K Nearest Neighbor

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Parametric vs. non-parametric models

So far…

All of our models have looked like

$$\hat{y} = f(x, w) = w_0 + w_1 x_1 + \dots + w_d x_d$$

A model class is more flexible if $f(x, w)$ can represent more possible functions.

- Some possibilities for $f(x, w) = w_0 + w_1 x_1$
- More possibilities for $f(x, w) = w_0 + w_1 x_1 + w_2 x_2$
- Even more possibilities for $f(x, w) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$

But until now, we had to "know" how to add flexibility - for example, by adding interaction terms or other basis functions.

A way to get more flexible models is with a **non-parametric** approach, where we don't a priori impose the functional form or a fixed number of parameters that the model should learn.

Note: "parametric" and "non-parametric" are not precisely defined terms, but this is how they are often understood.

Parametric models

- A particular model class is assumed (e.g. linear)
- Number of parameters fixed in advance

Note: even if you use K-fold CV to try different candidate models with different number of parameters, you are still defining each candidate model in advance.

Non-parametric models

- Minimal assumptions about model class
- Model structure determined by data

Nearest neighbor

- A kind of non-parametric model.
- Basic idea: Find labeled samples that are "similar" to the new sample, and use their labels to make prediction for the new sample.

We previously spoke about the inductive bias of the linear models - we assumed that the target variable can be modeled as a linear combination of features or transformed versions of features. What is the inductive bias here?

1-NN

- Given training data $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$
- And a new sample $\mathbf{x}_0$
- Find the sample in the training data $\mathbf{x}_{i'}$ with the least distance to $\mathbf{x}_0$.

$$i' = \operatorname*{argmin}_{i=1,\dots,n} d(\mathbf{x}_i, \mathbf{x}_0)$$

- Let $\hat{y}_0 = y_{i'}$

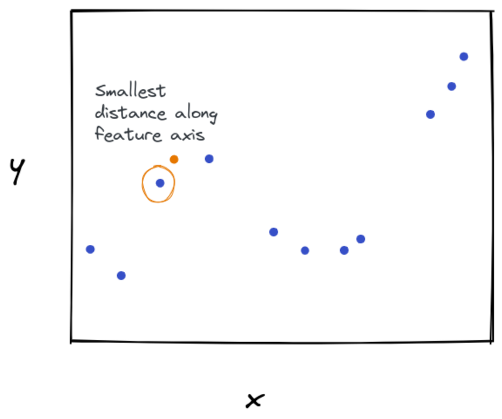


Figure 1: The nearest neighbor to the orange test point is the one that has the smallest distance in the feature space.

1-NN - runtime

- Training: just store data
- Inference: need to
  - compute distance to each of n points
  - distance metric typically scales with d

The runtime for predicting *each* test point is $O(nd)$. How does this compare to linear regression or logistic regression?

There, the training time could be long, but *inference* was only $O(d)$. We can tolerate a long training time more easily than a long inference time.

1NN - decision boundaries

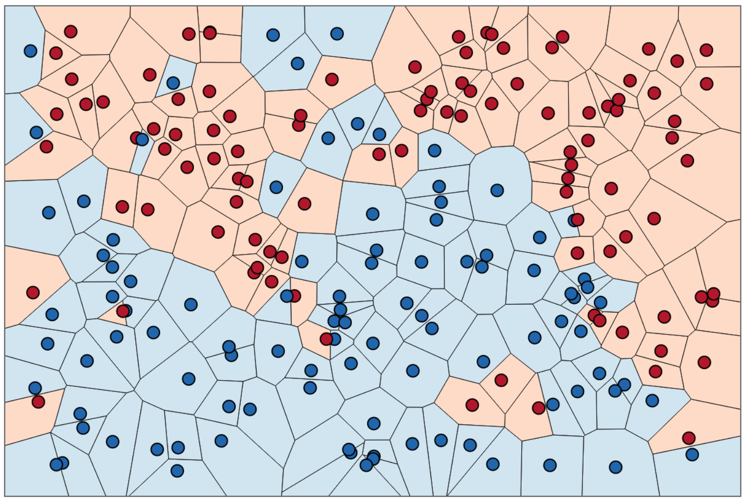


Figure 2: 1NN decision boundaries - Nearest neighborhoods for each point of the training data set.

