Lecture 8: Linear Classifiers and Model Validation

INFO 1998: Introduction to Machine Learning

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Agenda

1. Linear Classifiers
2. Validation: Classification vs Regression
3. Review: Bias-Variance trade-off
4. More Cross-Validation techniques
5. Train-Test Size

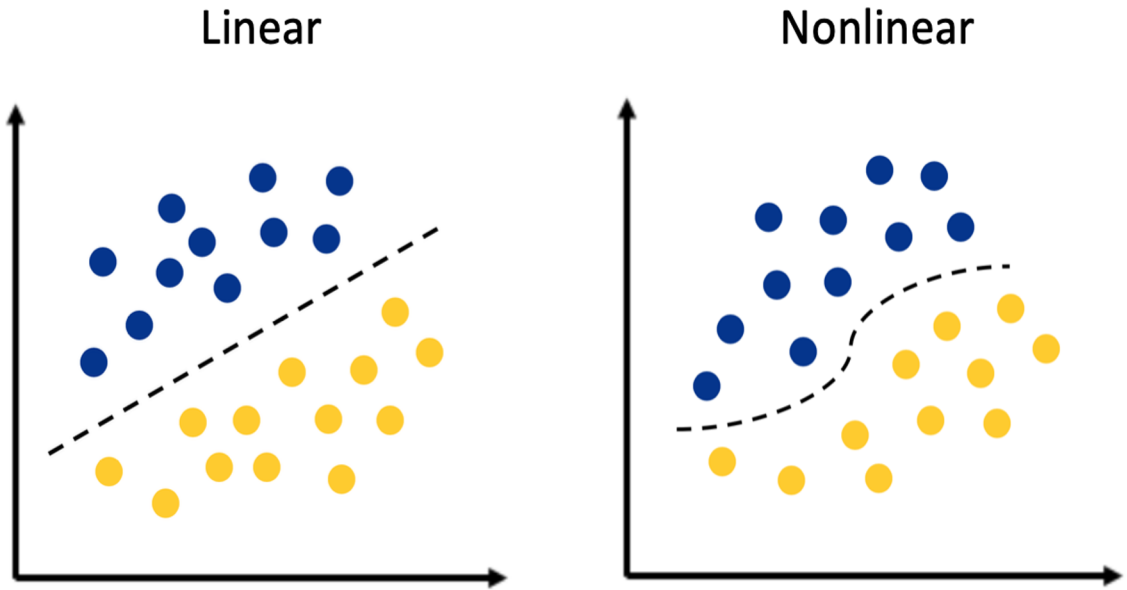
Linear Classifiers

Source

Linear Classifiers

A linear classifier is a hyper plane that is used to classify our data points

A hyperplane is our **decision boundary** and our goal is to find the hyper plane that best classifies our data

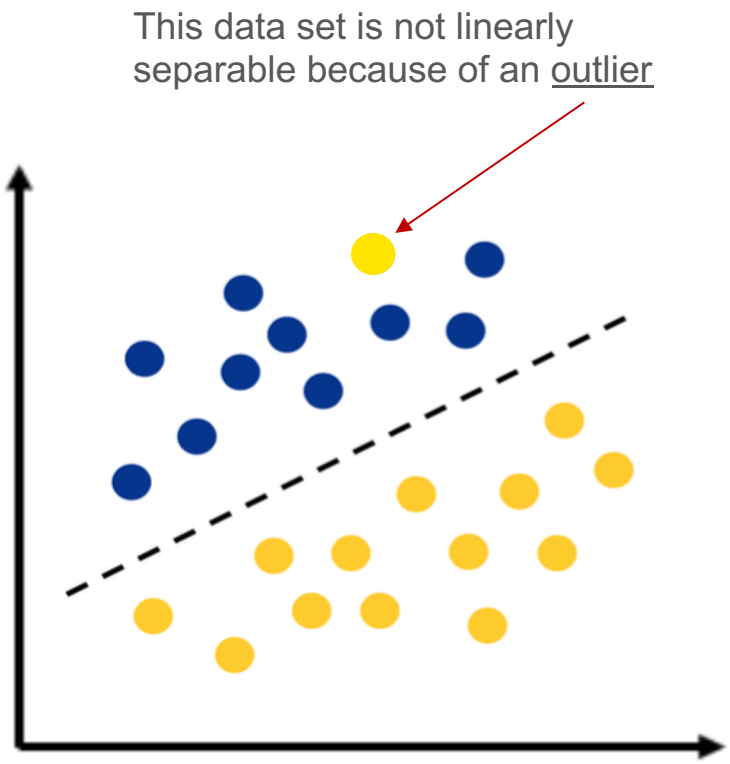


Source

Linearly Separable

In this example, we cannot partition our dataset into yellow and purple with a linear decision boundary. This means that our data is not **linearly separable.**

