

ML 1: Black Box Machine Learning

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November 29, 2017

Overview

- What is machine learning for?
- What is machine learning?
- How do I do it? (e.g. properly use an ML library)
- What can go wrong?
- Case study

Machine Learning Problems

What is Machine Learning for?

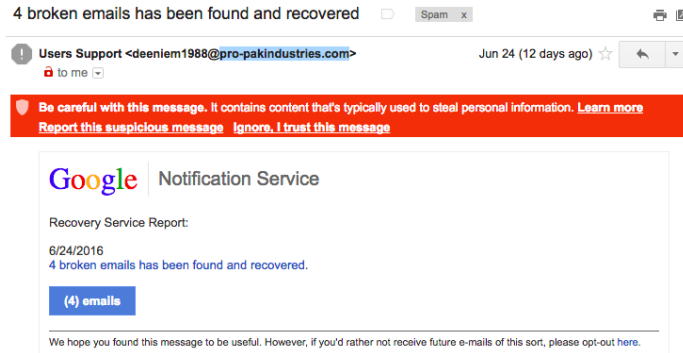
Common theme is to solve a prediction problem:

- given an **input** x ,
- **predict** an “appropriate” **output** y .

We'll start with a few canonical examples....

Example: Spam Detection

- **Input:** Incoming email



- **Output:** "SPAM" or "NOT SPAM"
- A **binary classification** problem, because only 2 possible outputs.

Example: Medical Diagnosis

- **Input:** Symptoms (fever, cough, fast breathing, shaking, nausea,...)
- **Output:** Diagnosis (pneumonia, flu, common cold, bronchitis, ...)
- A **multiclass classification** problem: choosing one of several [discrete] outputs.

How to express uncertainty?

- **Probabilistic classification** or **soft classification**:

$$\mathbb{P}(\text{pneumonia}) = 0.7$$

$$\mathbb{P}(\text{flu}) = 0.2$$

$$\vdots \quad \quad \vdots$$

Example: Predicting a Stock Price

- **Input:** History of stock's prices
 - **Output:** Predict stock's price at close of next day
 - A **regression** problem, because the output is a number.
- (Regression is **not** just “linear regression” from basic statistics.)

The Prediction Function

- A **prediction function** takes input x and produces an output y .
- We're looking for prediction functions that solve particular problems.
- **Machine learning** helps find the **best prediction function**.

What is Machine Learning?

What is **not** ML: Rule-Based Approaches

- Consider medical diagnosis.
 - ① Consult textbooks and medical doctors (i.e. “experts”).
 - ② Understand their diagnosis process.
 - ③ Implement this as an algorithm (a “**rule-based system**”)
- Doesn't sound too bad...
- Very popular in the 1980s.

(To be fair, these “**expert systems**” could be much more sophisticated than they sound here. For example, through “inference” they could make new logical deductions from knowledge bases.)

Rule-Based Approach

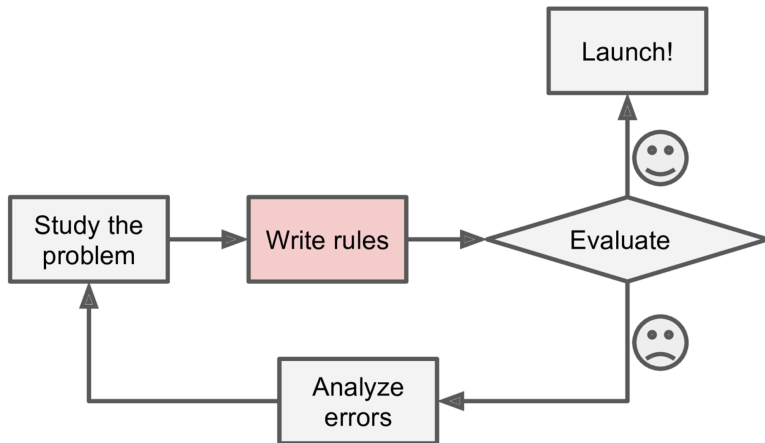


Fig 1-1 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

Issues with **rule-based systems**:

- Very labor intensive to build.
- Rules work very well for areas they cover
 - May not generalize well to unanticipated input combinations.
 - “Expert systems” had reputation of being “brittle”.

Disappointment in expert systems (late 80s / early 90s) led to an “**AI Winter**”.

