

# Intro to non-parametric machine learning models

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# We've been studying parametric models

- *Parametric models* have a finite number of parameters like linear model ( $\beta_i$ 's), multinomial Naïve Bayes ( $P(c)$ ,  $P(w|c)$ )
- 😊 *Nonparametric models* have an unbounded number of parameters (world's worst name)
- (If number of model parameters change with different  $n$  records, it's nonparametric. Neural nets have huge but finite number of parameters once net is constructed.)
- Random Forests (RF) and gradient boosting machines are nonparametric

# General advice for choosing a model

- If you know that the relationship between  $X$  and  $y$  is linear, use a linear model; or, if you need an extreme compression of the training data down to a few coefficients
- If you know the relationship is nicely summarized by conditional probabilities, Naïve Bayes approach is a good one
- For unstructured data such as images or signals, use deep learning neural networks (large number of parameters)
- For structured data like database tables or Excel spreadsheets, use decision tree-based methods: *Random Forests* (RF) or *Gradient Boosting Machines* (GBM)

# Some basic modeling advice

- That “choosing model” advice is solid in practice and reduces the number of models you need to study and understand (ignore SVM, ...)
- Remember: good features matter way more than the model
- Pick a decent model and then focus on feature engineering
- Know the strengths/weaknesses of your model; e.g., random forests don't extrapolate outside of support region but parametric models tend to extrapolate
- Compare your model to a weaker model
  - Sometimes a simpler model (e.g., linear model) just as good
  - Gives a good lower bound on accuracy
  - Helps identify bugs in your code; e.g., when weaker model is better

# Reinventing machine learning models

- Let's imagine creating model to predict SF rent prices
- What features, training data do we need? What's  $X$  and  $y$ ?
- Goal: generalize from training data
- How do people do it manually?  
Find a few comparable apts and then predict average price
- That's called a *k-Nearest-Neighbor* (kNN) model & is pretty good!  
(more on this shortly)

Features				Target
bedrooms	bathrooms	latitude	longitude	price
3	1.5	40.7145	-73.9425	3000
2	1.0	40.7947	-73.9667	5465
1	1.0	40.7388	-74.0018	2850
1	1.0	40.7539	-73.9677	3275
4	1.0	40.8241	-73.9493	3350

See <https://mlbook.explained.ai/intro.html>

# Starting with extreme models

- Recall our goal: to build an accurate model without being overly specific to training data

*dict* • What if we simply memorized the training set? How could we use such a dictionary method to make predictions?

*mean* • The other extreme would be to compute the average rent price from all apt data, ignoring all features, and make that our sole prediction

- How would you describe the differences / tradeoffs between them?
  - Dictionary has no bias (very accurate) but is not general (only works for training data)
  - Average has big bias but is very general (applies to any apartment)
- *Bias-generality tradeoff (bias-variance trade-off)*

↑  
*overfitting = not general*

# Dealing with uncertainty in target (prices)

- Aside from overfitting, what's wrong with the dictionary method?
- It can't handle multiple prices for identical apt feature vectors
- But, prices fluctuate from noise, errors, or exogenous features like square footage, view, proximity to BART, etc...
- Which/what price should our decent model return for data below?
- Merge identical records, recording mean(y) for prototype

	bedrooms	bathrooms	latitude	longitude	price
1470	0	1.0000	40.7073	-73.9664	2650
36509	0	1.0000	40.7073	-73.9664	2850
39241	0	1.0000	40.7073	-73.9664	2950
46405	0	1.0000	40.7073	-73.9664	2850

# Dealing with inexact feature matches

- Dictionaries are super rigid: they can't deal with mismatched keys
- Feature vectors not found in the training data dictionary will get a “key not found” error, rather than a prediction!
- How can we predict prices for inexact matches?
- Scan all apartment records, find the closest match  
(hard to measure distance for cat. variables like has\_parking)
- Or, find the closest  $k$  matches and predict the average price (this is what real estate agents do; they are called “comps”); this is  $k$ -nearest neighbor model, so let's look in more detail

