Black Box Machine Learning

David S. Rosenberg

Bloomberg ML EDU

September 20, 2017

Overview

Outline

- 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?

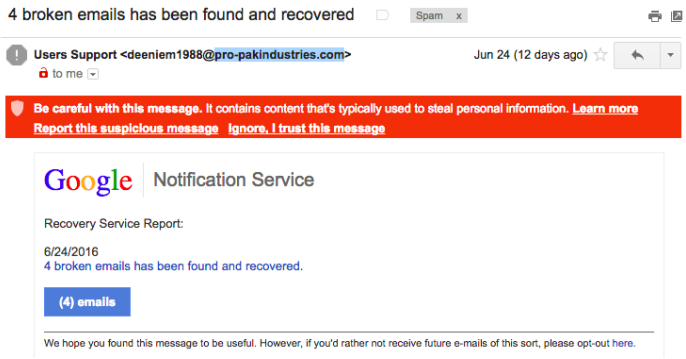
Common theme is to solve a prediction problem:

- 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**:

$$\begin{aligned} \mathbb{P}(\text{pneumonia}) &= 0.7 \\ \mathbb{P}(\text{flu}) &= 0.2 \\ \vdots &\quad \vdots \end{aligned}$$

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

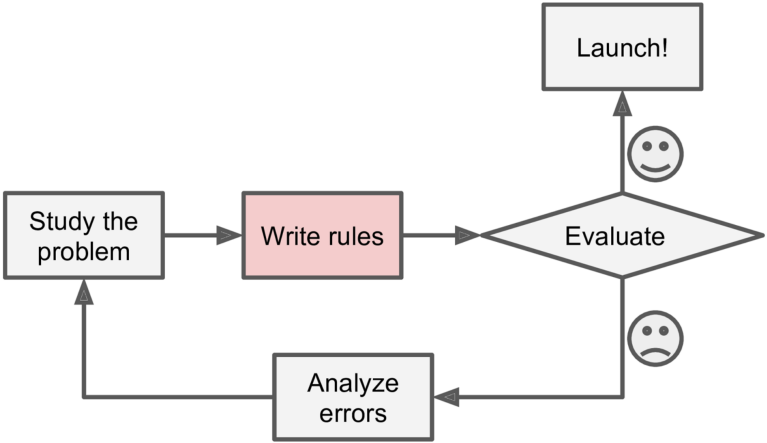


Fig 1-1 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

Rule-Based Systems

Issues with **rule-based systems**:

- Very labor intensive to build.
- Rules work very well for areas they cover
  - But cannot generalize to unanticipated input combinations.
- Don't naturally handle uncertainty.
- Expert systems seen as "brittle"

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

Modern AI: Machine Learning

- 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**.

Machine Learning Algorithm

- 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

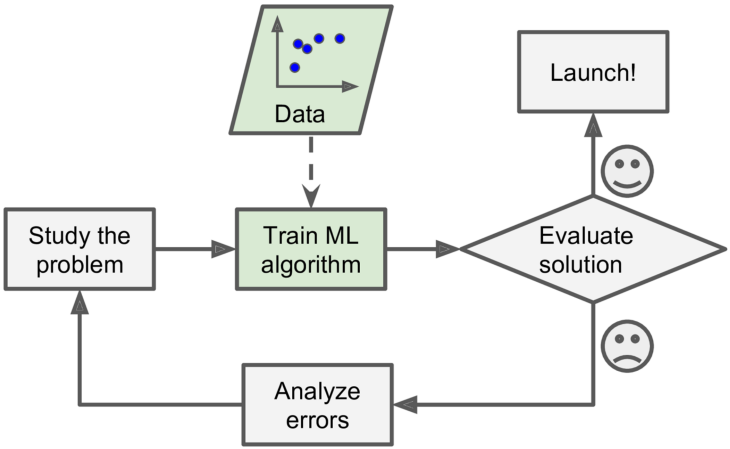


Fig 1-2 from *Hands-On Machine Learning with Scikit-Learn and TensorFlow* by Aurelien Geron (2017).

