Tree models

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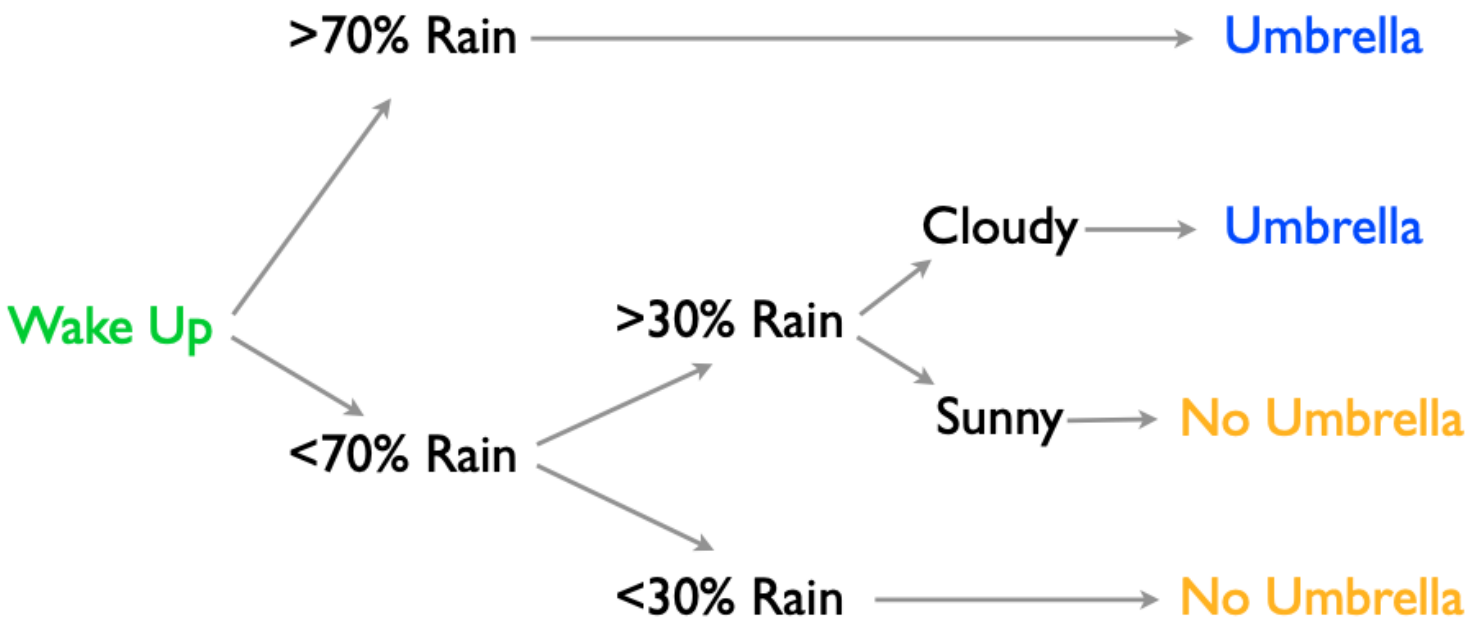
ECO 395M: Data Mining and Statistical Learning

Outline

1. Overview of tree models
2. Classification and regression trees: some examples
3. Fitting trees
4. Bagging: bootstrap aggregating
5. Random forests
6. Case study 1: back to the Houston power grid
7. Interpreting black-box models: feature importance and partial dependence plots
8. Boosting
9. Case study 2: Capital Metro ridership data

Tree models



Trees involve simple mini-decisions that, taken sequentially, result in a choice or prediction.

Each decision is a *node*; the final choice or prediction is a *leaf node.*

Tree models are among the most useful "general-purpose" function approximators in all of machine learning.

Tree models

You can think of a tree as a form of regression model:

- inputs x: forecast, current conditions
- output y: need for an umbrella

Based on previous data, the the goal is to specify branches/choices that lead to good predictions in new scenarios.

In other words, you want to estimate a **Tree Model**. Instead of linear coefficients, we need to find 'decision nodes': binary splitting rules defined by the x features.