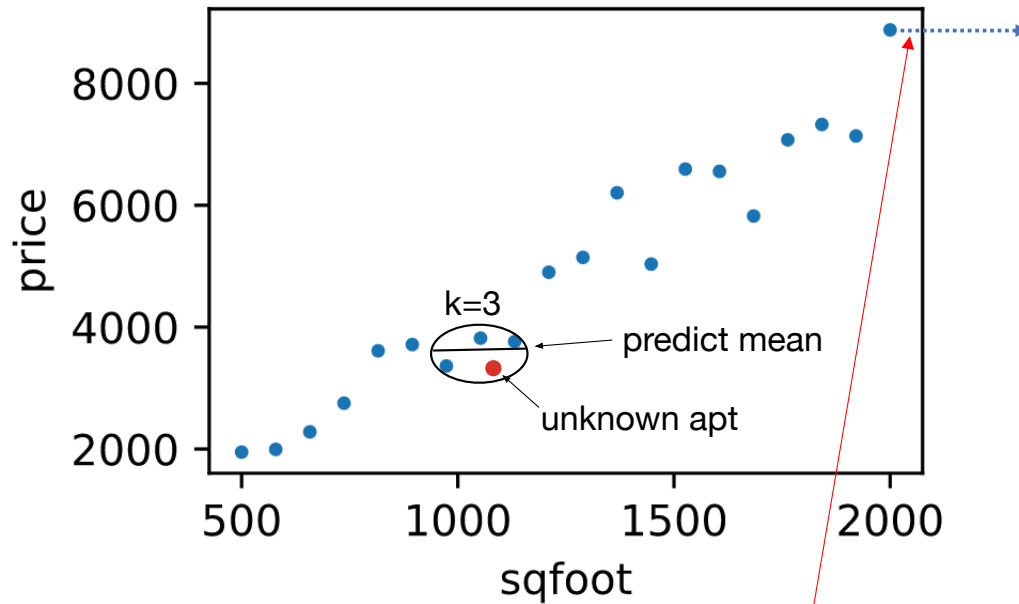


# Detour: $k$ -nearest neighbors ( $kNN$ )

- $kNN$  is less often used in practice, but it's part of your education to understand how they work and can still be very effective
- Regressor: get  $k$  observations closest to unknown  $x$  using Euclidean distance then predict average  $y$  from those  $k$
- Classifier: get  $k$  observations closest to unknown  $x$  using Euclidean distance then predict most common class from those  $k$
- Finding closest observations for large  $n$  can be slow
- Simple: there is no training process but must choose suitable  $k$
- Best if we normalize data due to Euclidean distances used
- Requires distance metric, which is problematic for categoricals

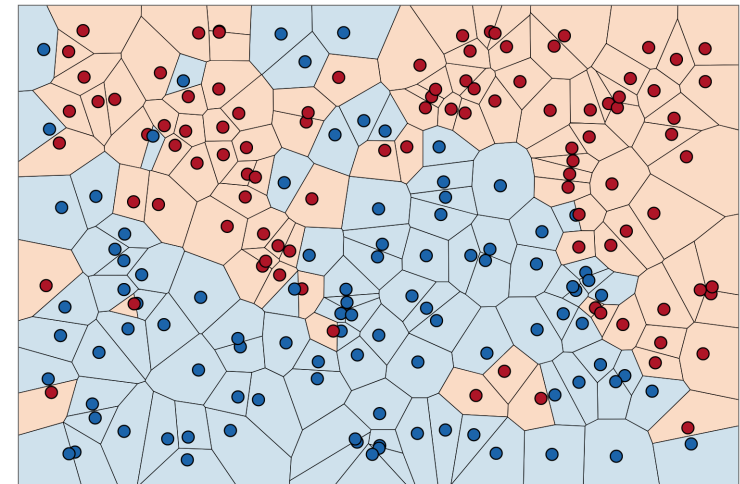
# Sample kNN models

1D k=3 regressor



Note: kNN regressors can't extrapolate

2D k=1 classifier



Classifier image credit:

<http://scott.fortmann-roe.com/docs/BiasVariance.html>

# From kNN to decision trees

# Feature space partitioning in rectangular hypervolumes not distance

- To avoid inefficiency and distance metric requirement of kNN, we can partition feature space into rectangular hypervolumes
- Each hypervolume would represent a prototypical apartment with similar features
- Predictions come from average  $y$  (regressor) or most common class (classifier) in hypervolume
- Note similarities with kNN but hypervolumes chosen by partitioning rather than Euclidean distance
- No distance computation means:
  - No need to normalize data
  - Can partition (nominal/ordinal) categorical variables by subsets as "regions"