Key Concepts

- 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

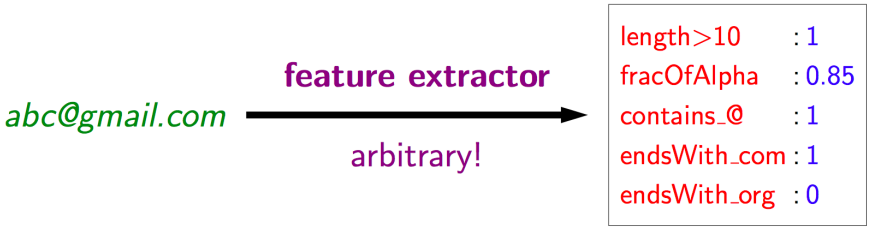
Definition

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

- 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:

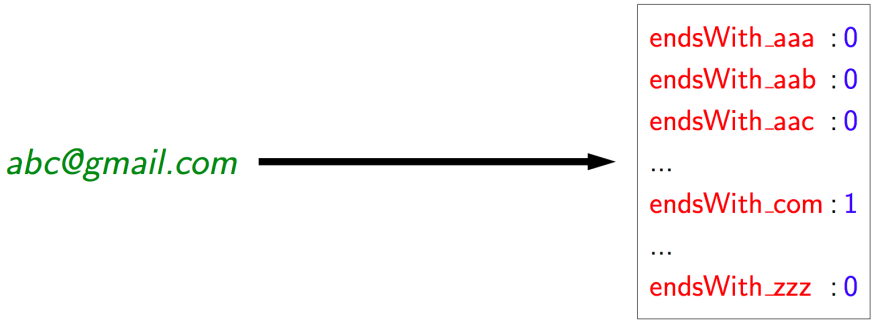


- This was a bit ad-hoc. Could we be more systematic? Yes ...

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Feature Template: Last Three Characters Equal ___

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



From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

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?

Labeled Data

- 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.

Unlabeled Data

- Just the feature vectors:

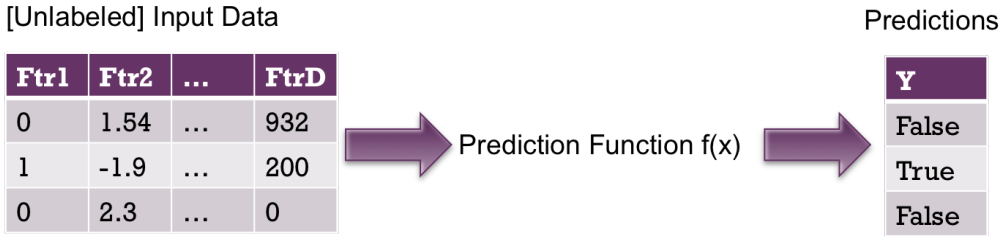
Ftr1	Ftr2	...	FtrD	Y
0	1.54	...	932	?
1	-1.9	...	200	?
0	2.3	...	0	?

- 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")

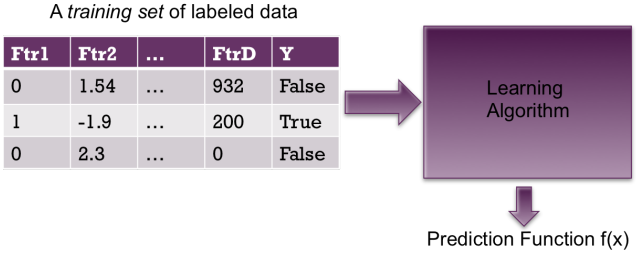


The prediction function is what gets **deployed**.

Learning Algorithm

A **learning algorithm** has

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



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

Key Concepts

- **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

Classic Loss Functions

- **Classification loss** or "**0/1 Loss**"
  - Loss is 1 if prediction is wrong.
  - Loss is 0 if prediction is correct.
- **Square loss** for regression
  - loss = (predicted - 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 $\leqslant 2\%$ 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 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!
- What can go wrong with random splitting of time series?
  - Suppose time series changes slowly over time.
  - To predict at test day d, just predict value at training day closest in time.
  - That trick won't work for very long during deployment.
- 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 good estimate of deployment performance.

