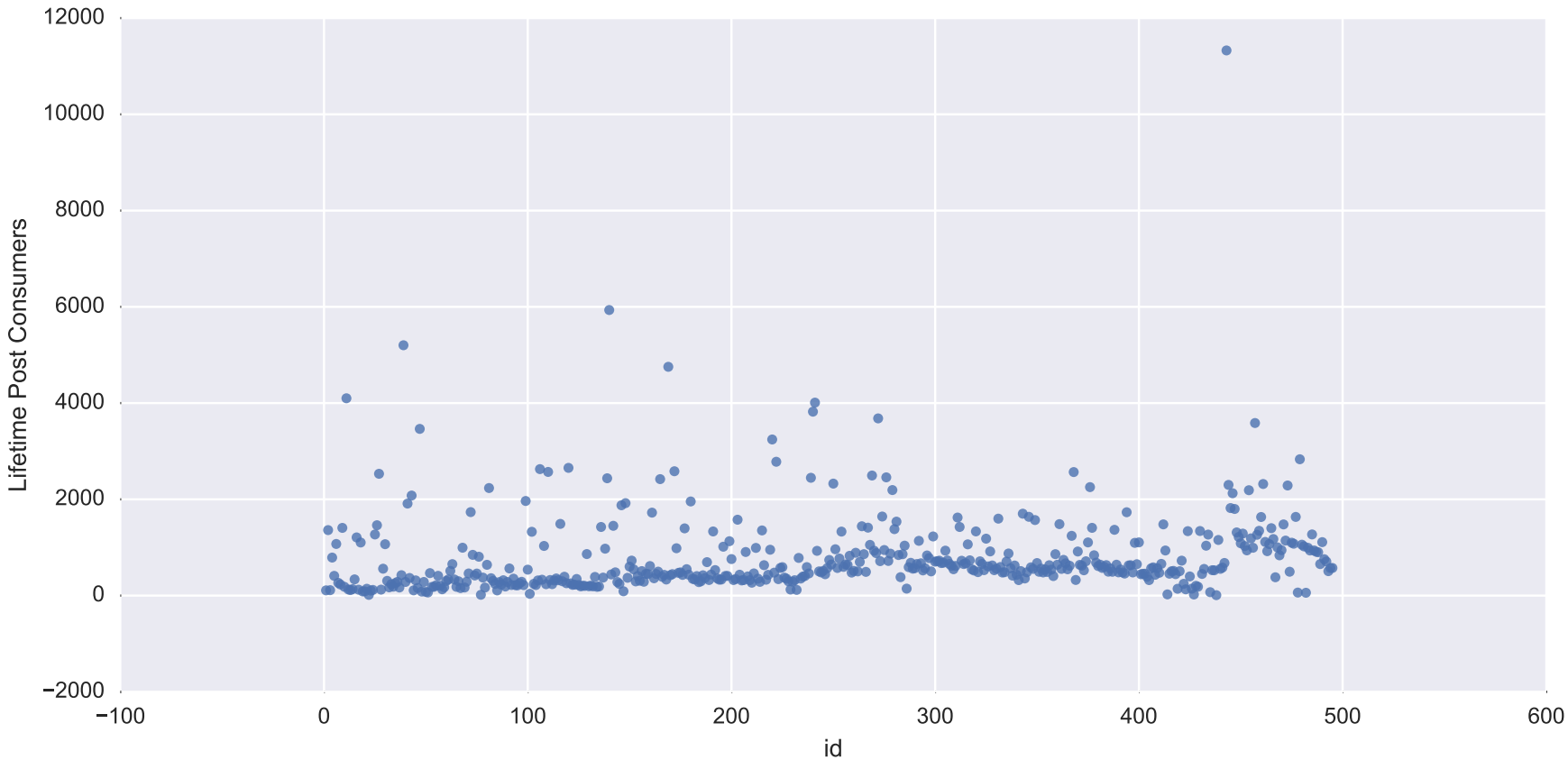
Some pandas trivia

```
# Adding a new column
y_df['id'] = range(1, len(df) + 1)
```

- If the column exists, it will replace it
- If the column does not, it will create it
- Make sure the data you are trying to insert have the same column length

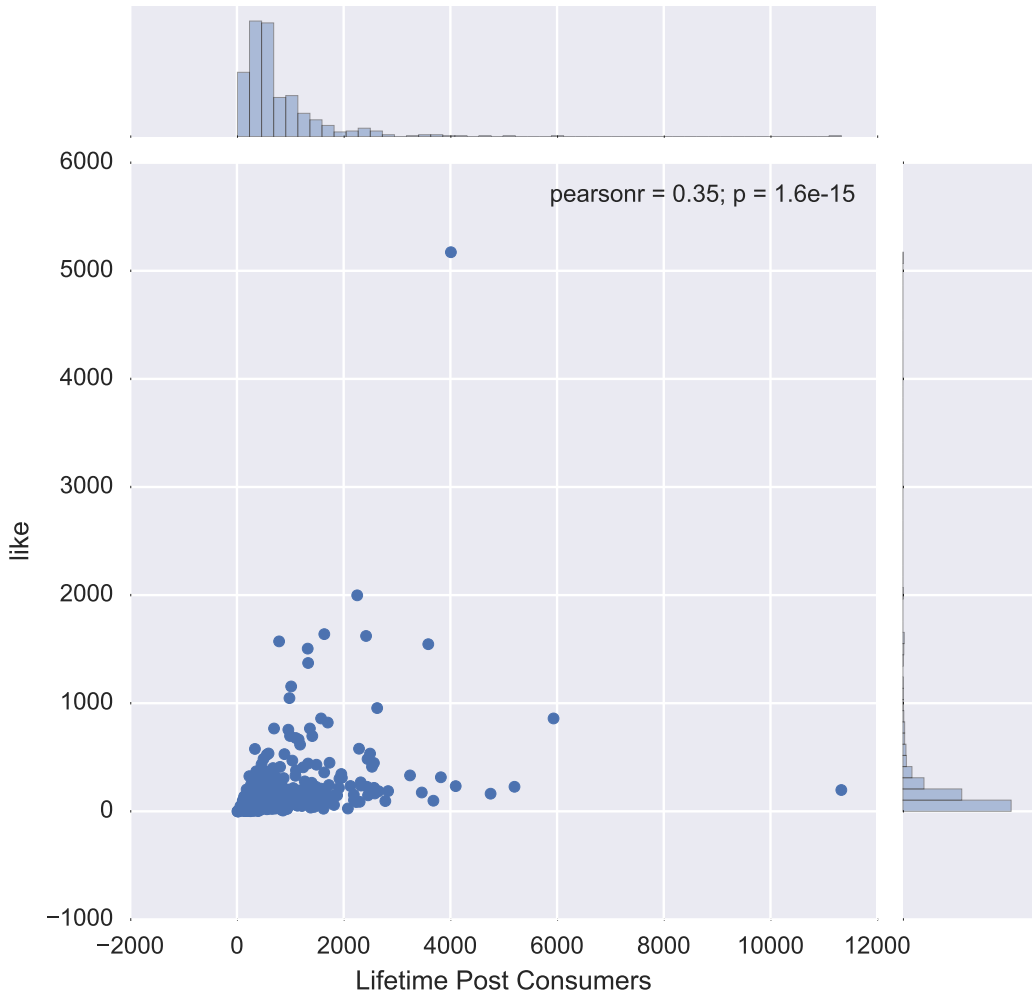
Plotting the data

```
# Notice how aspect changes the aspect ratio
sns_plot = sns.lmplot(x="id", y=attribute, data=y_df, fit_reg=False, aspect=2)
```