Outliers are frequently the reason a data set is not linearly separable.



Perceptron Learning Algorithm

Goal: find a normal vector w that perfectly classifies all the points in our data set
Algorithm:

Initialize classifier as some random hyperplane
While there exists a misclassified point x:
    Tilt classifier slightly so that it classifies x correctly
    (or, is a little closer to classifying x correctly)
End While

“Use your mistakes as your stepping stones”

Demo

Limitations of Perceptron

The training algorithm will never terminate if your training dataset is not linearly separable ☹

Is a great model to understand the intuition behind the training of a linear classifier: iteratively improve classifier by using misclassified points ☺

Review: Regression vs. Classification

Regression

- Predict Continuous Data
- “On average, **how wrong** are we?”

Classification

- Predict Discrete or Categorical data
- “**How many** points do we get wrong?”

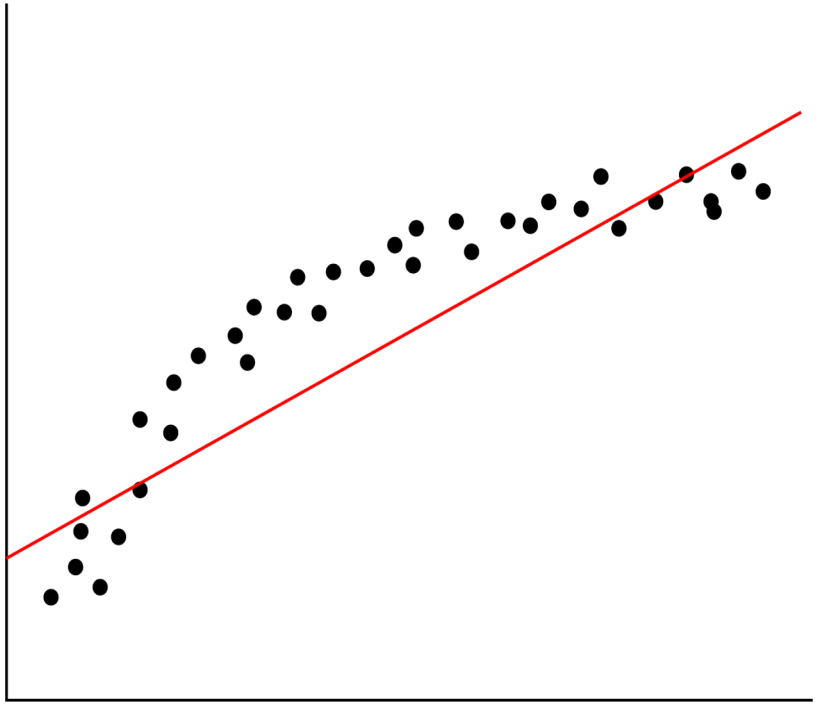
Numbers ≠ Continuous

Recap: Underfitting, Overfitting, Bias-Variance Tradeoff

Underfitting

Underfitting means we have high bias and low variance.

- Lack of relevant variables/factor
- Imposing limiting assumptions
  - Linearity
  - Assumptions on distribution
  - Wrong values for parameters