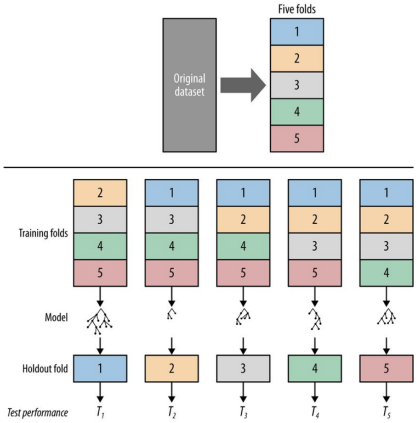
What Should the Intern Do?

- 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

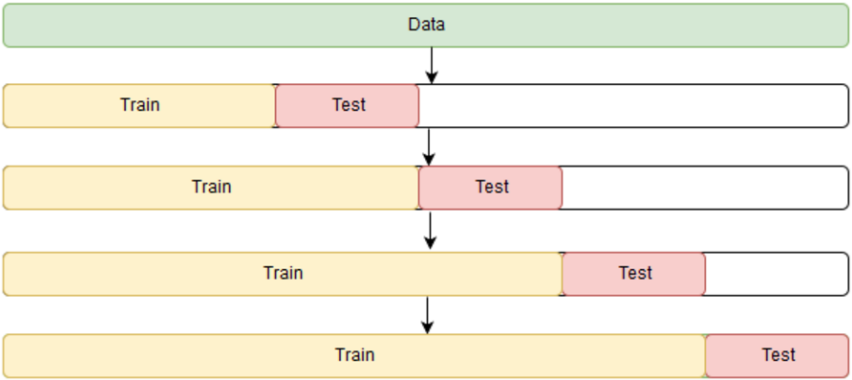
- Suppose test set too small for good performance estimate.
- Use k-**fold cross validation:**
  1. Randomly partition data $\mathcal{D}$ into k "folds" of equal size: $\mathcal{D}_1, \ldots, \mathcal{D}_k$.
  2. For $i = 1, \ldots, k$:
     1. Train model M_i on $\mathcal{D} - \mathcal{D}_i$.
     2.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

$$\begin{aligned} \hat{T} &= \text{Mean}(T_1, \ldots, T_k) \\ \text{SE}(\hat{T}) &= \text{SD}(T_1, \ldots, T_k)/\sqrt{k}. \end{aligned}$$



Provost and Fawcett *Data science for Business*, Figure 5-9.

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

Key Concepts

- **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

- **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

- **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).)

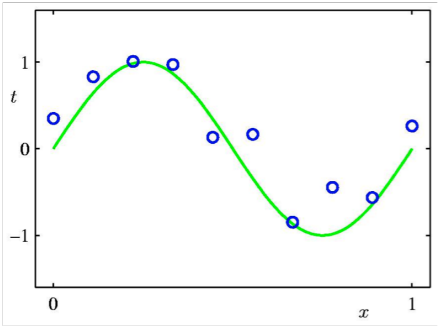
Nonstationarity

- **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.

$$f(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M$$

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

Polynomial Curve Fitting (an ML algorithm)

- Fit with polynomial $f(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M$
- Imagine a learning function:

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

- This function does the **"learning"**.
- Returns array of **parameters** $w_0, w_1, \ldots, w_M$.