Joint Plot with "likes"

```
# Notice how "aspect" changes the aspect ratio
sns_plot = sns.lmplot(x="id", y=attribute, data=y_df, fit_reg=False, aspect=2)
```



Modelling the data

- We would like to learn some model of the data that relates them to the outcome
- That is, if someone gives us a row of features we should be able to predict the corresponding outcome (e.g., how many likes will that post obtain)

Decision Trees and Random Forests

- For classification and regression we are going to use Classification And Regression Trees (CART)
- A tree creates a function between the features and an output attribute
- When you are predicting a certain type (e.g. “apples” vs “oranges”) it is called *classification*
- When this output is real-valued the procedure is called *regression*
- If you fit multiple decision trees on different bootstraps of the data (and features) and get the mean you have a random forest

Prediction

- Let's build a tree and fit on the data

```
from sklearn.tree import DecisionTreeRegressor

X = X_df.values
y = y_df.values.T[0]
y = (y - y.min())/(y.max() - y.min())

clf = DecisionTreeRegressor()
clf.fit(X, y)

print(mse(y, clf.predict(X))) # Mean Squared Error
```

Mean squared Error

- Reality is $f(x)$
- Our model is $\hat{f}(x)$ (e.g., a decision tree)
- The real labels are $\{y_0, ..., y_N\}$
  - $MSE = \frac{1}{N} \sum_{i=1}^{N} \left(y_i - \hat{f}(x_i) \right)^2$
  - $E\left[\left(y - \hat{f}(x) \right)^2 \right]$
- Let's say MSE = 1.5083614548e-05
  - Is this number meaningful?

Noise in the data

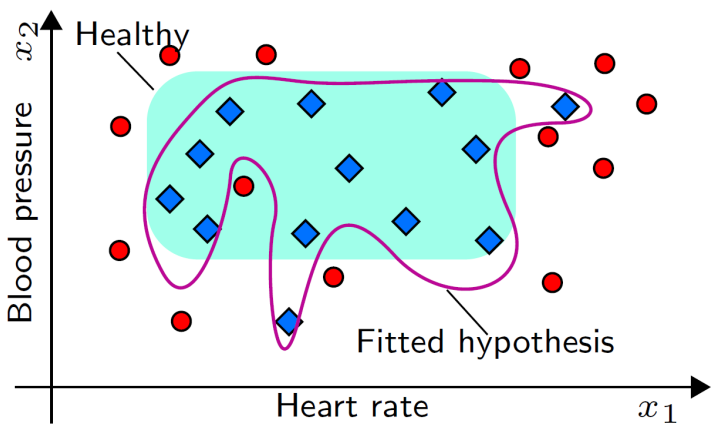
- Data typically contain errors
- Possible causes:
  - imprecision in recording the input attributes (e.g., measurement errors, human mistakes...)
  - imprecision affecting the target value measurement (e.g., errors of expert judgement)
  - random errors: effect of additional attributes that affect the label of an instance but are unavailable (neglected/hidden/unobservable)
- We refer to all of these as **noise**

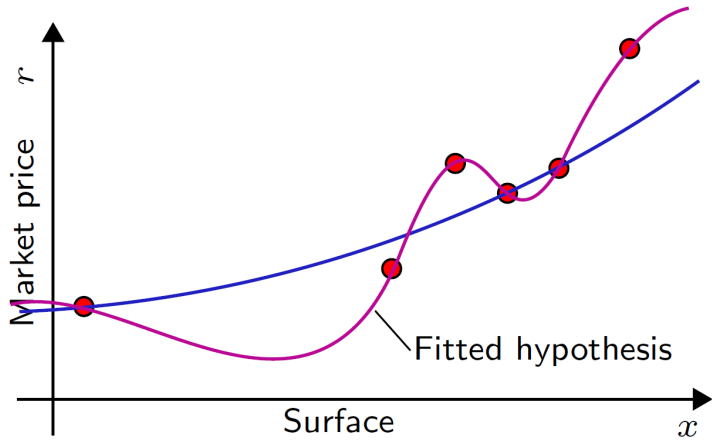
Consequences of noise

The main consequence of noise in the training data is **overfitting**, i.e., the **fitted hypothesis reflects the random error** instead of the underlying relationship between the features and the target.