- Don't reverse engineer an expert's decision process.
- Machine “learns” on its own.
- We provide “**training data**”, i.e.
 - many examples of (input x , output y) pairs.
 - e.g. A set of videos, and whether or not each has a cat.
 - e.g. A set of emails, and whether or not each is SPAM.
- Learning from training data of this form is called **supervised learning**.

- A machine learning algorithm:
 - **Input:** Training Data
 - “Learns” from the training data.
 - **Output:** A “prediction function” that produces output y given input x .

Machine Learning Approach

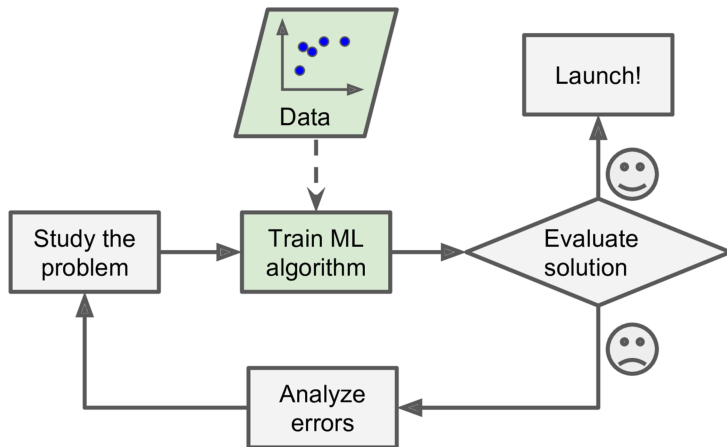


Fig 1-2 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

- **most common ML problem types**
 - classification (hard or soft/probabilistic)
 - multiclass (hard or soft/probabilistic)
 - regression
- **prediction function**
 - predicts output y given input x
- **training data**
 - a set of (input x , output y) pairs
- **supervised learning algorithm**
 - takes training data and produces a prediction function

Elements of the ML Pipeline

Feeding Inputs to ML Algorithms

- Raw input types can be
 - Text documents
 - Variable-length time series
 - Image files
 - Sound recordings
 - DNA sequences
- But most ML prediction functions like their input as
 - **fixed-length arrays of numbers**
 - `double[d]` – for the computer scientists
 - \mathbf{R}^d – for the mathematicians

Feature Extraction

Definition

Mapping raw input x to \mathbb{R}^d is called **feature extraction** or **featurization**.

Raw Input

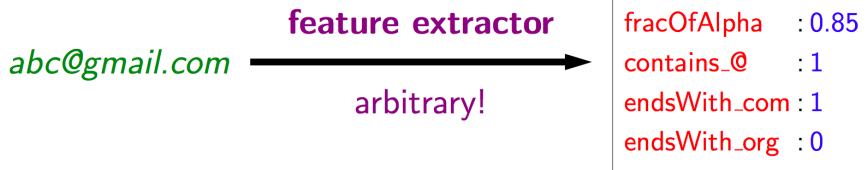
Feature Vector



- Better features \implies less “smart” ML needed (makes things easier)
 - Limiting case: a single feature is already the correct output
- **Feature vectors** are often called **input vectors**.

Example: Detecting Email Addresses

- **Task:** Predict whether a string is an email address
- Could use domain knowledge and write down:



- This was a bit ad-hoc. Could we be more systematic? Yes ...

Feature Template: Last Three Characters Equal ___

- Don't think about which 3-letter suffixes are meaningful...
- Just **include them all**.

abc@gmail.com



```
endsWith_aaa : 0  
endsWith_aab : 0  
endsWith_aac : 0  
...  
endsWith_com : 1  
...  
endsWith_zzz : 0
```

Feature Template: One-Hot Encoding

- **one-hot encoding**: a set of binary features that always has **exactly one** nonzero value.
- **categorical variable**: a variable that takes one of several discrete possible values:
 - *NYC Boroughs*: "Brooklyn", "Bronx", "Queens", "Manhattan", "Staten Island"
- Categorical variables can be encoded numerically using one-hot encoding.
 - In statistics, called a **dummy variable encoding**

Concept Check: How many features to one-hot encode the boroughs?

- Package feature vectors together with output “labels”:

Ftr1	Ftr2	...	FtrD	Y
0	1.54	...	932	False
1	-1.9	...	200	True
0	2.3	...	0	False

- Each **row** is an “example” or “labeled datum”.
- The last column is the **output** or “label” column.