Tree models

Tree models come in two flavors.

- Classification tree: the leaf nodes are predicted class labels/probabilities for a categorical outcome. (**"The predicted probability of rain is 90%, so take an umbrella."**)
- Regression tree: the leaf nodes specify $E(y \mid x)$ for a numerical outcome. (**"The predicted amount of rain is 2 cm, so take an umbrella."**)

The basic idea is the same for both; just a few of the details change.

Tree models

The goal of tree modeling: specify the sequence of mini-decisions that get you to the leaves.

- How many?
- What decisions? (Which features, which values of the features?)
- What order?

The space of possible trees is *huge*.

We'll talk about fitting the tree later; for now, let's see some examples to build our intuition.

A classification tree

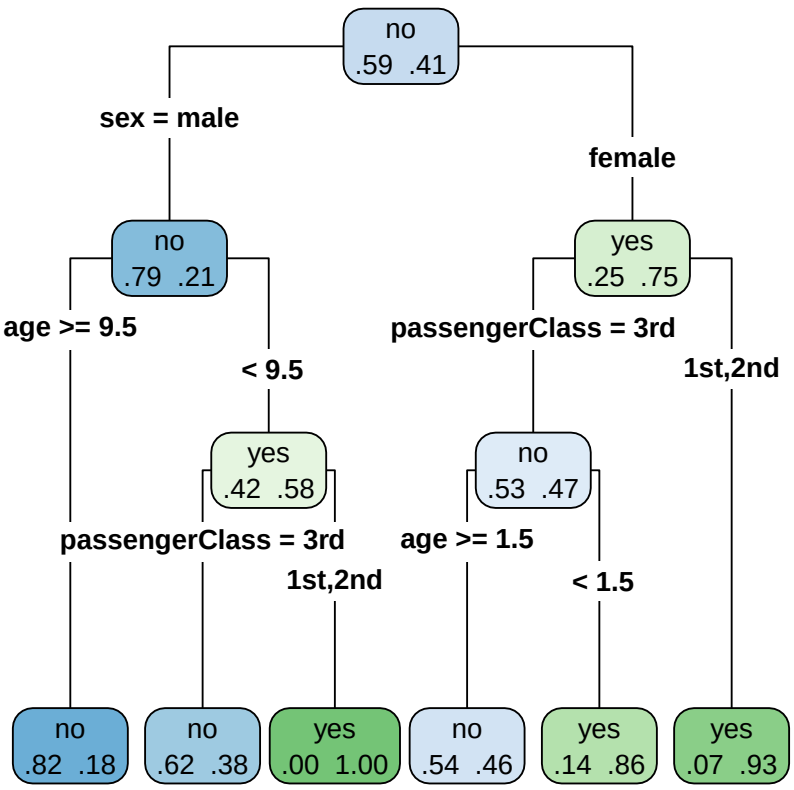
Classification trees are for categorical outcomes (with binary outcomes as a special case).

Let's see an example trained on data from the Titanic:

- x: a passenger's sex, age, class of travel
- y: whether the passenger survived the sinking of the ship