In turn, overfitting causes:

- *Solutions that are more complex than necessary* and hard to interpret
- *Solutions that don't generalize*, i.e., poor accuracy on new unseen data



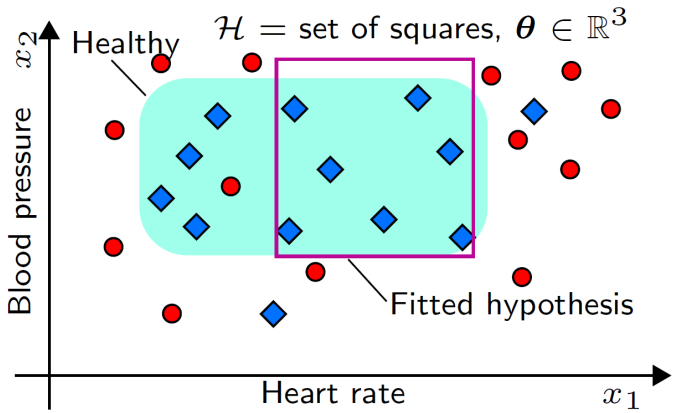


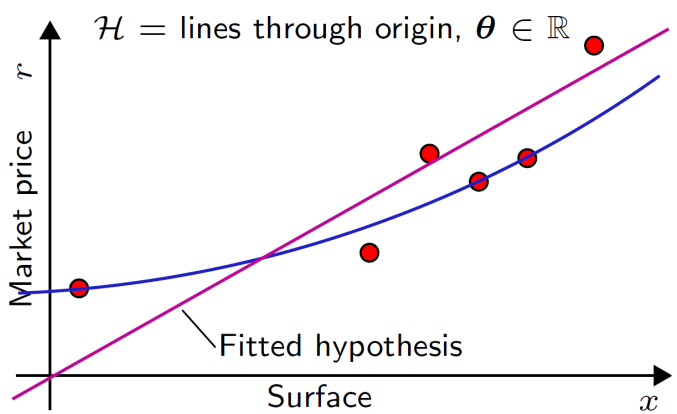
Alleviate effect of noise

To alleviate these harmful effects of noise, we have to prevent overfitting.

The common approach is to **simplify induced hypotheses**, i.e., use models that require a smaller number of parameters to be estimated from the data.

On the other hand, if the hypothesis is too simple, we incur in the opposite type of error: **underfitting**.





Errors in predictions

After analysing possible sources of error in the training data, we are interested in the errors we make when **predicting unseen examples**.

Possible sources of error:

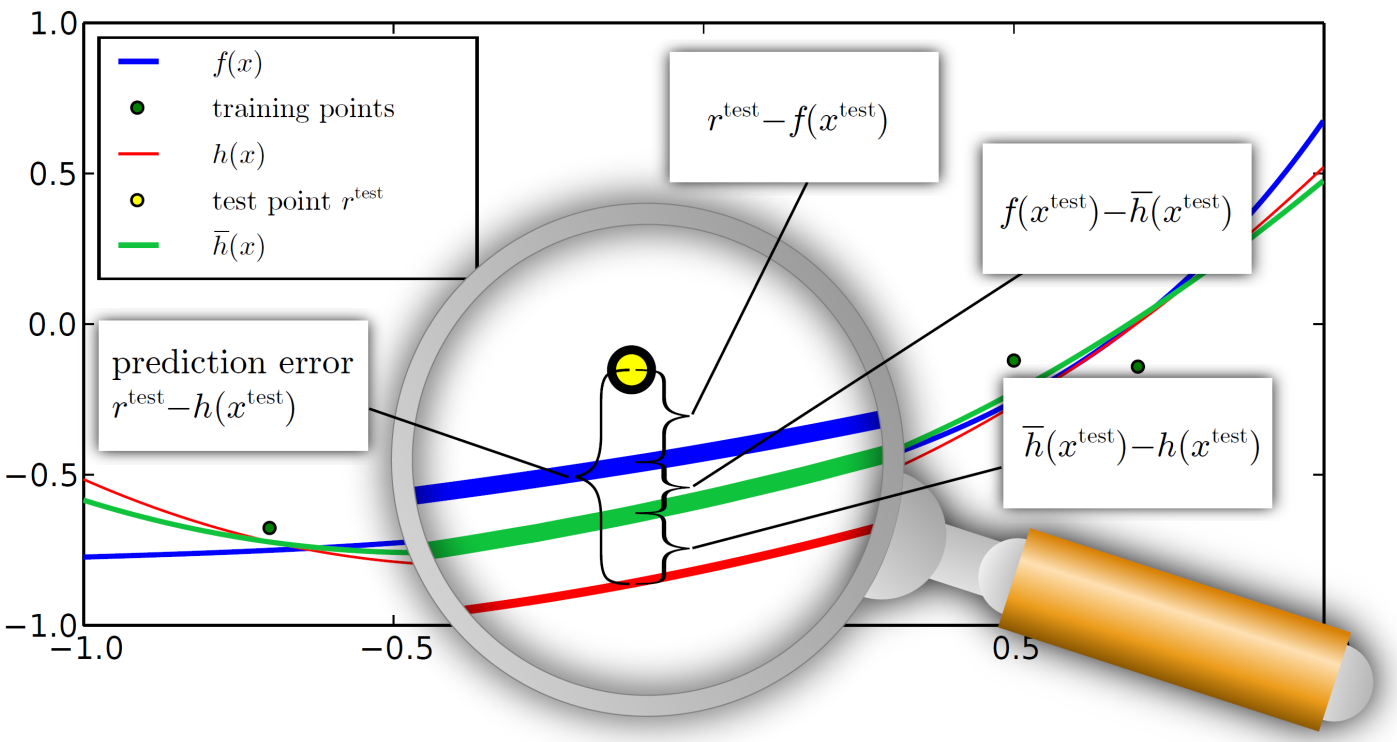
- Same as in the training data (after all, we made the assumption that training data and test data are drawn from the same population)
- Errors due to a model that underfits the training data
- Errors due to a model that overfits the training data

Can we quantify the errors we make when predicting unseen examples?