- Just the feature vectors:

Ftr1	Ftr2	...	FtrD	Y
0	1.54	...	932	?
1	-1.9	...	200	?
0	2.3	...	0	?

- We want to be able to predict the missing labels.

Prediction Functions

A **prediction function** has

- **input:** a feature vector (a.k.a. “input vector”)
- **output:** a “label” (a.k.a. “prediction”, “response”, “action”, or “output”)

[Unlabeled] Input Data

Ftr1	Ftr2	...	FtrD
0	1.54	...	932
1	-1.9	...	200
0	2.3	...	0



Prediction Function $f(x)$



Predictions

Y
False
True
False

The prediction function is what gets **deployed**.

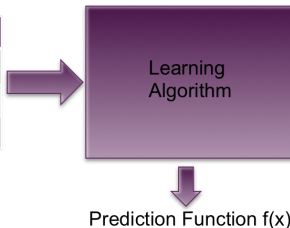
Learning Algorithm

A learning algorithm has

- **input:** labeled data (i.e. the **training set**)
- **output:** a **prediction function**

A training set of labeled data

Ftr1	Ftr2	...	FtrD	Y
0	1.54	...	932	False
1	-1.9	...	200	True
0	2.3	...	0	False



Today is about what's outside the "purple box". ML101 is about the inside of the box.

- **feature extraction**
 - maps raw inputs into arrays of numeric values
 - ideally, extracts essential features of the input
- **one-hot encoding for categorical variables**
- **labeled data / unlabeled data**

Evaluating a Prediction Function

Evaluating a Prediction Function

- Brilliant data science intern gives you a prediction function.
- How do we evaluate performance?
- Very important part of machine learning.
 - It can be subtle.
 - Evaluation should reflect business goals as closely as possible.

Evaluating a Single Prediction: The Loss Function

A **loss function** scores how far off a prediction is from the desired “target” output.

- `loss(prediction, target)` returns a number called “**the loss**”
- Big Loss = Bad Error
- Small Loss = Minor Error
- Zero Loss = No Error

- **Classification loss** or “0/1 Loss”
 - Loss is 1 if prediction is wrong.
 - Loss is 0 if prediction is correct.
- **Square loss** for regression
 - $\text{loss} = (\text{predicted} - \text{target})^2$

Evaluating a Prediction Function

- Data science intern gives you a prediction function $f(x)$.
 - “Average classification loss on training data was 0.01” (i.e. 1% error)
- Product manager says “we can deploy if $\leq 2\%$ error.”
- Deploy this prediction function?
 - No!
- Prediction function needs to do well on **new inputs**.
- (Don't test somebody with problems they've seen in advance.)

The Test Set

- A “**test set**” is labeled data that is **independent** of training data.
- e.g. Split labeled data **randomly** into 80% training and 20% test.
- **Training set**: only for **training prediction functions**.
- **Test set**: only for **assessing performance**.
- Larger test set gives more accurate assessment of performance.
- How big? We can review “**confidence intervals**” from statistics.

Train/Test vs. Train/Deploy

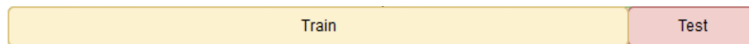
- Train/Test:
 - Build model on training data (say 80% of all labeled data).
 - Get performance estimate on test data (remaining 20%).
- Train/Deploy:
 - Build model on all labeled data.
 - Deploy model into wild.
 - Hope for the best.
- A large part of real-world machine learning is ensuring that
 - **Test performance is a good estimate of deployment performance.**
- How can we do this, and what can go wrong?

Main Principal of Train/Test Splitting

- **Train/Test setup should represent Train/Deploy scenario as closely as possible.**
- Random split of labeled data into train/test is usually the right approach.
 - (why random?)
- But consider **time series prediction**: 1000 days of historical data
 - Should we randomly split the days into training and test?