# Example partitioning rules

- The goal is to split each feature into as many ranges as necessary to get accuracy but w/o creating so many tight regions we kill generality by overfitting to training data
- Rules for partitioning might look like:

```
if bedrooms == 1 and bathrooms == 1.0 and \  
    latitude >= 40.6661 and latitude <= 40.6663 and \  
    longitude >= -73.9882 and longitude <= -73.9402:  
    price = 2143 # average of apts in that range  
if bedrooms == 2 and bathrooms == 1.0 and \  
    latitude >= 40.6661 and latitude <= 40.6663 and \  
    longitude >= -73.9882 and longitude <= -73.9402:  
    price = 2462 # average of apts in that range
```

Predict by testing rules until we find a match and get a price

# Partitioning rules prediction efficiency

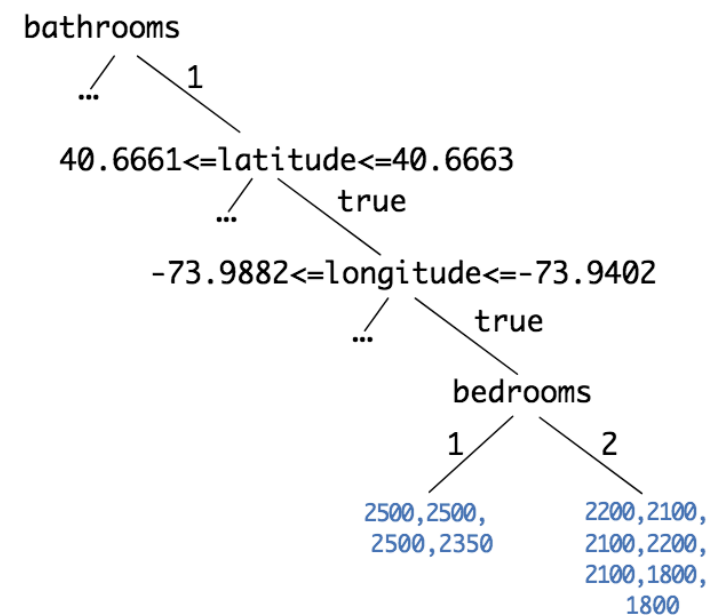
- Unlike a dictionary, partitioning rules automatically:
  - handle multiple identical apartments with different prices
  - can make predictions for previously unseen feature combinations
- The number of feature ranges or “splits” tested by the model are a kind of a bias-generality “knob” we can turn up or down
- Potentially very slow walking through a large number of partitioning rules so factor / nest the IF-rules to avoid redundant tests

```
if bathrooms == 1.0:  
    if latitude >= 40.6661 and latitude <= 40.6663 and \  
        longitude >= -73.9882 and longitude <= -73.9402:  
        if bedrooms == 1:  
            price = 2143  
        elif bedrooms == 2:  
            price = 2462  
if ...
```



# Encoding partitioning rules as a tree

- Can encode those nested rules as tree data structure
- Internal nodes perform feature comparisons, leaves make predictions
- Leaves contain prices for all apts fitting criteria on path from root down to that leaf
- Leaves represent feature-hypervolumes
- These are called *decision trees*
- By testing same feature many times, can carve up feature space arbitrarily tightly
- Training finds feature & value to test in each decision node (and when to stop splitting feature space)

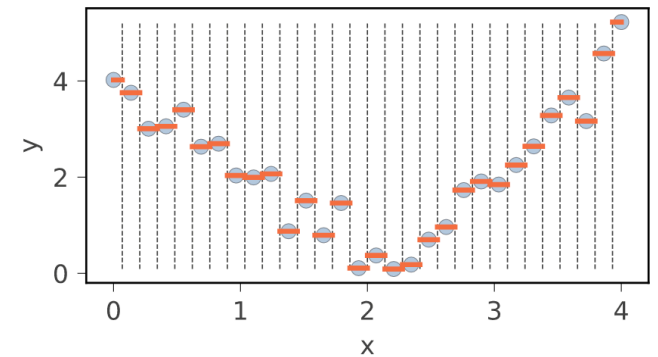


# From decision trees to random forests



# The problem with decision trees

- Decision trees overfit like crazy to the training data
- By default, they split feature space until each leaf has a single observation (apartment in this case); that is precise like dictionary but does not generalize very well
- We can control overfitting partially by requiring a min number of observations for leaf or restricting tree height
- A single-node decision tree degenerates to our extreme model that predicts the mean