Note that there will be zero error on training set (unless there are training data points that have identical feature values, but different labels).

K nearest neighbors

Instead of 1 closest sample, we find K: Let N_0 be the set of K training points that are closest to $\mathbf{x}_0$.

How do we use this set for (1) classification? (2) regression?

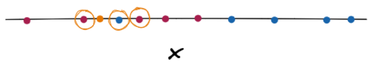


Figure 3: 3 nearest neighbors.

KNN for classification

Idea: Estimate conditional probability for a class as fraction of points among neighbors with the class label.

Remember: Let N_0 be the set of K training points that are closest to $\mathbf{x}_0$.

Then, we can estimate the per-class conditional probability given the sample x_0.

For each class $m \in M$:

$$P(y = m|\mathbf{x_0}) = \frac{1}{K} \sum_{(\mathbf{x}_i, y_i) \in N_0} I(y_i = k)$$

where $I(y_i = m)$ is 1 if $(\mathbf{x}_i, y_i) \in N_0$ is a member of class m, 0 otherwise.

- We can then select the class with the highest probability.
- Practically: select the most frequent class among the neighbors.

KNN for regression

Idea: Use the the combined label of the K nearest neighbors. For example, we can take their mean:

$$\hat{y}_0 = \frac{1}{K} \sum_{(\mathbf{x}_i, y_i) \in N_0} y_i$$

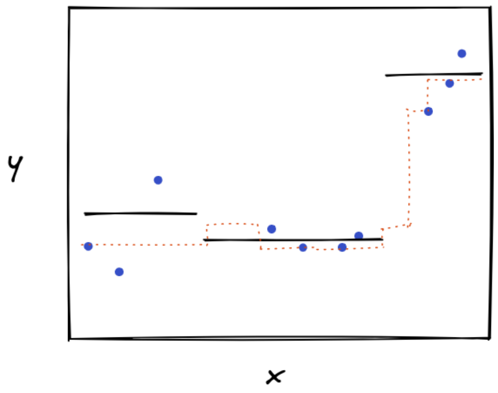


Figure 4: Example of a regression using median vote of the 3NN. The “true function” is shown in black, the orange dashed line shows the prediction of the regression model.

Model choices

We're letting the data dictate the form of the solution, but we still need to make many model choices:

- What value of K?
- What distance measure?
- How to combine K labels into prediction?

Question: does larger K mean "more flexible" or "less flexible" model?

What value of K? Illustration (1NN)

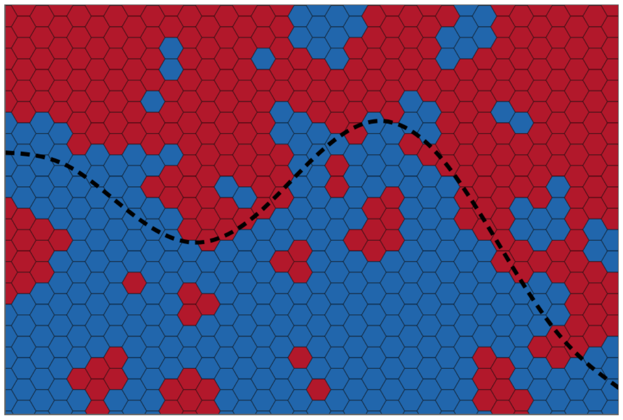


Figure 5: 1NN

What value of K? Illustration (2NN)