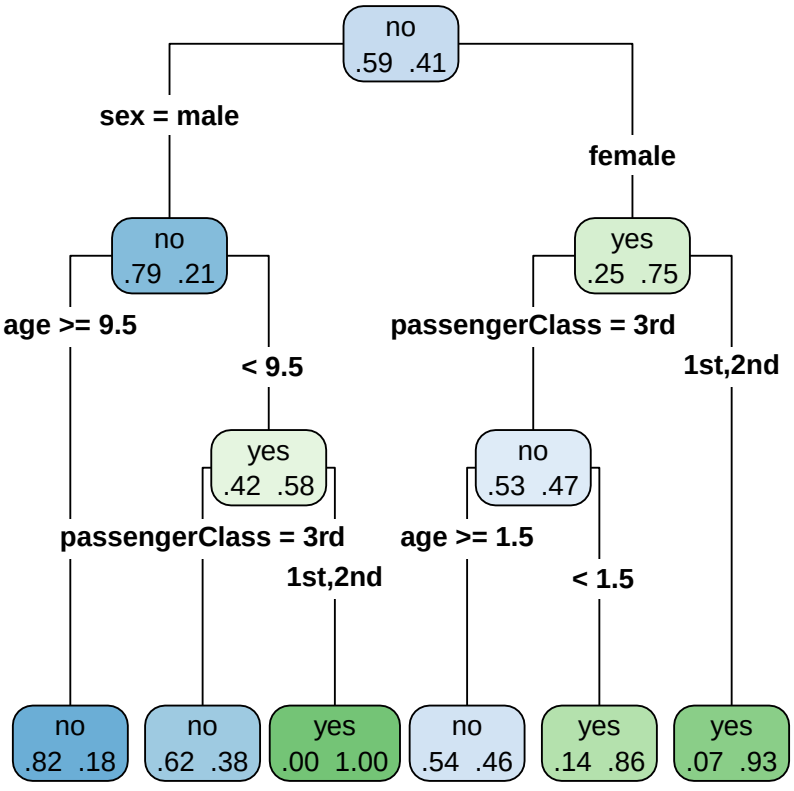
Goal: estimate $P(y \mid x)$

A classification tree



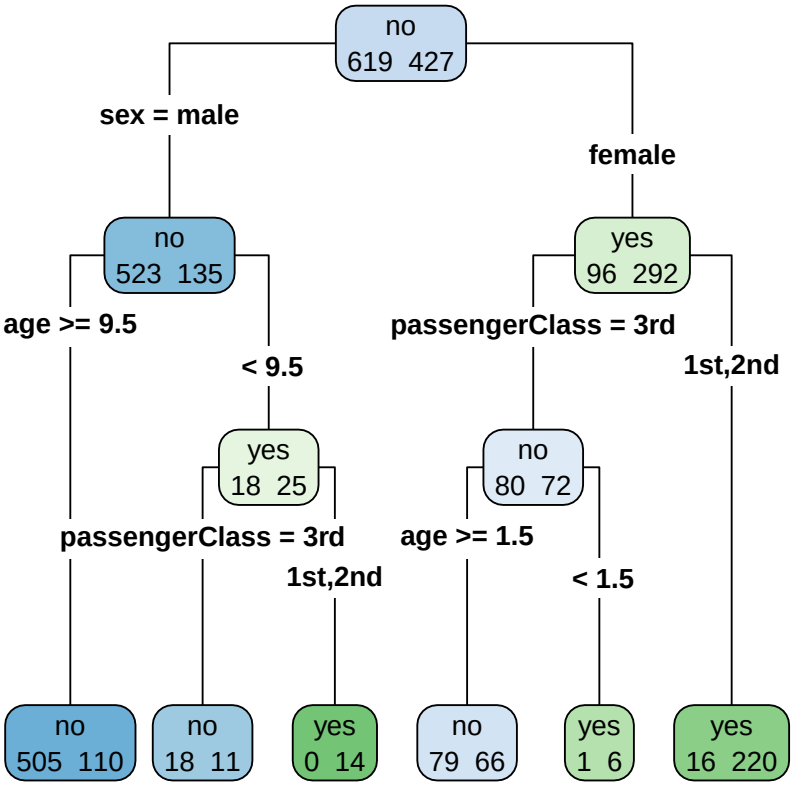
- Each split involves a yes/no question about a single variable.
- For numerical features (age), the yes/no question is whether x exceeds some threshold t.
- You might see/hear this called a "dendrogram," which is just a fancy Latin word for "tree picture."

A classification tree



- At each leaf node, we see fitted class probabilities. These come from the training data.
- To make a prediction, you "drop" your x down the tree, answering each yes/no question in turn.
- Notice the interactions! E.g. the questions we ask about age at later splits depend on which branch we're on.

A classification tree



- It's easier to see where the fitted probabilities come from if we show the number of observations per class in each leaf node.
- Let's reason through two quick examples.
  - x = {male, 3rd, 5 years}
  - x = {female, 1st, 25 years}.