Decomposing the prediction error

We fit a model $h(x)$ from our training set.

Given a new data point $(x^{\text{test}}, r^{\text{test}})$, what prediction error $r^{\text{test}} - h(x^{\text{test}})$ should we expect?



Decomposing the squared prediction error

$$E\left[(y-\hat{f}(x))^2\right] = \left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma^2$$

$$E\left[(y-\hat{f}(x))^2\right] = Bias^2 + Variance + Noise$$

$$Bias = \left(E[\hat{f}(x)] - f(x)\right)$$

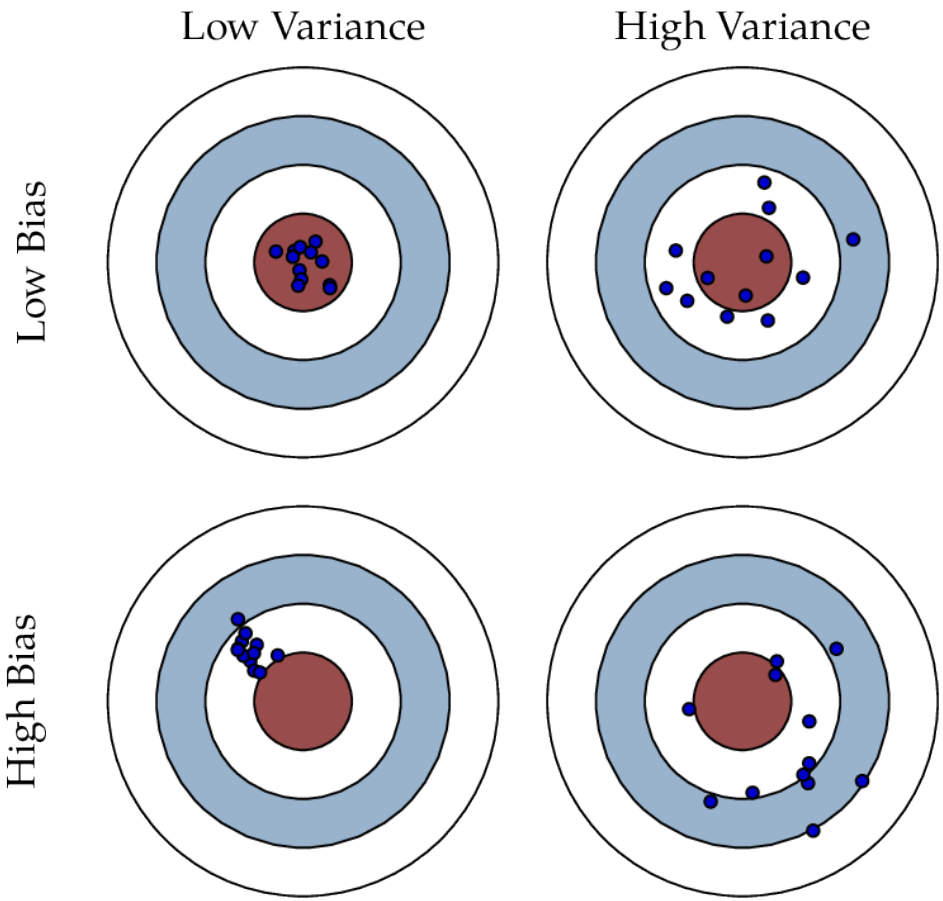
$$Variance = E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] = Var[\hat{f}(x)]$$

$$Noise = \sigma^2$$

Bias-variance decomposition

- What does this error represent?
- One way of understanding the quality of a regressor is to use the bias-variance decomposition of the error
- Bias is the error you expect because reality and your model are different (i.e., $f(x) \neq \hat{f}(x)$)
- Variance is the error you expect due to random noise and only seeing a sample of your data

Intuition



http://tex.stackexchange.com/questions/307117/reconstructing-the-following-bias-variance-diagram

Bias

- A high bias model is strongly opinionated vs the data
  - A constant function (predicting "0" all the time)
  - A linear function on very non-linear data
  - i.e., a model that's too simple for the data we're modelling
- A low bias fits the data closely
  - A model that was created to fit the data
    - A decision tree when the data was created using rules
  - A linear function when the data is generated by a linear process

Variance

- A high variance model changes opinions about the data based on the samples it sees
  - A decision tree on very few data points
  - A very complex model on a very simple function
- A low variance model is not impacted by the training data that much
  - A constant function
  - The mean
- Variance comes from randomness in the training set