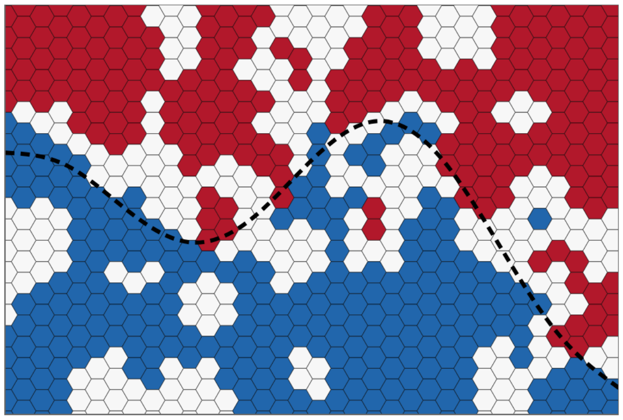


Figure 6: 2NN

What value of K? Illustration (3NN)

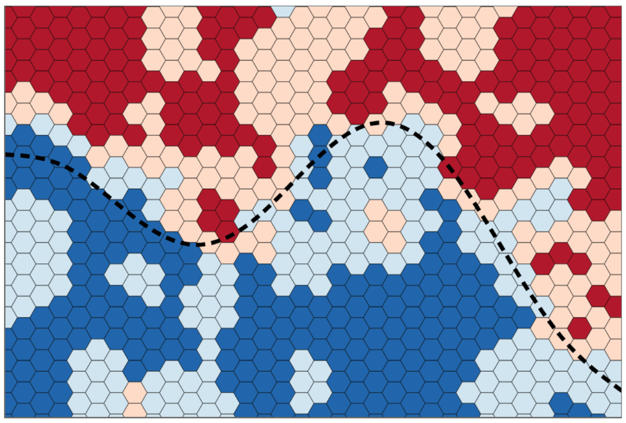


Figure 7: 3NN

What value of K? Illustration (9NN)

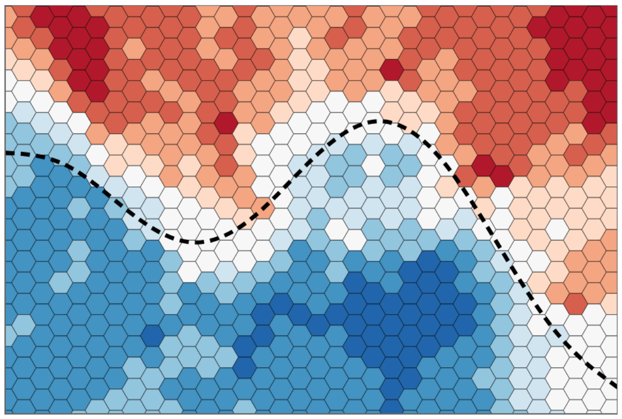


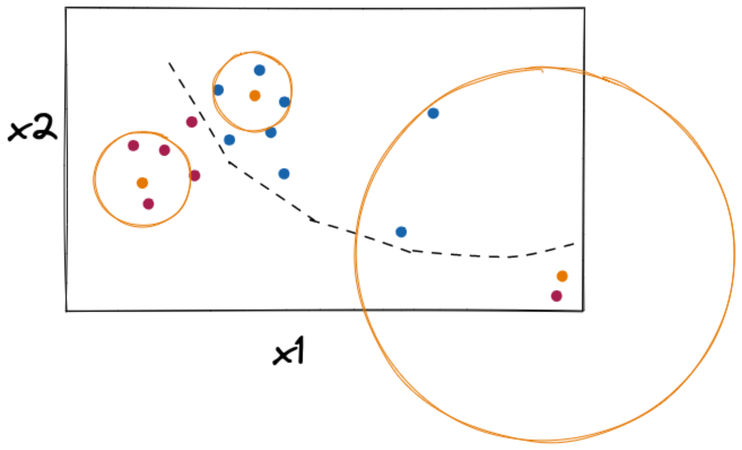
Figure 8: 9NN

What value of K? (1)

- In general: larger K, less complex model
- K can be selected by CV.
- Often cited “rule of thumb”: use $K = \sqrt{N}$

What value of K? (2)

- Alternative to fixed K: Radius-based neighbor learning.
- A fixed radius r is specified, can be selected by CV.
- Number of neighbors depends on local density of points.