Train/Test Split for Time Series

- Consider **Train/Deploy** scenario:
 - Prediction function trained on days occurring before deployment time period.
- Consider **Train/Test** scenario with **random splitting**:
 - Some test days occur before some training days.
 - No good!
- Create train/test split by splitting in time:
 - Training set is everything before time T
 - Test set everything after time T



Jatin Garg (<https://stats.stackexchange.com/users/123886/jatin-garg>), Using k-fold cross-validation for time-series model selection, URL (version: 2017-03-22): <https://stats.stackexchange.com/q/268847>

Summary: What to Give your Data Science Intern

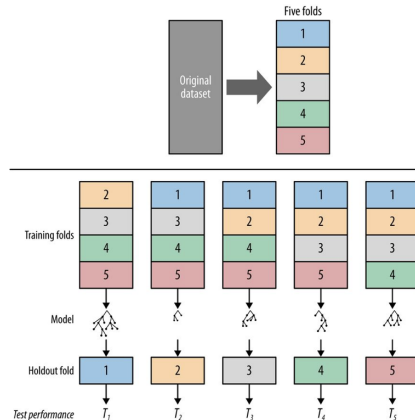
- Split data into **train** and **test**.
- Give training set to intern, you keep the test set.
- Intern gives you a prediction function.
- You evaluate prediction function on test set.
- No matter what intern did with training set,
 - test performance should give you a good estimate of deployment performance.

What Should the Intern Do?

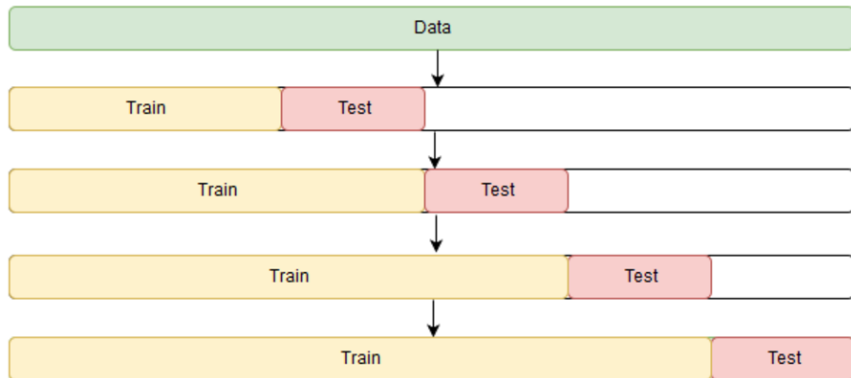
- Intern wants to try many fancy ML models.
- Each gives a different prediction function.
- Intern needs her own test set to evaluate prediction functions.
- Intern should randomly split data again into
 - **training set** and
 - **validation set**
- This split could again be 80/20.
- Validation set is like test set, but used to choose best among many prediction functions.
- Test set is just used to evaluate the final chosen prediction function.

k-Fold Cross Validation

- Suppose test set too small for good performance estimate.
- Use **k-fold cross validation**:
 - 1 Randomly partition data \mathcal{D} into k “folds” of equal size: $\mathcal{D}_1, \dots, \mathcal{D}_k$.
 - 2 For $i = 1, \dots, k$:
 - 1 Train model M_i on $\mathcal{D} - \mathcal{D}_i$.
 - 2 Let T_i be M_i 's performance on \mathcal{D}_i .
 - 3 Performance estimate is $\hat{T} = \text{Mean}(T_1, \dots, T_k)$.



Forward Chaining (Cross Validation for Time Series)



Jatin Garg (<https://stats.stackexchange.com/users/123886/jatin-garg>), Using k-fold cross-validation for time-series model selection, URL (version: 2017-03-22): <https://stats.stackexchange.com/q/268847>

- **loss functions**
 - e.g. **0/1 loss** (for classification)
 - e.g. **square loss** (for regression)
- **training set, validation set, test set**
 - train/test should resemble train/deploy as closely as possible
 - random split often reasonable
 - for time series, split data in time, rather than randomly
 - validation and test sets are often called “hold-out data”
- **k-fold cross validation** for small datasets

Other Sources of Test \neq Deployment

- **Leakage:** Information about labels sneaks into features.
- Examples:
 - identifying cat photos by using the title on the page
 - including sales commission as a feature when ranking sales leads
 - using star rating as feature when predicting sentiment of Yelp review

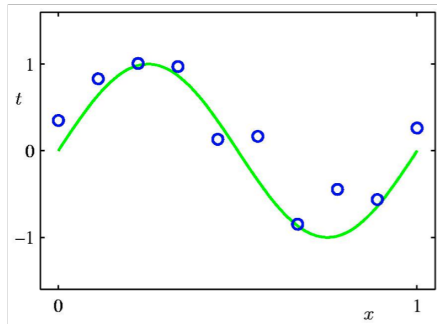
- **Sample bias:** Test inputs and deployment inputs have different distributions.
- Examples:
 - create a model to predict US voting patterns, but phone survey only dials landlines
 - building a stock forecasting model, but training using a random selection of companies that exist today – what's the issue?
 - US census slightly undercounts certain subpopulations in a way that's somewhat predictable based on demographic and geographic features.
 - If predictable, can it be corrected? Hotly debated topic ~2000 – some of the world's top statisticians couldn't agree (Stephen Fienberg vs David Freedman).)