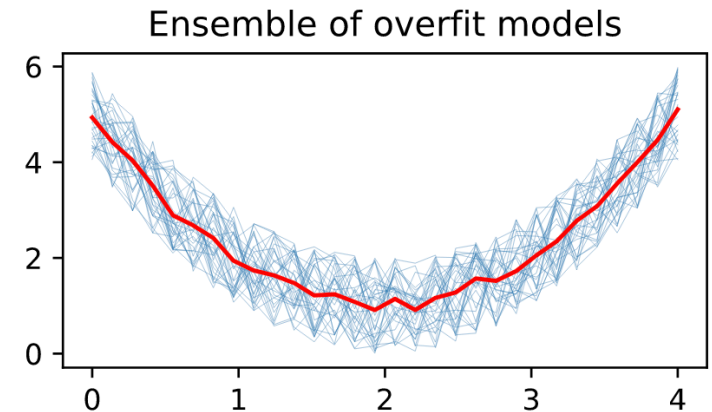


# Randomness is your friend

- To prevent overfitting, we can weaken a decision tree by showing it a random subset of the training data (*bagging*)
- *Bagging* uses *bootstrapping*: from  $n$  records, randomly select  $n$  w/replacement
- To go further, degrade training so that it always forgets that some features exist when making splitting decisions
- Such individual decision trees are weaker and less accurate than regular decision trees but...

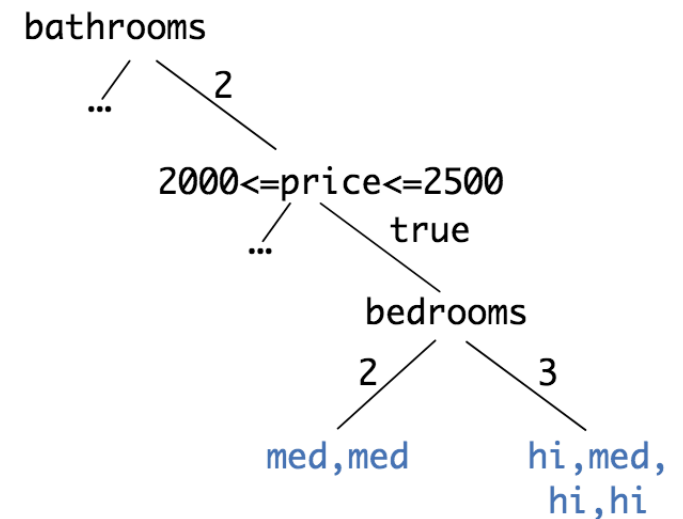
# Random Forest (RF) regressors

- To compensate for weaker learners, we can create lots of them
- Take the average of their predictions to get overall prediction
- This is called *ensemble learning* and is excellent technique to increase accuracy without a tendency to overfit
- RFs are crowd-sourcers; analogous to group of real estate agents looking for comparable apartments, and cooperating to estimate apartment price
- During training, agents independently select and visit apts
- Randomize to avoid visiting, say, only 1-bedroom apts
- Agents find different apt subsets with some overlap



# RF classifiers

- RFs can predict classes too but take a majority vote among the decision tree classifiers, rather than predicting average  $y$  value
- Each decision tree classifier leaf predicts the most common category from observations in that leaf
- Example classifier: predicting website interest in apartments (low, medium, hi)
- (full lecture on RFs soon)



# Key takeaways

- Parametric vs nonparametric models (fixed vs arbitrary parameters)
- Default model choice for structured data: RF or GBM
- Feature engineering much more important than the model
- Bias-generality tradeoff
- kNN: Find  $k$  **nearest** feature vectors and then predict average  $y$  (regressor) or most common  $y$  (classifier); tessellates feature space
- Decision tree: partitions feature space into rectangular **hypervolumes**; predict average/most common  $y$  in volume
- Random Forest: collection of decision trees trained on subset of training data and sometimes ignoring features; avg or majority vote among trees