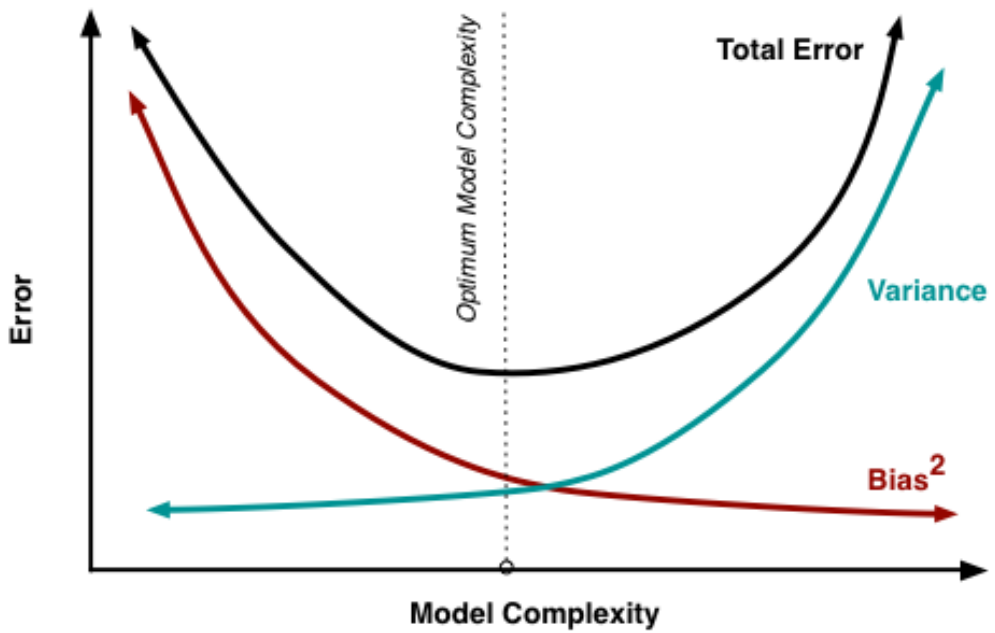
The tradeoff

- We can't really measure the noise easily
  - It's also the lower bound on our performance
- Models with high variance have low bias
- Models with high bias have low variance

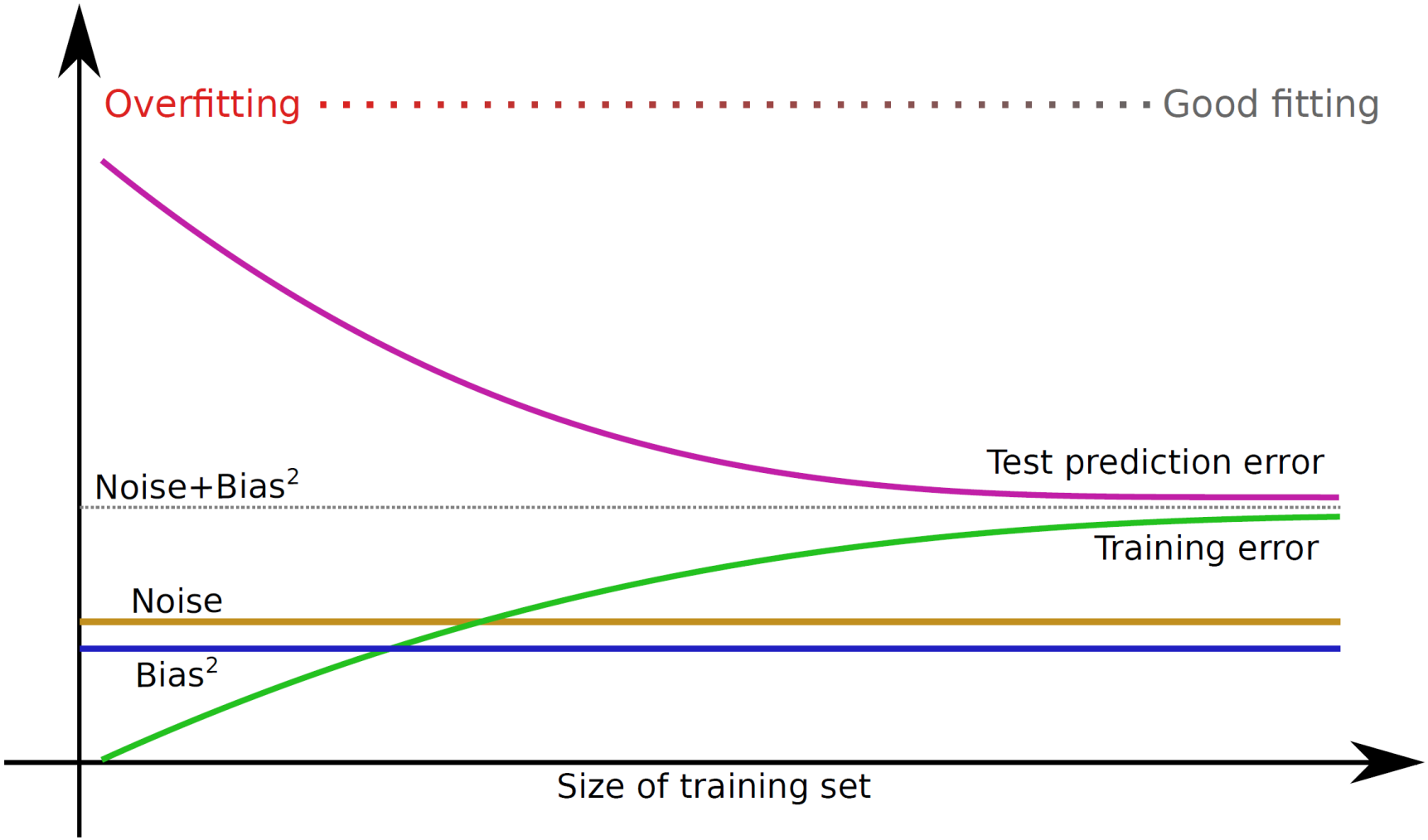
A very nice article on the bias-variance tradeoff:
`http://scott.fortmann-roe.com/docs/BiasVariance.html`

Bias and variance as a function of model complexity

In general, increasing complexity reduces bias (i.e. the error related to underfitting) and increases variance (i.e. the error related to overfitting).



Bias and variance as a function of size



Bias-variance - using the bootstrap (1)

Let's assume noise is zero, hence:

$$E\left[(y - \hat{f}(x))^2\right] = \left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right]$$

We don't have access to all the samples - what should we do?