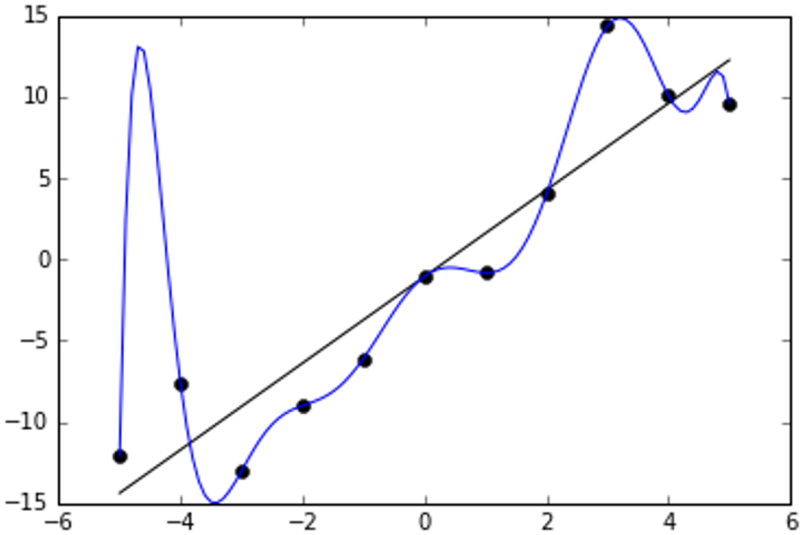


Source

Overfitting

Overfitting means we have low bias and high variance.

- Model fits too well to specific cases
- Model is over-sensitive to sample-specific noise
- Model introduces too many variables/complexities than needed



Source

Bias-Variance Tradeoff

When evaluating the models we are using, one property that we would often refer to is the bias-variance tradeoff.

Bias-variance tradeoff is the property of a set of predictive models where:

- Models with higher flexibility would typically have lower bias and higher variance;
- Models with lower flexibility would typically have higher bias and lower variance.

The graph gives a visualization on the outcomes of different bias and variance if we are doing experiment of throwing darts.

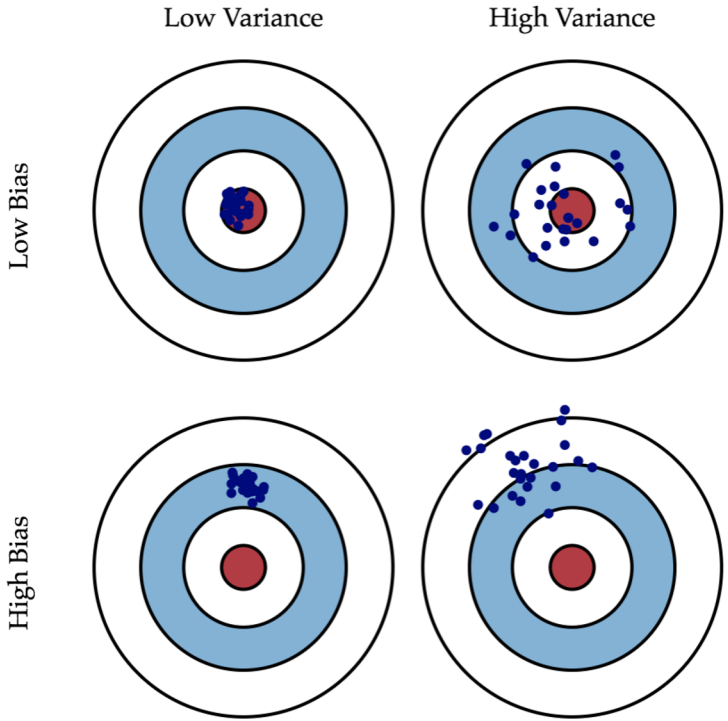


Fig. 1 Graphical illustration of bias and variance.

Graph source: http://scott.fortmann-roe.com/docs/BiasVariance.html

Bias-Variance Tradeoff

Say:

- θ is an unknown quantity we want to estimate
- $\hat{\theta}$ is an estimator of θ (computed from data, random)

The mean squared error (MSE) decomposes as:

$$\underbrace{\mathbb{E}(\hat{\theta} - \theta)^2}_{\text{MSE}} = \underbrace{\left(\mathbb{E}\hat{\theta} - \theta\right)^2}_{\text{bias}^2} + \underbrace{\text{Var}(\hat{\theta})}_{\text{variance}}$$

$$\text{MSE} = \text{bias}^2 + \text{variance}$$

Bias-Variance Tradeoff

In regression:

Want to predict y for a fixed test data point x

y is generated from the true model $y = f(x) + \epsilon$
(ϵ has zero mean and independent of everything else)

