CS440/ECE448 Lecture 3: Decision Theory

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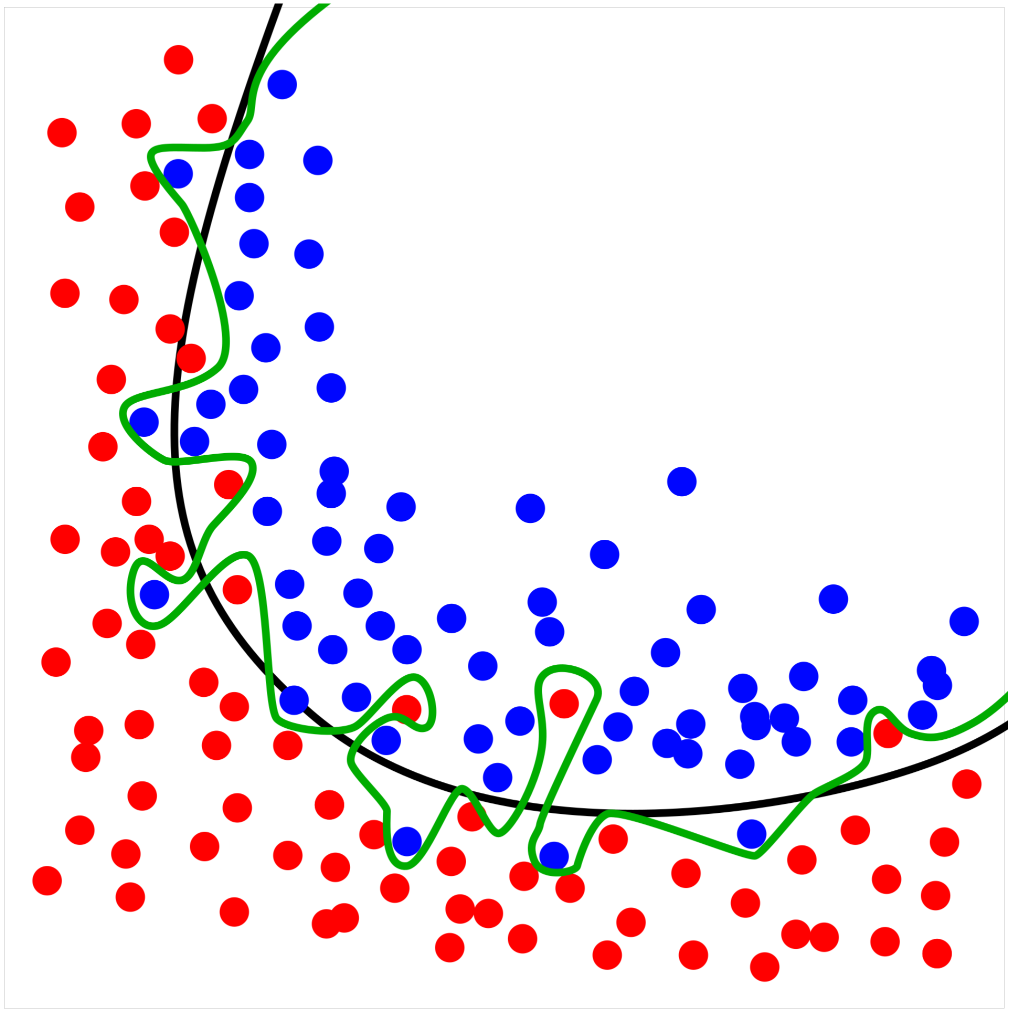

Diagram showing overfitting of a classifier. CC-BY 4.0, Ignacio Icke, 2008

Outline

- Decision Theory
- Minimum Probability of Error
- Bayes' Rule
- Accuracy, Error Rate, and the Bayes Error Rate
- Confusion Matrix, Precision & Recall
- Train, Dev, and Test Corpora
- Overfitting

Decision Theory

- Suppose we have an experiment with two random variables, X and Y.
  - X is something we can observe, like the words in an email.
  - Y is something we can't observe, but we want to know. For example, Y=1 means the email is spam (junk mail), Y=0 means it's ham (desirable mail).
- Can we train an AI to read the email, and determine whether it's spam or not?