Bias-variance - using the bootstrap (2)

```
n_test = 100
n_repeat = 1000

#estimator = DecisionTreeRegressor()
estimator = RandomForestRegressor()

# Compute predictions
y_predicts = np.zeros((n_repeat, len(X)))
for i in range(n_repeat):

    sample  = np.random.choice(range(len(X)),replace=True, size=len(X))

    train_ids = sample[:-n_test]
    test_ids  = sample[-n_test:]
    test_ids = np.setdiff1d(test_ids, train_ids)
    if(len(test_ids) == 0 ):
        continue

    X_train,y_train = X[train_ids], y[train_ids]
    X_test, y_test = X[test_ids], y[test_ids]

    estimator.fit(X_train, y_train)
    y_predict = estimator.predict(X_test)
    y_predicts[i,test_ids] = y_predict
```

Bias-variance - using the bootstrap (3)

```
y_bias = (y - np.mean(y_predicts, axis=0)) **2

y_error = ((y - y_predicts)**2).mean()
y_var = np.var(y_predicts, axis=0, ddof=1)

clf_type = "Decision tree"
print("{0}: {1:.4f} (error) = {2:.4f} (bias^2) "
          "+ {3:.4f} (var)".format(clf_type,
                                   np.mean(y_error),
                                   np.mean(y_bias),
                                   np.mean(y_var)))

print("{0}: {1:.4f} ((bias^2) + (var)) = {2:.4f} (bias^2) "
          "+ {3:.4f} (var)".format(clf_type,
                                   np.mean(y_bias) + np.mean(y_var),
                                   np.mean(y_bias),
                                   np.mean(y_var)))
```

Measuring error

Decision tree: 0.0110 (error) = 0.0100 (bias^2) + 0.0010 (var)

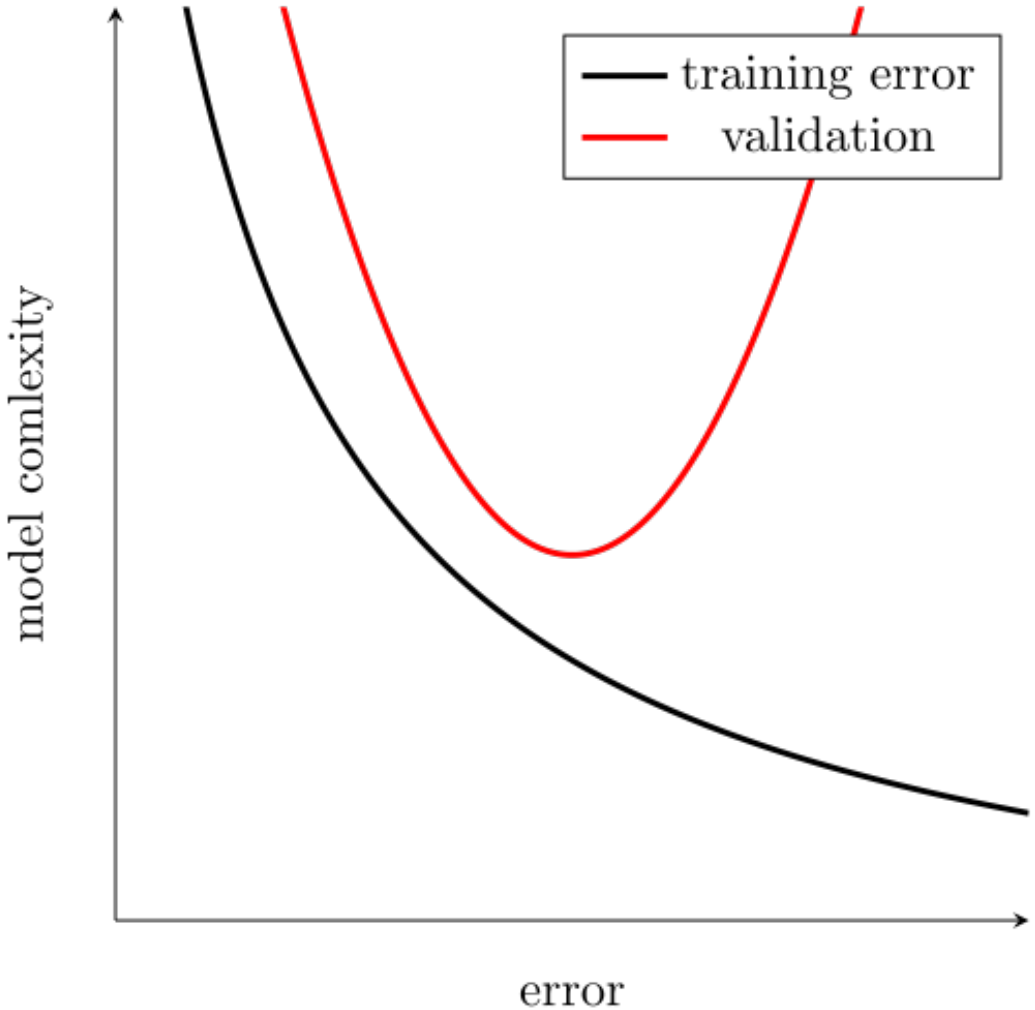
Decision tree: 0.0110 ((bias^2) + (var)) = 0.0100 (bias^2) + 0.0010 (var)

Random Forest: 0.0107 (error) = 0.0099 (bias^2) + 0.0008 (var)

Random Forest: 0.0107 ((bias^2) + (var)) = 0.0099 (bias^2) + 0.0008 (var)

- The procedure for using the bootstrap to find better values for a model is called "Bagging"
  - Mostly minimises the variance
  - Very commonly used trick

Error vs validation (or test set)



https://github.com/MartinThoma/LaTeX-examples/tree/master/tikz/bias-variance

Cross validation (1)

- One of the most common procedures used when evaluating a model
- We take data X,y
- Split into 10 different random chunks (called **folds**)
- Learn a model using 9 of them
- Test performance on the 10^{th} (the one you did not use for learning)
- Pick another 9, test on another set
- Keep on going until you test on all test subsets
- K-fold cross-validation
  - There are other methods, but all related to this basic principle

Cross validation (2)

It is largely automated on scikit-learn

```
clf = RandomForestRegressor(n_estimators=1000,max_depth=2)
dummy_clf = DummyRegressor()
scores = cross_val_score(clf, X, y, cv=10,scoring=make_scorer(mse))
dummy_scores = cross_val_score(dummy_clf, X, y, cv=10, scoring=make_scorer(mse))

print("MSE: %0.8f (+/- %0.8f)" % (scores.mean(), scores.std()))
print("Dummy MSE: %0.8f (+/- %0.8f)" % (dummy_scores.mean(), dummy_scores.std()))
```

MSE: 0.00699996 (+/- 0.00748646)

Dummy MSE: 0.00616020 (+/- 0.00521769)

What can we say about our model?