- **Nonstationarity:** when the thing you're modeling changes over time
- Nonstationarity often takes one of two forms:
 - **Covariate shift:** input distribution changed between training and deployment.
 - (covariate is another term for input feature)
 - e.g. once popular search queries become less popular – new ones appear
 - mathematically similar to sample bias
 - **Concept drift:** correct output for given input changes over time
 - e.g. season changes, and given person no longer interested in winter coats
 - e.g. last week I was looking for a new car, this week I'm not

Model Complexity & Overfitting

Toy Example

- Green line is truth; Blue points are our noisy data



- What's the input? What's the output?

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Polynomial Curve Fitting (an ML algorithm)

- Fit data with a polynomial.

$$f(x) = w_0 + w_1x + w_2x^2 + \cdots + w_Mx^M$$

- **Concept Check:** What is $f(x)$ in our ML vocabulary?

Polynomial Curve Fitting (an ML algorithm)

- Fit with polynomial $f(x) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M$
- Imagine a learning function:

```
double[] fitPolynomial(Data data, int M)
```

- This function does the “**learning**”.
- Returns array of **parameters** w_0, w_1, \dots, w_M .
- With parameters and M we can create **prediction function**:

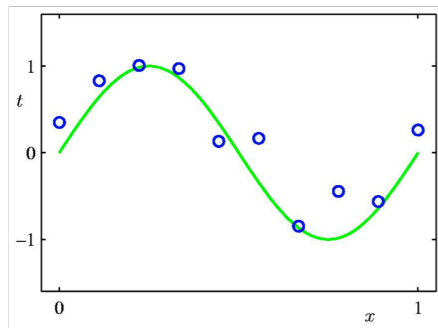
```
double predictPolynomial(double[] w, int M, double x)
```

Polynomial Curve Fitting (an ML algorithm)

- A polynomial model $f(x) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M$
- **Learning algorithms** find the best **parameters** w_0, w_1, \dots, w_M .
- A **hyperparameter** is a parameter of the ML algorithm itself.
 - Here, M is a hyperparameter.
- Generally, the data scientist adjusts the hyperparameters.
- Though it can also be chosen by an ML algorithm.

Example: Polynomial Curve Fitting

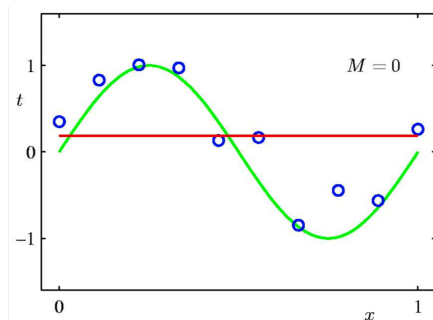
- Green curve is truth



From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Example: Polynomial Curve Fitting

- Fit with $M = 0$:

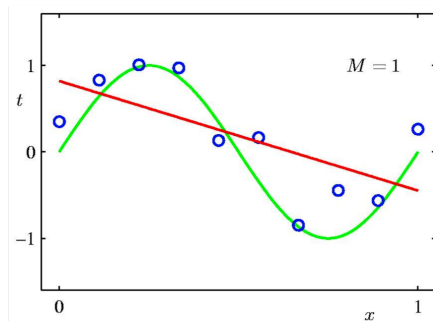


UNDERFIT (not fitting data well enough)

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Example: Polynomial Curve Fitting

- Fit with $M = 1$

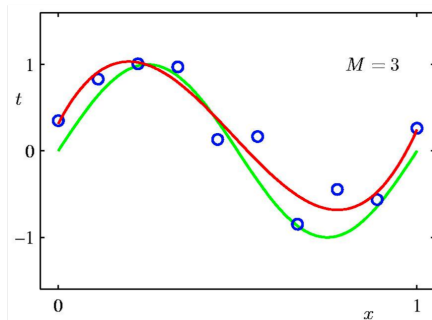


UNDERFIT (not fitting data well enough)