Decision Theory

- Y $=$ the correct label
  - Y $=$ the correct label as a random variable (“in general”)
  - y $=$ the label observed in a particular experiment (“in particular”)
- $f(X)$ $=$ the decision that we make, after observing the datum, X
  - $f(X)$ $=$ the function applied to random variable X (“in general”)
  - $f(x)$ $=$ the function applied to a particular value of x (“in particular”)

Deciding how to Decide: Loss and Risk

- Suppose that deciding $f(x)$, when the correct label is $Y = y$, costs us a certain amount of money (or prestige, or safety, or points, or whatever) – call that the **loss**, $l(f(x), y)$
- In general, we would like to lose as few points as possible (negative losses are good…)
- Define the **risk**, $R(f)$, to be the expected loss incurred by using the decision rule $f(X)$:

$$R(f) = E[l(f(X), Y)] = \sum_y \sum_x l(f(x), y) P(X = x, Y = y)$$

Minimum-Risk Decisions

- If we want to the smallest average loss (the smallest risk), then our decision rule should be

$$f = \operatorname{argmin} R(f)$$

- In other words, for each possible x, we find the value of $f(x)$ that minimizes our expected loss given that x, and that is the $f(x)$ that our algorithm should produce.

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Zero-One Loss

Suppose that $f(x)$ is an estimate of the correct label, and

- We lose one point if $f(x) \neq y$
- We lose zero points if $f(x) = y$

$$l(f(x), y) = \begin{cases} 1 & f(x) \neq y \\ 0 & f(x) = y \end{cases}$$

Then the risk is

$$R(f) = E[l(f(X), Y)] = \Pr(f(X) \neq Y)$$

Minimum Probability of Error

We can minimize the probability of error by designing f(x) so that $f(x) = 1$ when $Y = 1$ is more probable, and $f(x) = 0$ when $Y = 0$ is more probable.

$$f(x) = \begin{cases} 1 & P(Y = 1|X = x) > P(Y = 0|X = x) \\ 0 & P(Y = 1|X = x) < P(Y = 0|X = x) \end{cases}$$

MPE = MAP

- The "minimum probability of error" (MPE) decision rule is the rule that chooses f(X) in order to minimize the probability of error:
$$f(x) = \operatorname{argmin} P(\text{Error}|X = x)$$

- The "maximum *a posteriori*" (MAP) decision rule is the rule that chooses $f(X)$ in order to maximize the *a posteriori* probability:
$$f(x) = \operatorname{argmax} P(Y = f(x)|X = x)$$

- Those two decision rules are the same. MPE = MAP.

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The Bayesian Scenario

- Let's use $x \sim X$ to mean that x is an instance of random variable X, and similarly $y \sim Y$.
- In order to minimize the probability of error, we just need to know $P(Y = y | X = x)$ for every pair of values $x \sim X$ and $y \sim Y$. Then we choose $f(x) = \operatorname*{argmax}_{y} P(Y = y | X = x)$.

Example: spam detection

- But how can we estimate $P(Y = y|X = x)$?
- The prior probability of spam might be obvious. If 80% of all email on the internet is spam, that means that

$$P(Y = 1) = 0.8, P(Y = 0) = 0.2$$

- The probability of X given Y is also easy. Suppose we have a database full of sample emails, some known to be spam, some known to be ham. We count how often any word occurs in spam vs. ham emails, and estimate:

$$P(X = x|Y = 1) = \text{frequency of the words } x \text{ in emails known to be spam}$$
$$P(X = x|Y = 0) = \text{frequency of the words } x \text{ in emails known to be ham}$$

- Now we have $P(X = x|Y = y)$ and $P(Y = y)$. How do we get $P(Y = y|X = x)$?