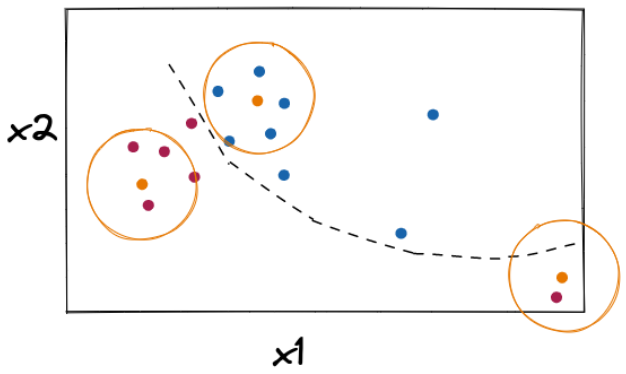


Figure 9: Comparison of KNN (top) and radius-based neighbor learning (bottom) when the density of training points in the feature space is uneven.

What distance measure? (1)

Some popular choices: for two vectors a_i, b_i,

- Euclidean (L2): $\sqrt{\sum_{i=1}^{d}(a_i - b_i)^2}$
- Manhattan (L1): $\sum_{i=1}^{d}|a_i - b_i|$

(L2 distance prefers many medium-sized disagreements to one big one.)

There are many more choices - for example, look at the distance metrics implemented in sklearn.

Problems with the basic distance metrics:

- When features have different scale/range, need to standardize
- KNN implicitly weights all features equally: this is a problem if you have features that are not relevant for the target variable!
- For images: pixel-wise distance doesn't necessarily equate to perceptual similarity

Distance measure - standardization (1)

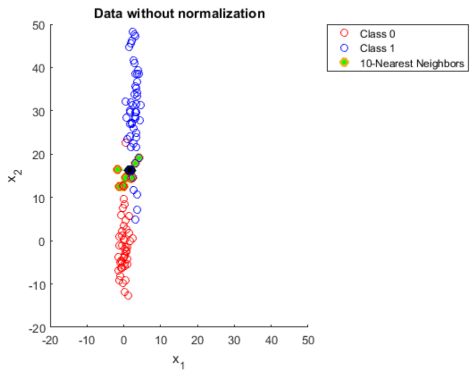


Figure 10: Without standardization, via https://stats.stackexchange.com/a/287439/. The x2 feature dominates the distance measure.

Distance measure - standardization (2)

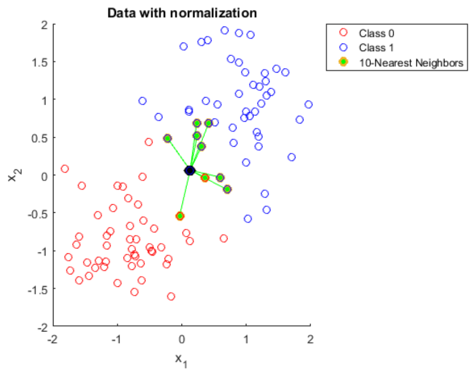


Figure 11: With standardization, via https://stats.stackexchange.com/a/287439/

Distance measure - equal weighted features

Suppose you are trying to predict a student's course grade using their previous GPA and how far they live from the NYU campus:

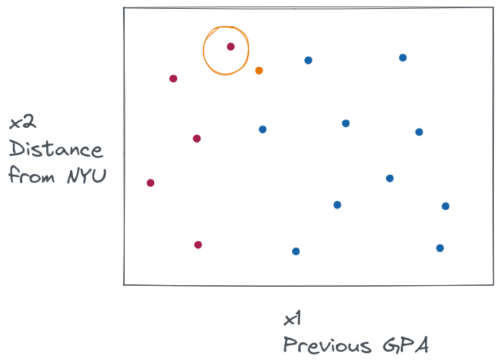


Figure 12: The training point circled in orange is the nearest neighbor, but it's not the most similar according to the only feature that matters (previous GPA). All features are weighted equally in the distance metric, regardless of their importance.