- It is bad
- We are worse than just predicting the average!
- Hence we can't really say much about if there is any relationship between our variables of interest
  - You can't prove a negative
  - Maybe our regressor is not good enough?
- We are not seeing any predictive effect here

Ridge Regression

Maybe we can get better results with a different regressor?

```
cat_features = ["Category", "Type", "Paid"]

X_df = pd.get_dummies(X_df, cat_columns=features)
```

Here is how "category" is converted to dummy

	Category_1	Category_2	Category_3
0	0.0	1.0	0.0
1	0.0	1.0	0.0
2	0.0	0.0	1.0
3	0.0	1.0	0.0
4	0.0	1.0	0.0

BayesianRidge Regression

```
from sklearn.linear_model import  BayesianRidge
clf = BayesianRidge(normalize=True)
dummy_clf = DummyRegressor()
scores = cross_val_score(clf, X, y, cv=10,scoring=make_scorer(mse))
dummy_scores = cross_val_score(dummy_clf, X, y, cv=10, scoring=make_scorer(mse))

print("MSE: %0.8f (+/- %0.8f)" % (scores.mean(), scores.std()))
print("Dummy MSE: %0.8f (+/- %0.8f)" % (dummy_scores.mean(), dummy_scores.std()))
```

MSE: 0.00479575 (+/- 0.00511744)

Dummy MSE: 0.00616020 (+/- 0.00521769)

Not great (at all!), but better

Binning samples

- Maybe we can try to create classes out of the data

```
outcomes_of_interest = ["Lifetime Post Consumers", "like"]
n_bins = 20

X_df = df[features].copy()
y_df = df[outcomes_of_interest].copy()

bins =  pd.qcut(y_df[outcomes_of_interest[0]].values,n_bins)
y_df = df[outcomes_of_interest].copy()
y_df[outcomes_of_interest[0]] = bins
y_df[outcomes_of_interest] = y_df[outcomes_of_interest].apply(LabelEncoder().fit_transform)
```

Metrics for classification

- Each row is now assigned to a class of $y_i \in 0, ..., 19$
- Accuracy is the obvious one
  - $accuracy = \frac{1}{N} \sum_{i=0}^{N-1} y_i = \hat{f}(x)$
  - The higher the accuracy the better
- What if the dataset is unbalanced - how informative is accuracy then?
- There are multiple metric functions
  - Use the one appropriate for your problem

Now with the classifier

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import ExtraTreesClassifier

clf = ExtraTreesClassifier(n_estimators=1000,max_depth=4)

dummy_clf = DummyClassifier()
scores = cross_val_score(clf, X, y, cv=10,scoring=make_scorer(acc))
dummy_scores = cross_val_score(dummy_clf, X, y, cv=10, scoring=make_scorer(acc))

print("ACC: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std()))
print("Dummy ACC: %0.2f (+/- %0.2f)" % (dummy_scores.mean(), dummy_scores.std()))
```

ACC: 0.18 (+/- 0.06) Dummy ACC: 0.05

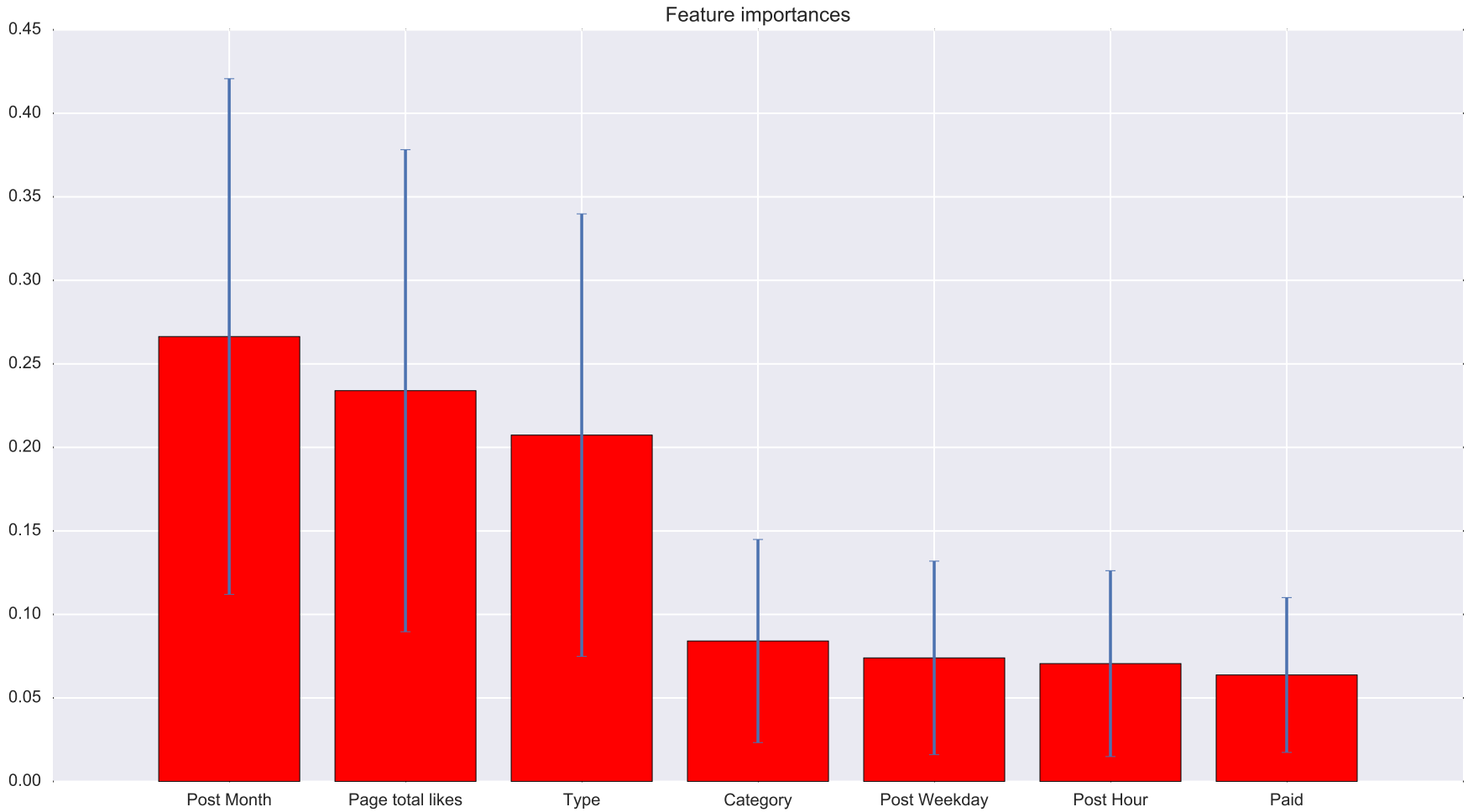
Generate feature importances