Estimate using some model $\hat{f}$: $\hat{y} = \hat{f}(x)$

Then:

$$\text{test error} = \mathbb{E}(\hat{f}(x) - y)^2 = \underbrace{\left(\mathbb{E}\hat{f}(x) - f(x)\right)^2}_{\text{bias}^2} + \underbrace{\text{Var}(\hat{f}(x))}_{\text{variance}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

Proof (not required, only for reference)

Suppose we have test set data: ***y = f(x) + ε***. The test data *y* is random, since ***ε*** is random. The estimator ***f hat*** is also random, because it is fitted on random training data.
Then from the previous slide “MSE = bias^2 + variance” for unknown quantity ***θ*** and its random estimator ***θ*** hat, we have:

$$
\begin{aligned}
&\mathbb{E}(\hat{f}(x) - y)^2 \\
=&\mathbb{E}\Big[\mathbb{E}\big[(\hat{f}(x) - y)^2 \big| y\big]\Big] \\
=&\mathbb{E}\Big[\big(\mathbb{E}\hat{f}(x) - y\big)^2 + \mathrm{Var}(\hat{f}(x))\Big] \\
=&\mathbb{E}\big(\mathbb{E}\hat{f}(x) - f(x) - \epsilon\big)^2 + \mathrm{Var}(\hat{f}(x)) \\
=&\mathbb{E}\big(\mathbb{E}\hat{f}(x) - f(x)\big)^2 + 2\mathbb{E}\Big[\big(\mathbb{E}\hat{f}(x) - f(x)\big)\epsilon\Big] + \mathbb{E}\epsilon^2 + \mathrm{Var}(\hat{f}(x))
\end{aligned}
$$

(For some part of this lecture material, credit goes to Professor Damek Davis, Cornell ORIE department.)

Bias-Variance Tradeoff

$$\underbrace{\mathbb{E}(\hat{f}(x) - y)^2}_{\text{test error}} = \underbrace{\left(\mathbb{E}\hat{f}(x) - f(x)\right)^2}_{\text{bias}^2} + \underbrace{\text{Var}(\hat{f}(x))}_{\text{variance}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

- Less flexible model:

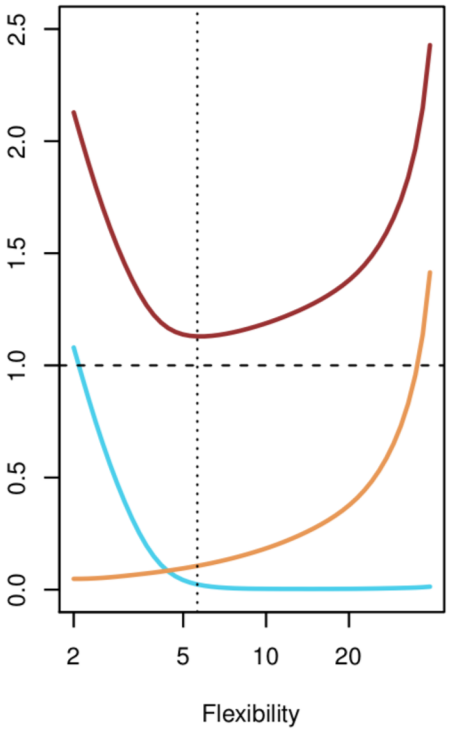
$$\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}_1 x$$

bias high, variance low

- More flexible model:

$$\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}_1 x + \hat{\beta}_2 x^2 + \hat{\beta}_3 x^3$$

bias low, variance high



More Validation Techniques

Leave-P-out

Let **D** be our whole dataset

Choose a **P**

For every combination of **P** points in **D**:

Use a train/test split with those **P** points as test, the rest as train

Leave-P-out: different from K-fold!

Let's say **D** has a size of 4. There are four data points: *a*, *b*, *c*, and *d*.

K-fold:

- K = 2.
- Each fold has a size of 2: {*a*,*b*} and {*c*,*d*}
- So, we only have 2 possible test sets:

  {*a*,*b*} and {*c*,*d*}

Leave-P-out:

- P = 2.
- We have 6 possible test sets:

  {*a*,*b*}, {*a*,*c*}, {*a*,*d*}, {*b*,*c*}, {*b*,*d*}, and {*c*,*d*}

Leave-P-out

Pros:

- Dependable (not random)
- Representative — checks all combinations

Cons:

- Slow!
  - Runtime increases with larger datasets
  - Runtime explodes with larger P

Monte Carlo CV

- Getting accuracy **1** time doesn't tell us much
- Getting accuracy **2** times tells us a bit
- Getting accuracy **3** times tells us a bit more
- ...
- Getting accuracy **N** times might be good enough!