Alternative to equal weighted features: assign feature weights

$$d(\mathbf{a}, \mathbf{b}) = \left(\sum_{i=1}^{k} (w_i |a_i - b_i|)^q \right)^{\frac{1}{q}}$$

But then we need a way to learn feature weights!

With L1 regularization, we had a data-driven way to do feature selection. The nearest neighbor method doesn't have any "built-in" way to do feature weighting or feature selection as part of the training process, so we need to do it ourselves as part of the pre-processing steps.

We'll go back to this at the end.

Distance measure - perceptual distance

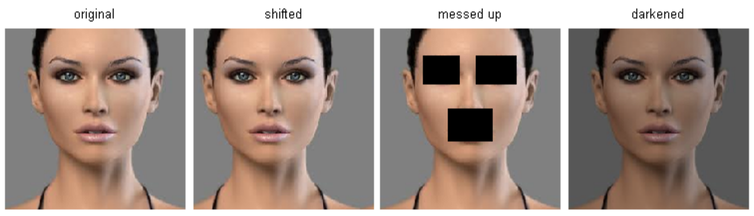


Figure 13: An original image (left) and three other images next to it that are all equally far away from it based on L2 pixel distance. Image via CS321n.

This is a little more difficult to overcome. In practice, KNN is often just not very useful for image data.

How to combine labels into prediction?

- **Basic voting**: use mode of neighbors for classification, mean or median for regression.
- **Distance-weighted**: weight of vote inversely proportional to distance from the query point. ("More similar" training points count more.)

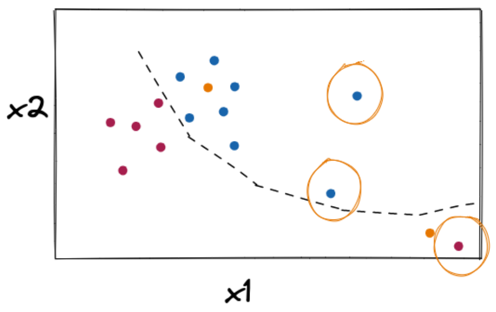


Figure 14: In this example, the red training point will get a bigger "vote" in the class label because it is closest to the test point. The point can be classified as red, even though 2 of the 3 neighbors are blue.

Bias and variance of KNN

True function

Suppose data has true relation

$$y = t(\mathbf{x}) + \epsilon, \quad \epsilon \sim N(0, \sigma_\epsilon^2)$$

and our model predicts $\hat{y} = f(\mathbf{x})$.

Assumption of fixed training set

For this derivation, we consider the expectation over:

- the test points
- the error ϵ
- the randomness in the y values in the training set!

We do not consider randomness in the x values - we assume a fixed training set.

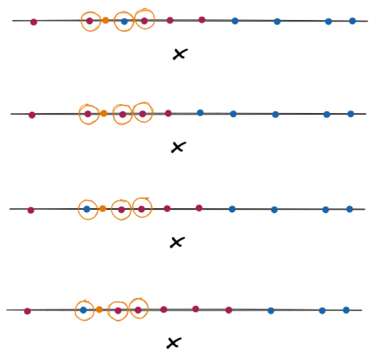


Figure 15: Assume the x values in the training set are fixed (and therefore, the neighbors of any given test point), but there is randomness in the y values.

Expected loss

We will use an L2 loss function, so that the expected error of the prediction $\hat{y}$ for a given test point $\mathbf{x_t}$ is:

$$\begin{aligned} MSE(\mathbf{x_t}) :=& E[(y-\hat{y})^2] \\ =& \left(t(\mathbf{x_t}) - E[f(\mathbf{x_t})]\right)^2 + \\ & E[(f(\mathbf{x_t}) - E[f(\mathbf{x_t})])^2] + \\ & \sigma_\epsilon^2 \end{aligned}$$

i.e. squared bias, variance, and irreducible error.