Bayes' Rule

Rev. Thomas Bayes (1702-1761)

By Unknown - [2][3], Public Domain, https://commons.wikimedia.org/w/index.php?curid=14532025

The reverend Thomas Bayes solved this problem for us in 1763. His proof is really just the definition of conditional probability, applied twice in a row:

$$P(Y = y|X = x) = \frac{P(X = x, Y = y)}{P(X = x)}$$

$$= \frac{P(X = x|Y = y)P(Y = y)}{P(X = x)}$$

The four Bayesian probabilities

$$P(Y = y|X = x) = \frac{P(Y = y)P(X = x|Y = y)}{P(X = x)}$$

This equation shows the relationship among four probabilities. This equation has become so world-famous, since 1763, that these four probabilities have standard universally recognized names that you need to know:

- $P(Y = y|X = x)$ is the ***a posteriori*** (after-the-fact) probability, or **posterior**
- $P(Y = y)$ is the ***a priori*** (before-the-fact) probability, or **prior**
- $P(X = x|Y = y)$ is the **likelihood**
- $P(X = x)$ is the **evidence**

Bayes' rule: the posterior equals the prior times the likelihood over the evidence.

MPE = MAP using Bayes' rule

- MPE = MAP: to minimize the probability of error, design f(X) so that
$$f(x) = \underset{y}{\operatorname{argmax}}\, P(Y = y|X = x)$$
- Bayes' rule:
$$P(Y = y|X = x) = \frac{P(Y = y)P(X = x|Y = y)}{P(X = x)}$$
- Putting the two together:
$$f(x) = \underset{y}{\operatorname{argmax}} \frac{P(Y = y)P(X = x|Y = y)}{P(X = x)}$$
$$= \underset{y}{\operatorname{argmax}}\, P(Y = y)P(X = x|Y = y)$$

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Accuracy

When we train a classifier, the metric that we usually report is “accuracy.”

$$\text{Accuracy} = \frac{\text{\# tokens correctly classified}}{\text{\# tokens total}}$$

Error Rate

Equivalently, we could report error rate, which is just 1-accuracy:

$$\text{Error Rate} = \frac{\text{\# tokens incorrectly classified}}{\text{\# tokens total}}$$

Bayes Error Rate

The "Bayes Error Rate" is the smallest possible error rate of any classifier with labels y and features x:

$$\text{Error Rate} = \sum_{x} P(X = x) \min_{y} P(Y \neq y | X = x)$$

It's called the "Bayes error rate" because it's the error rate of the Bayesian classifier.

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The problem with accuracy

- In most real-world problems, there is one class label that is much more frequent than all others.
  - Words: most words are nouns
  - Animals: most animals are insects
  - Disease: most people are healthy
- It is therefore easy to get a very high accuracy. All you need to do is write a program that completely ignores its input, and always guesses the majority class. The accuracy of this classifier is called the “chance accuracy.”
- It is sometimes very hard to beat the chance accuracy. If chance=90%, and your classifier gets 89% accuracy, is that good, or bad?

The solution: Confusion Matrix

<u>Confusion Matrix</u> =

- $(m, n)^{\text{th}}$ element is
- the number of tokens of the m^{th} class
- that were labeled, by the classifier, as belonging to the n^{th} class.

```
title: Consonant Confusions in CV utterances, for V=/a/, for S/N = +12db and
Phones involved: 16, namely p t k f T (th) s S (sh) b d g v D (dh) z Z (zh) m
```

	p	t	k	f	T	s	S	b	d	g	v	D	z	Z	m	n		Total
p	228	7	7	1	0	0	1	0	0	0	0	0	0	0	0	0	p	244
t	0	236	8	0	0	0	0	0	0	0	0	0	0	0	0	0	t	244
k	26	5	213	0	0	0	0	0	0	0	0	0	0	0	0	0	k	244
f	6	1	1	194	35	0	0	3	0	0	1	3	0	0	0	0	f	244
T	0	2	2	96	146	2	0	2	1	0	1	8	0	0	0	0	T	260
s	0	2	0	1	31	204	1	1	9	4	0	7	0	0	0	0	s	260
S	0	0	0	0	0	1	243	0	0	0	0	0	0	0	0	0	S	244
b	0	0	0	13	12	0	0	207	2	3	19	8	0	0	0	0	b	264
d	0	0	0	0	0	0	0	0	240	9	0	0	0	3	0	0	d	252
g	0	0	0	0	0	0	0	1	41	199	0	0	2	1	0	0	g	244
v	0	0	0	3	3	0	0	20	0	2	182	47	2	0	0	1	v	260
D	0	0	0	0	7	0	0	10	3	22	49	170	19	0	0	0	D	280
z	0	0	0	0	1	0	0	3	8	24	2	22	145	3	0	0	z	208
Z	0	0	0	0	0	0	1	0	2	0	0	0	13	264	0	0	Z	280
m	0	0	0	0	0	0	0	0	0	0	0	0	0	0	213	11	m	224
n	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	248	n	248

Plaintext versions of the Miller & Nicely matrices, posted by Dinoj Surendran, http://people.cs.uchicago.edu/~dinoj/research/nicely.html

Confusion matrix for a binary classifier

Suppose that the correct label is either 0 or 1. Then the confusion matrix is just 2x2.