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Example: Polynomial Curve Fitting

- Fit with $M = 3$

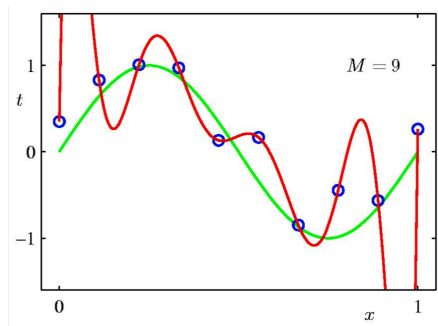


PRETTY GOOD!

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Example: Polynomial Curve Fitting

- Fit with $M = 9$



OVERFIT (fits data **too well**)

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

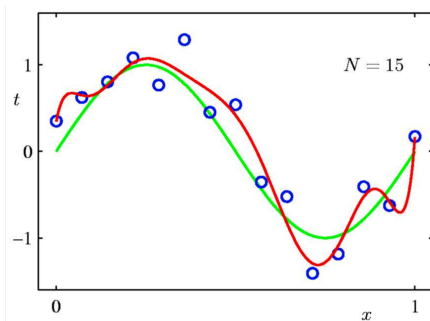
Polynomial Model Complexity

- M controls the **model complexity**.
- Bigger M allows more “complex” prediction functions.
 - i.e. more “squiggly” functions
- Larger model complexity means
 - Better fit to training data
 - NOT necessarily better performance on test data

- Loosely speaking, we say a model **overfits** when
 - training performance is good but
 - test/validation performance is poor.
- Fix overfitting by
 - Reducing model complexity
 - **Getting more training data**

Example: Polynomial Curve Fitting

- Fit with $M = 9$ (more data)

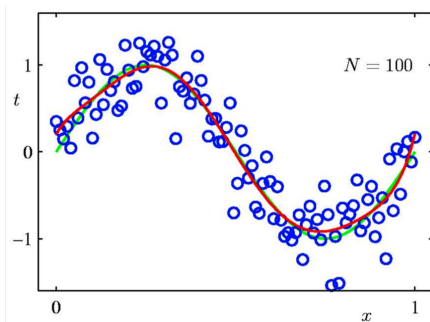


Pretty good - slightly overfit?

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Example: Polynomial Curve Fitting

- Fit with $M = 9$ (even more data)



NAILED IT?

From Bishop's *Pattern Recognition and Machine Learning*, Ch 1.

Hyperparameters (or “Tuning Parameters”)

- Almost every learning algorithm has
 - at least one “**hyperparameter**” or “**tuning parameter**”
- You (the data scientist) must tune these values.
- Hyperparameter control various things
 - **model complexity** (e.g. polynomial order)
 - **type of model complexity** control (e.g. L1 vs L2 regularization)
 - **optimization algorithm** (e.g. learning rate)
 - **model type** (e.g. loss function, kernel type,...)

Overall Machine Learning Workflow

Basic Machine Learning Workflow

- 1 Split labeled data into **training**, **validation**, and **test** sets.
- 2 Repeat until happy with performance on validation set:
 - 1 Build / revise your feature extraction methodology.
 - 2 Choose some ML algorithm.
 - 3 Train ML model with various hyperparameter settings.
 - 4 Evaluate prediction functions on validation set.
- 3 Retrain model on (train + validation)
- 4 Evaluate performance on test set. [Report this number to product manager.]
- 5 Retrain on all labeled data (training + validation + test).
- 6 Deploy resulting prediction function.

Case Study: Cell Phone Churn Prediction

The Cell Phone Churn Problem

- Cell phone customers often switch carriers. Called “churn”.
- Often cheaper to retain a customer than to acquire a new one.
- You can try to retain a customer by giving a promotion, such as a discount.
- If you give a discount to somebody who was going to churn, you probably saved money.
- If you give a discount to somebody who was NOT going to churn, you wasted money.

The Cell Phone Churn Problem

- Suppose you have 2 years of customer data.
- For each customer, you know whether they “churned” (i.e. changed service), and the date of churn if they did churn.
- How can we use machine learning to find the most likely churners?

Lift Curves for Predicting Churners