KNN output

The output of a KNN regression at the test point is

$$f(\mathbf{x_t}) = \frac{1}{K} \sum_{\ell \in K_x} t(\mathbf{x}_\ell) + \epsilon_\ell$$

where K_x is the set of K nearest neighbors of $\mathbf{x_t}$. (We assume that these neighbors are fixed.)

Bias of KNN

When we take expectation of bias over test samples:

$$\begin{aligned} Bias^2 &= \left(t(\mathbf{x_t}) - E[f(\mathbf{x_t})]\right)^2 \\ &= \left(t(\mathbf{x_t}) - E\left(\frac{1}{K} \sum_{\ell \in K_x} t(\mathbf{x}_\ell) + \epsilon_\ell\right)\right)^2 \\ &= \left(t(\mathbf{x_t}) - \frac{1}{K} \sum_{\ell \in K_x} t(\mathbf{x}_\ell)\right)^2 \end{aligned}$$

The expectation is over the training sample draw - but note that the x values in the training samples are fixed! So the only randomness is in ϵ_ℓ.

Since the x values in the training samples are fixed, the $\frac{1}{K} \sum_{\ell \in K_x} t(\mathbf{x}_\ell)$ can come out of the expectation as a constant. Then $E[\epsilon_\ell] = 0$.

Variance of KNN (1)

$$\begin{aligned}
Var(\hat{y}) &= E[(f(\mathbf{x_t}) - E[f(\mathbf{x_t})])^2] \\
&= E\left[\left(f(\mathbf{x_t}) - \frac{1}{K}\sum_{\ell \in K_x} t(\mathbf{x}_\ell)\right)^2\right] \\
&= E\left[\left(\frac{1}{K}\sum_{\ell \in K_x} (t(\mathbf{x}_\ell) + \epsilon_\ell) - \frac{1}{K}\sum_{\ell \in K_x} t(\mathbf{x}_\ell)\right)^2\right] \\
&= E\left[\left(\frac{1}{K}\sum_{\ell \in K_x} \epsilon_\ell\right)^2\right]
\end{aligned}$$

Variance of KNN (2)

$$\begin{aligned}
&= E\left[\left(\frac{1}{K}\sum_{\ell \in K_x} \epsilon_\ell\right)^2\right] = \frac{1}{K^2}E\left[\left(\sum_{\ell \in K_x} \epsilon_\ell\right)^2\right] \\
&= \frac{1}{K^2}Var\left(\sum_{\ell \in K_x} \epsilon_\ell\right) = \frac{1}{K^2}\sum_{\ell \in K_x} Var\left(\epsilon_\ell\right) = \frac{K\sigma_\epsilon^2}{K^2} \\
&= \frac{\sigma_\epsilon^2}{K}
\end{aligned}$$

Note: we use the fact that the ϵ terms are independent, so the variance of sum is equal to sum of variances.

Error of KNN

Then the expected error of KNN is

$$\left(t(\mathbf{x_t}) - \frac{1}{K}\sum_{\ell \in K_x} t(\mathbf{x}_\ell)\right)^2 + \frac{\sigma_\epsilon^2}{K} + \sigma_\epsilon^2$$

where K_x is the set of K nearest neighbors of $\mathbf{x}$.

Bias variance tradeoff

- Variance decreases with K
- Bias likely to increase with K, if function $t()$ is smooth.

Why does bias increase with K? For a smooth function, the few closest neighbors to the test point will have similar values, so average will be close to $t(\mathbf{x})$; as K increases, neighbors are further way, and average of neighbors moves away from $t(\mathbf{x})$.

You can think about the extreme case, where $K = n$ so you use the average of *all* of the training samples. This is equivalent to "prediction by mean".