Classified As:

Correct Label:

	0	1
0		
1		

For example, in this box, you would write the # tokens of class 1 that were misclassified as class 0

False Positives & False Negatives

- TP (True Positives) = tokens that were correctly labeled as “1”
- FN (False Negatives) = tokens that should have been “1”, but were mislabeled as “0”
- FP (False Positives) = tokens that should have been “0”, but were mislabeled as “1”
- TN (True Negative) = tokens that were correctly labeled as “0”

Classified As:

Correct Label:

	0	1
0	**TN**	**FP**
1	**FN**	**TP**

Summaries of a Binary Confusion Matrix

The binary confusion matrix is standard in many fields, but different fields summarize its content in different ways.

- In medicine, it is summarized using Sensitivity and Specificity.
- In information retrieval (IR) and AI, we usually summarize it using Recall and Precision.

Classified As:

Correct Label:

	0	1
0	TN	FP
1	FN	TP

Specificity and Sensitivity

Specificity = True Negative Rate (TNR):

$$TNR = P(f(X) = 0 | Y = 0) = \frac{TN}{TN + FP}$$

Classified As:

Correct Label:

	0	1
0	**TN**	**FP**
1	**FN**	**TP**

Sensitivity = True Positive Rate (TPR):

$$TPR = P(f(X) = 1 | Y = 1) = \frac{TP}{TP + FN}$$

How IR and AI summarize confusions

Precision:

$$P = P(Y = 1 | f(X) = 1) = \frac{TP}{TP + FP}$$

Recall = Sensitivity = TPR:

$$R = P(f(X) = 1 | Y = 1) = \frac{TP}{TP + FN}$$

Classified As:

Correct Label:	0	1
0	TN	FP
1	FN	TP

The Misdiagnosis Problem: Example

1% of women at age forty who participate in routine screening have breast cancer. The test has sensitivity of 80%, and selectivity of 90.4%.

$$P(f(X)=0, Y=0) = P(f(X)=0|Y=0)P(Y=0)$$
$$= (0.904)(0.99) \approx 0.895$$

$$P(f(X)=1, Y=0) = P(f(X)=1|Y=0)P(Y=0)$$
$$= (0.096)(0.99) \approx 0.095$$

$$P(f(X)=0, Y=1) = P(f(X)=0|Y=1)P(Y=1)$$
$$= (0.2)(0.01) = 0.002$$

$$P(f(X)=1, Y=1) = P(f(X)=1|Y=1)P(Y=1)$$
$$= (0.8)(0.01) = 0.008$$

Classified As:

Correct Label:

	0	1
0	**0.895**	**0.095**
1	**0.002**	**0.008**

The Misdiagnosis Problem

1% of women at age forty who participate in routine screening have breast cancer. 80% of women with breast cancer will get positive mammographies. 9.6% of women without breast cancer will also get positive mammographies.

A woman in this age group had a positive mammography in a routine screening. What is the probability that she actually has breast cancer?

$$P(\text{Cancer} = T|\text{Test} = T) = \frac{P(\text{Test} = T|\text{Cancer} = T)P(\text{Cancer} = T)}{P(\text{Test} = T)}$$

$$= \frac{P(\text{Test} = T|\text{Cancer} = T)P(\text{Cancer} = T)}{P(\text{Test} = T|\text{Cancer} = T)P(\text{Cancer} = T) + P(\text{Test} = T|\text{Cancer} = F)P(\text{Cancer} = F)}$$

$$= \frac{(0.8)(0.01)}{(0.8)(0.01) + (0.096)(0.99)} = 0.0776$$

Recall:

$R = P(f(X) = 1|Y = 1)$

$= 0.8$

Precision:

$P = P(Y = 1|f(X) = 1)$

$= 0.0776$

Quiz

- You are worried that you might be a zombie, so you ask your doctor to test you. The test comes back positive. The zombie virus is still quite rare in the United States: the *a priori* probability that you are a zombie is only 1/8. The sensitivity of the test is 4/5. The specificity of the test is also 4/5. Given that your test came back positive, what is the probability that you are, nevertheless, not a zombie? In other words, what is the probability of a misdiagnosis?
- $P(Y=0,f(X)=0) = P(Y=0)P(f=0|Y=0) = (7/8) * (4/5) = 28/40$
- $P(Y=0, f(X)=1) = P(Y=0)P(f=1|Y=0) = (7/8) * (1/5) = 7/40$
- $P(Y=1, f(X)=0) = P(Y=1)P(f=0|Y=1) = (1/8) * (1/5) = 1/40$
- $P(Y=1, f(X)=1) = P(Y=1)P(f=1|Y=1) = (1/8) * (4/5) = 4/40$
- $P(Y=0 \mid f(X)=1) = P(Y=0, f(X)=1) / P(f(X)=1)$

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Accuracy on which corpus?

Consider the following experiment: among all of your friends' pets, there are 4 dogs and 4 cats.

1. Measure several attributes of each animal: weight, height, color, number of letters in its name…
2. You discover that, among your friends' pets, all dogs have 1-syllable names, while the names of all cats have 2+ syllables.
3. Your classifier: an animal is a cat if its name has 2+ syllables.
4. Your accuracy: 100%

Is it correct to say that this classifier has 100%? Is it useful to say so?

Training vs. Test Corpora

Training Corpus = a set of data that you use in order to optimize the parameters of your classifier (for example, optimize which features you measure, how you use those features to make decisions, and so on).

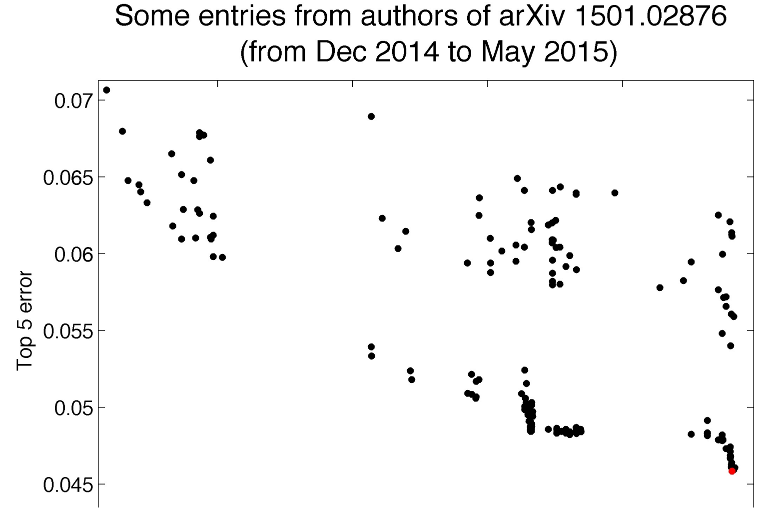
Test Corpus = a set of data that is non-overlapping with the training set (none of the test tokens are also in the training dataset) that you can use to measure the accuracy.

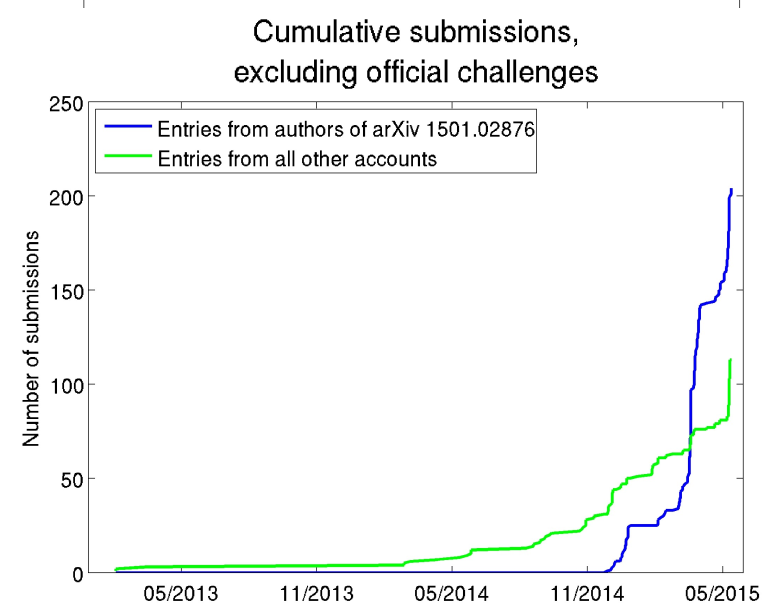
- Measuring the training corpus accuracy is useful for debugging: if your training algorithm is working, then training corpus accuracy should always go up.
- Measuring the test corpus accuracy is the only way to estimate how your classifier will work on new data (data that you’ve never yet seen).