```
importances = clf.feature_importances_
std = np.std([tree.feature_importances_ for tree in clf.estimators_], axis=0)
indices = np.argsort(importances)[::-1]

print("Feature ranking:")
for f in range(X.shape[1]):
    print("%d. %s (%f)" % (f + 1, features[indices[f]],  importances[indices[f]]))

# Plot the feature importances of the forest
fig = plt.figure()
plt.title("Feature importances")
plt.bar(range(X.shape[1]), importances[indices], color="r", yerr=std[indices], align="center")
plt.xticks(range(X.shape[1]), np.array(features)[indices])
plt.xlim([-1, X.shape[1]])
fig.set_size_inches(15, 8)
axes = plt.gca()
axes.set_ylim([0,None])
```

Feature importances

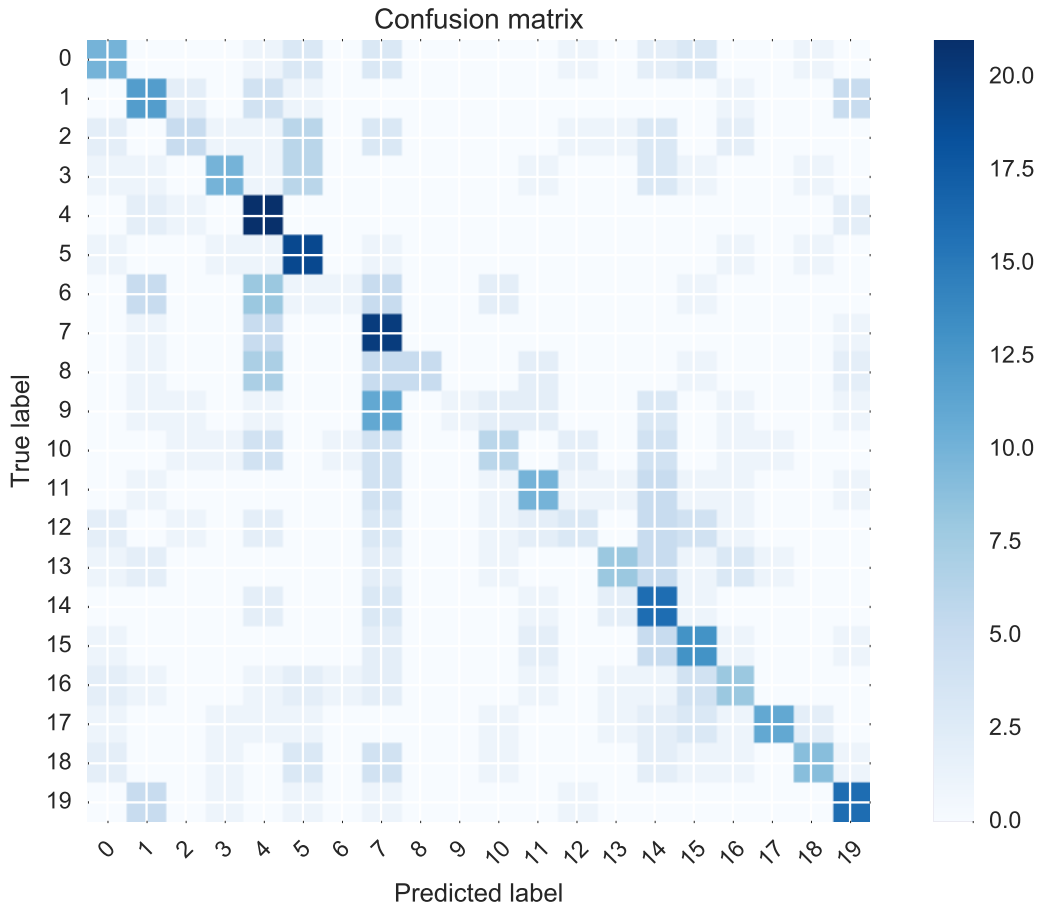


Generate a confusion matrix

```
# Compute confusion matrix
y_pred = clf.predict(X)
cnf_matrix = confusion_matrix(y, y_pred)
np.set_printoptions(precision=2)

# Plot non-normalized confusion matrix
plt.figure()
plot_confusion_matrix(cnf_matrix, classes=range(len(set(y))), normalize = False,
                      title='Confusion matrix')
```

Confusion Matrix?



Conclusion

- We have just touched the subject
- More in the labs
- We will revisit some of these concepts later on
- After today, you should be able to train a basic model
- If you are to optimise hyperparameters, you need to do nested cross-validation
  - Hyperparameters are things like tree size, depth etc.
  - Again, we will see this later on.