The Curse of Dimensionality

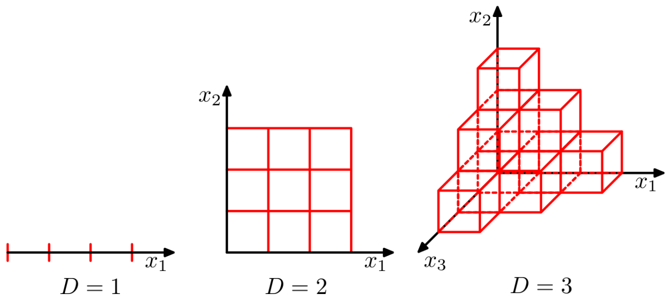


Figure 16: Feature space grows exponentially with dimension. From Bishop PRML, Fig. 1-21

KNN in 1D

- Consider a dataset $(x_1, y_1), \ldots, (x_N, y_N), N = 100$
- x is uniformly distributed in [0,1]
- On average, one data point is located every 1/100 units along 1D feature axis.
- To find 3NN, would expect to cover 3/100 of the feature axis.

KNN in 2D

- Now consider the same dataset with two features.
- Each feature is uniformly distributed in [0,1]
- To find 3NN, would expect to cover $0.03^{\frac{1}{2}}$ of the unit rectangle.

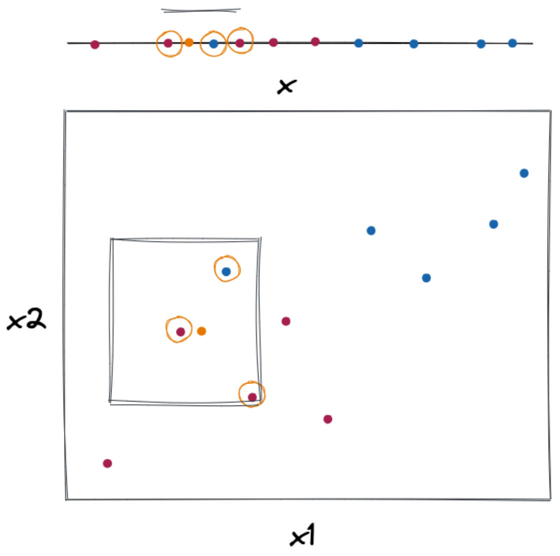


Figure 17: When d goes from 1 to 2, the density of the training points decreases and we need to cover more of the feature space to find the same number of neighbors.

Density of samples decreases with dimensions

To get 3NN,

- need to cover 3% of space in 1D
- need to cover 17% of space in 2D
- need to cover 70% of space in 10D. At this point, the nearest neighbors are not much closer than the rest of the dataset.

Density of samples decreases with dimensions - general

The length of the smallest hyper-cube that contains all K-nearest neighbors of a test point:

$$\left(\frac{K}{N}\right)^{\frac{1}{d}}$$

for N samples with dimensionality d.

Solutions to the curse (1)

Add training data?

$$\left(\frac{K}{N}\right)^{\frac{1}{d}}$$

As number of dimensions increases linearly, number of training samples must increase exponentially to counter the “curse”.

Solutions to the curse (2)

Reduce d?

- Feature selection
- Dimensionality reduction: a type of unsupervised learning that *transforms* high-d data into lower-d data.

Summary of NN method

NN learning

Learning:

- Store training data
- Don't do anything else until you have a new point to classify

In practice, we will usually store training data in a data structure that makes it faster to compute nearest neighbors.

NN prediction

Prediction:

- Find nearest neighbors using distance metric
- Classification: predict most frequently occuring class among nearest neighbors
- Regression: predict mean value of nearest neighbors

The good and the bad (1)

Good:

- Good interpretability
- Fast "learning" (*memory-based*)
- Works well in low dimensions for complex decision surfaces

The good and the bad (2)

Neutral:

- Assumes similar inputs have similar outputs

The good and the bad (3)

Bad:

- Slow prediction (especially with large N)
- Curse of dimensionality

Feature selection and feature weighting

Feature selection is actually two problems:

- best number of features
- best subset of features

These problems can be solved separately:

- find best subset of feature of every possible size
- then among those, select the best

or they can be solved together, for example:

- keep adding features until improvement due to another feature is less than some threshold t
- keep features whose "score" exceeds some threshold t
- etc.