Accuracy on which corpus?

This happened:

- Large Scale Visual Recognition Challenge 2015: Each competing institution was allowed to test up to 2 different fully-trained classifiers per week.
- One institution used 30 different e-mail addresses so that they could test a lot more classifiers (200, total). One of their systems achieved <46% error rate – the competition's best, at that time.
- Is it correct to say that that institution's algorithm was the best?





Training vs. development test vs. evaluation test corpora

Training Corpus = a set of data that you use in order to optimize the parameters of your classifier (for example, optimize which features you measure, what are the weights of those features, what are the thresholds, and so on).

Development Test (DevTest or Validation) Corpus = a dataset, separate from the training dataset, on which you test 200 different fully-trained classifiers (trained, e.g., using different training algorithms, or different features) to find the best.

Evaluation Test Corpus = a dataset that is used only to test the ONE classifier that does best on DevTest. From this corpus, you learn how well your classifier will perform in the real world.

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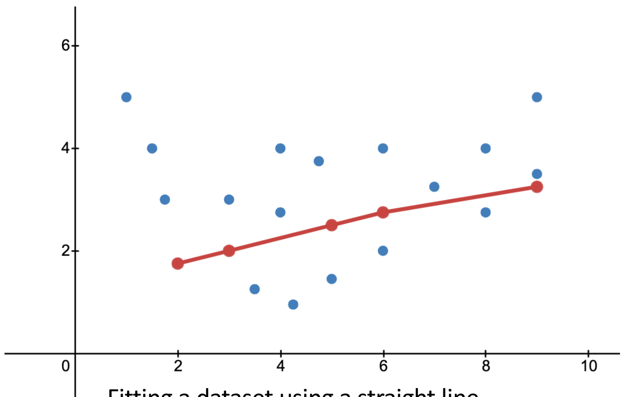
Overfitting

- Underfitting = your model has too few parameters. It is not able to get good accuracy on the training data.
- Overfitting = your model has too many parameters. It gets great accuracy on the training data, but very poor accuracy on the dev data.
- Overfitting is good! It proves that your code works.
- …but now that you've proven that your code works, now you need to do something to solve the overfitting.

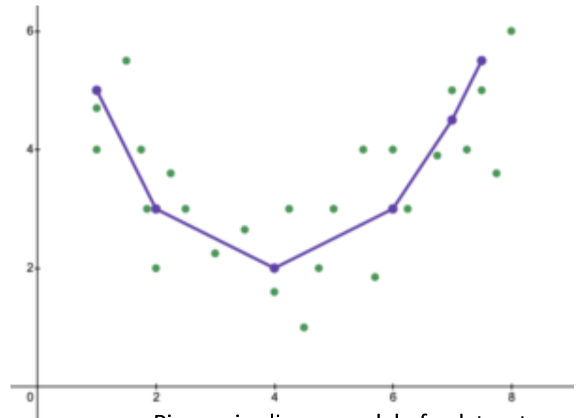
Example (from Wikipedia): curve fitting

- Suppose you have some examples of (x,y) training data points, where X and Y are both scalars.
- You want to try to find a polynomial, f(x) that
    1. Fits the training data points pretty well
    2. You think it is likely to also fit a test corpus pretty well

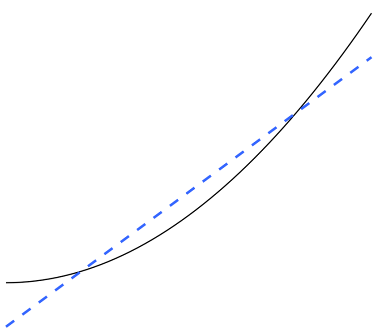
Which of these models of the data is best?