Take the average of those **N** times

Monte Carlo CV

- Need to use **new**, **random** train/test split each time
  - If you use the same train/test split each time, you're not getting any new information!
- Pros:
  - easy to implement
  - easy to make faster/slower by changing number of iterations
- Cons:
  - random -> train/test splits not guaranteed to be representative of dataset
  - harder to calculate how many iterations you need

The Bootstrap

What if we don’t have enough data?

- Use **bootstrap datasets** to approximate the test error
- **Sample with replacement** from the original training dataset (with n samples) to generate **bootstrap datasets** of size n
  - Some data points may appear more than once in the generated data
  - Some data points may not appear
- Estimate of test error = average error among bootstrap datasets

Pipeline of the Bootstrap

Algorithm 1 Estimating prediction error via the bootstrap

1: **Input**: dataset $\{(x_i, y_i)\}_{i=1}^n$, loss function ℓ.
2: **for** $b = 1, 2, \ldots, B$ **do**
3: generate set $\mathcal{S}_b$ by sampling n items with replacement from $\{(x_i, y_i)\}_{i=1}^n$.
4: form prediction $\hat{f}^b$ by fitting the logistic regression model with training data $\mathcal{S}_b$.
5: compute $\widehat{\text{err}}_b := \frac{1}{n} \sum_{i=1}^n \ell(y_i, \hat{f}^b(x_i))$
6: **end for**
7: **return** $\widehat{\text{err}}_{\text{boot}} := \frac{1}{B} \sum_{b=1}^B \widehat{\text{err}}_b$

- Does this give very good estimate of the prediction error?
- If **no,** why not? Does it **underestimate** or **overestimate** the prediction error?

Pipeline of the Bootstrap

No.

Since the bootstrap is sampling with replacement for B validation folds, each fold would have significant overlap with the original data used for training. Approximately, **2/3** of the training data would appear in each validation fold.

This leads to significant **underestimation** of the prediction error.

- Why **2/3**?

Proof

Suppose there are n samples *(yi, xi)* in the training set data, then for each of the bootstrap validation fold b, every sample has probability **1/n** of being selected into b. The probability of each data sample *(yi, xi)* not being in fold b is **(1 - 1/n)**, respectively.

Probability of **avoid selecting** all n data points in fold b: **(1 - 1/n)^n**.

When n gets large, we have this probability converges to 1/e.
(Why this converges? Probably should review Calc I, or see:
https://math.stackexchange.com/questions/882741/limit-of-1-x-nn-when-n-tends-to-infinity.)

Therefore, the fraction of overlapping data points in each fold is **(1-1/e)**, which is about **2/3**.

How we fix the problem

- Requires some thoughts when generating validation set, especially for real-world complex data.
- Can partly fix this problem by only using predictions for those observations that did not (by chance) occur in the current bootstrap sample.
- But the method gets complicated.

Bootstrap vs. k-fold

In K-fold validation, each of the K folds is distinct from the other (K − 1) folds used for training: there is **no overlap**.

This is crucial for its success in estimating prediction error.

Why we still use bootstrap

- Bootstrap allows us to use a computer to mimic the process of obtaining new data sets.
- Can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- Provides an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.
  - i.e., the variability of the model!

Measures of overfitting

- Compare *train* accuracy with *test* accuracy!
- Method 1: **Generalization error**
  - (Generalization error) = (test error) - (train error)
  - Error introduced from trying to *generalize* to new data
- Method 2: **Prediction variation**
  - VAR(predictions for a specific point x)
  - How much do predictions change for point x, based on the training data?

Reminder: don't mix up error and accuracy! They're nearly equivalent measures, but confusing them in your code can cause problems

Demo

Coming Up

- **Assignment 8**: Due at 5:30pm, Dec. 9
- **Next Lecture**: Applications of *Un*supervised Learning

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