For some models, like KNN, we can also do feature weighting (compute a weight for each feature, scale feature by that weight) as an alternative to (or in addition to) feature selection.

Feature selection is hard!

Computationally **hard** - even on small problems.

Optimization in two parts

- **Search** the space of possible feature subsets
- **Evaluate** the goodness of a feature subset

Search: exhaustive search

Optimal search: consider every combination of features

- Given d features, there are 2^d possible feature subsets
- Too expensive to try all possibilities for large d!

Search: naive heuristic

- sort d features in order of "goodness"
- select top k features from the list

Problem: this approach considers each feature independently.

- Doesn't consider redundancy: if you have two copies of an informative features, they'll both score high (but you wouldn't necessarily want to include both in your model).
- Doesn't consider interaction: if you are going to use a model that can learn interactions "natively" (like a tree-based model), this type of feature selection may exclude features that are not informative themselves but whose combination is informative.

Search: sequential forward selection

- Let S^{t-1} be the set of selected features at time $t-1$
- Train and evaluate model for all combinations of current set + one more feature
- For the next time step S^t, add the feature that gave you the best performance.

("Backward" alternative: start with all features, and "prune" one at a time.)

This is not necessarily going to find the best feature subset! But, it is a lot faster than the exhaustive search, and considers relationship between features (which naive approach dose not.)

Evaluation: methods

- **Filter methods**: consider only the statistics of the training data, don't use the model.
- **Wrapper methods**: evaluate subsets of features on a model.

Evaluation: filter methods (1)

Pseudocode:

```
for j in X.shape[1]:
  score[j] = score_fn(X[:,j], y) )
```

Once you have a score for each feature, pick k features that have highest score (use CV to choose k?)

Can also include multivariate scoring functions:

```
for j, feat_set in enumerate(feat_sets):
  score[j] = score_fn(X[:,feat_set], y) )
```

You can also use the score for feature weighting: Compared to feature selection, feature weighting does not have the benefit of faster inference time, but it does have the advantage of not throwing out useful information.

Evaluation: filter methods (2)

- Usually much faster!
- Finds "generally" good features
- Need to choose "scoring" function that is a good fit for the model

- Scoring function measures the relationship between `X` and `y`.
- For example: correlation coefficient, or F-statistic both of which measures linear relationship between `X` and `y`.

Problem: correlation coefficient scoring metric only captures linear relationship.

- If you expect the relationship to be linear, it's fine!
- If you are using a model (e.g. linear regression) that is only capable of learning linear relationships, it's fine! You don't want your feature selection method to give a high score to a column if the model won't be able to learn from it anyway.

Evaluation: filter methods (3)

Evaluation: wrapper methods (1)

- Tuned to specific interaction of dataset + model!
- Usually much more expensive (especially considering model hyperparameter tuning…)

An option for some models

- **Embedded methods**: use something built-in to training algorithm (e.g. LASSO regularization). (Not available for KNN!)

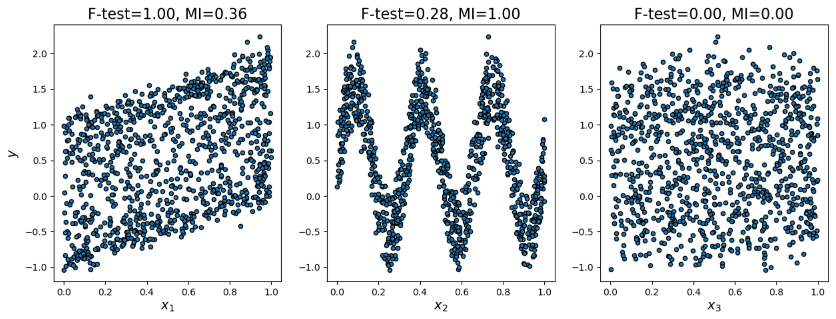


Figure 18: F-test selects x_1 as the most informative feature, MI selects x_2.

Recap

- Feature selection approach should "match" the data, model
- Computation is a concern - it won't be possible to optimize everything