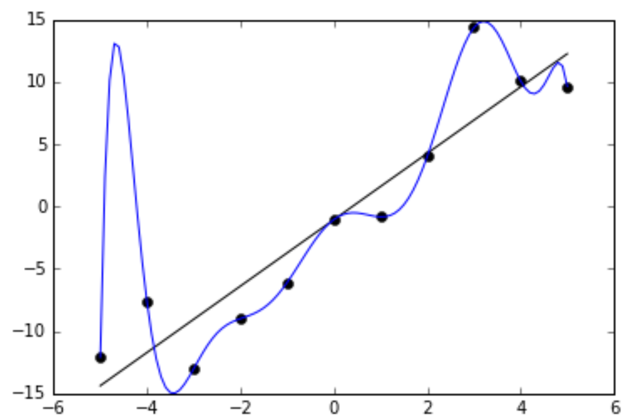
Fitting a dataset using a straight line.
Figure by AAStein, CC-BY-4.0, 2021



Piece-wise linear model of a dataset
Figure by AAStein, CC-BY-4.0, 2021



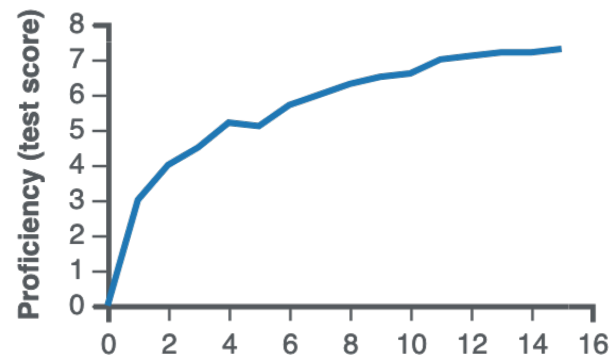
Fitting a dataset with a parabola.
Figure by Dfrankow, CC-BY-4.0, 2019



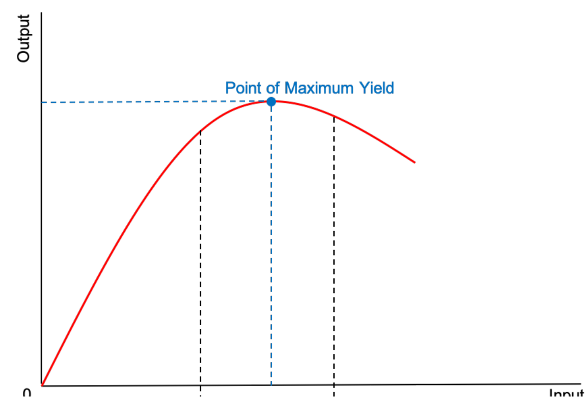
Fitting 11 data points using a 12th-order polynomial.
Figure by Ghiles, CC-BY-4.0, 2016

How to avoid both underfitting and overfitting

- Start with a model that has few trainable parameters
  - Train it on the training set.
  - Test it on the dev set.
  - Make sure you have similar accuracy on both the training set and dev set.
- Increase the number of trainable parameters in your model
  - Train on training data. As # parameters increases, accuracy on training set will always increase.
  - Test on dev data. As # parameters increases, accuracy on dev data will increase until it reaches a maximum, then start falling.
  - Best model = model that achieved lowest error rate on the dev set.



Accuracy on **training** data vs. # params.
https://en.wikipedia.org/wiki/Learning_curve, 2021



Accuracy on **dev** data vs. # params.
Happyavocado, CC-BY-4.0, 2021

Summary

- Bayes Error Rate:

$$\text{Bayes Error Rate} = \sum_x P(X = x) \min_y P(Y \neq y | X = x)$$

- Confusion Matrix, Precision & Recall

$$\text{Precision} = \frac{TP}{TP + FP}, \text{Recall} = \frac{TP}{TP + FN}$$

- Train, Dev, and Test Corpora
- Overfitting: increase # parameters in your model until you get the best accuracy on the dev data.