- With parameters and M we can create **prediction function**:

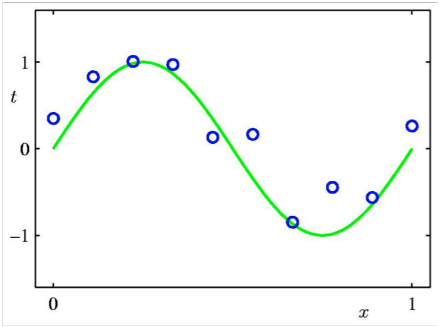
```
double predictPolynomial(double[] w, int M, double x)
```

Polynomial Curve Fitting (an ML algorithm)

- A polynomial model $f(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M$
- **Learning algorithms** find the best **parameters** $w_0, w_1, \ldots, w_M$.
- 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

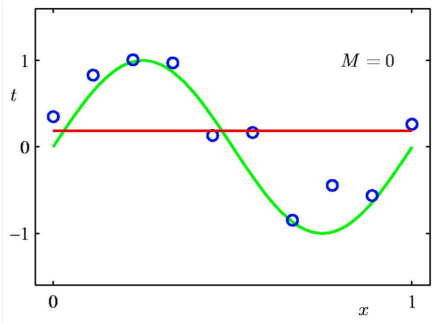
- Green curve is truth



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

Example: Polynomial Curve Fitting

- Fit with $M = 0$:

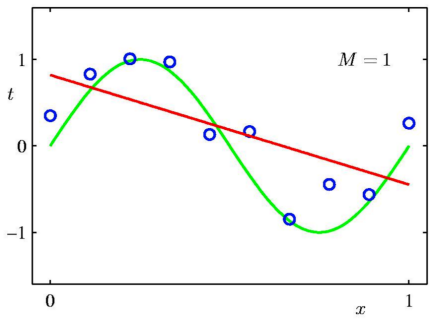


UNDERFIT (not fitting data well enough)

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

Example: Polynomial Curve Fitting

- Fit with $M = 1$

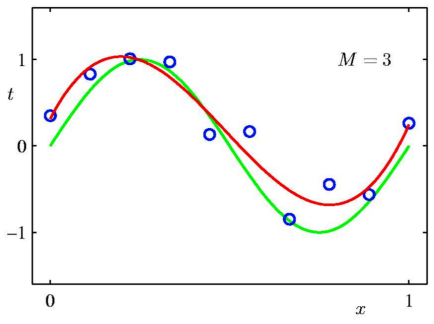


UNDERFIT (not fitting data well enough)

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

Example: Polynomial Curve Fitting

- Fit with $M = 3$

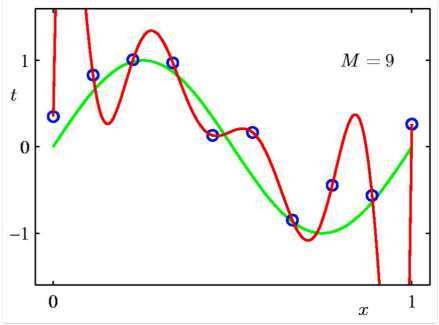


PRETTY GOOD!

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

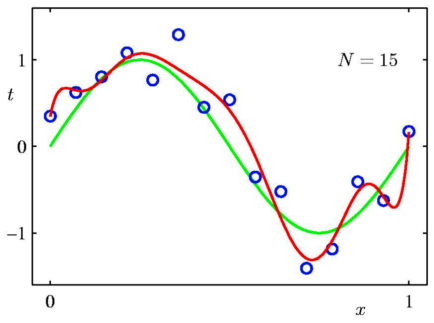
- M controls the **model complexity.**
- Bigger M allows more "complex" prediction functions.
  - i.e. more "squiggly" functions
- Larger model complexity means
  - Better fit to training data
  - NOT necessarily better performance on test data

Overfitting

- 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)

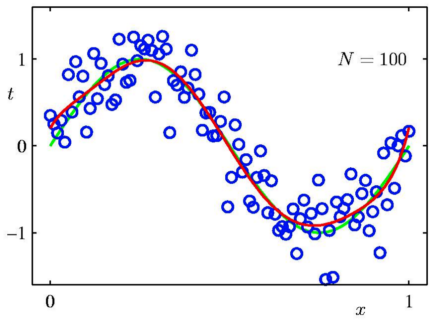


Pretty good - slightly overfit?

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