A regression tree

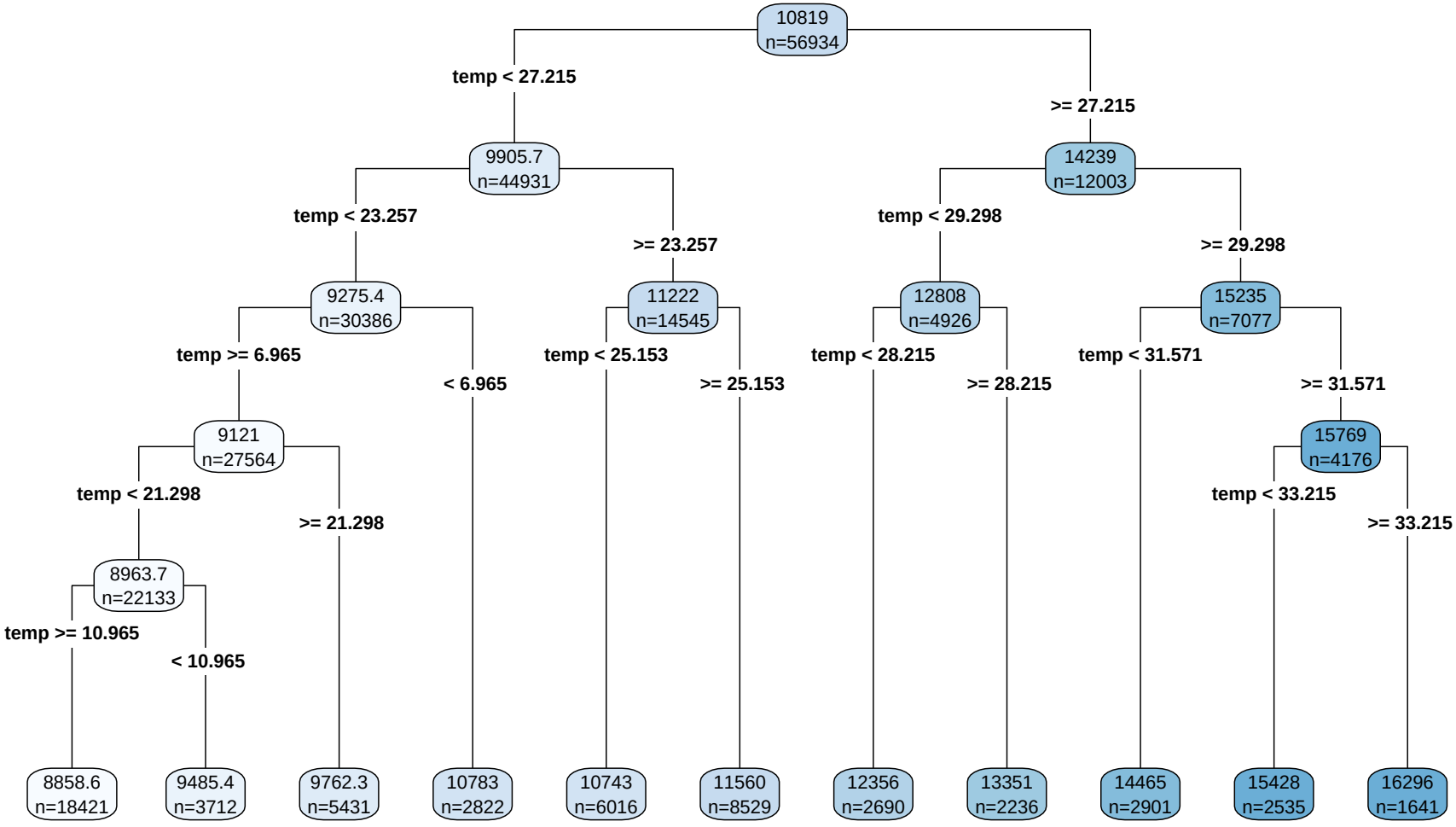
Regression trees are for numerical (as opposed to categorical) outcomes.

Let's see one on a familiar data set:

- y = peak power consumption in the ERCOT coast region
- x = temperature at Houston's Hobby airport in degrees C (so all splits are of the form $\mathrm{temp} < t$ for some threshold t).

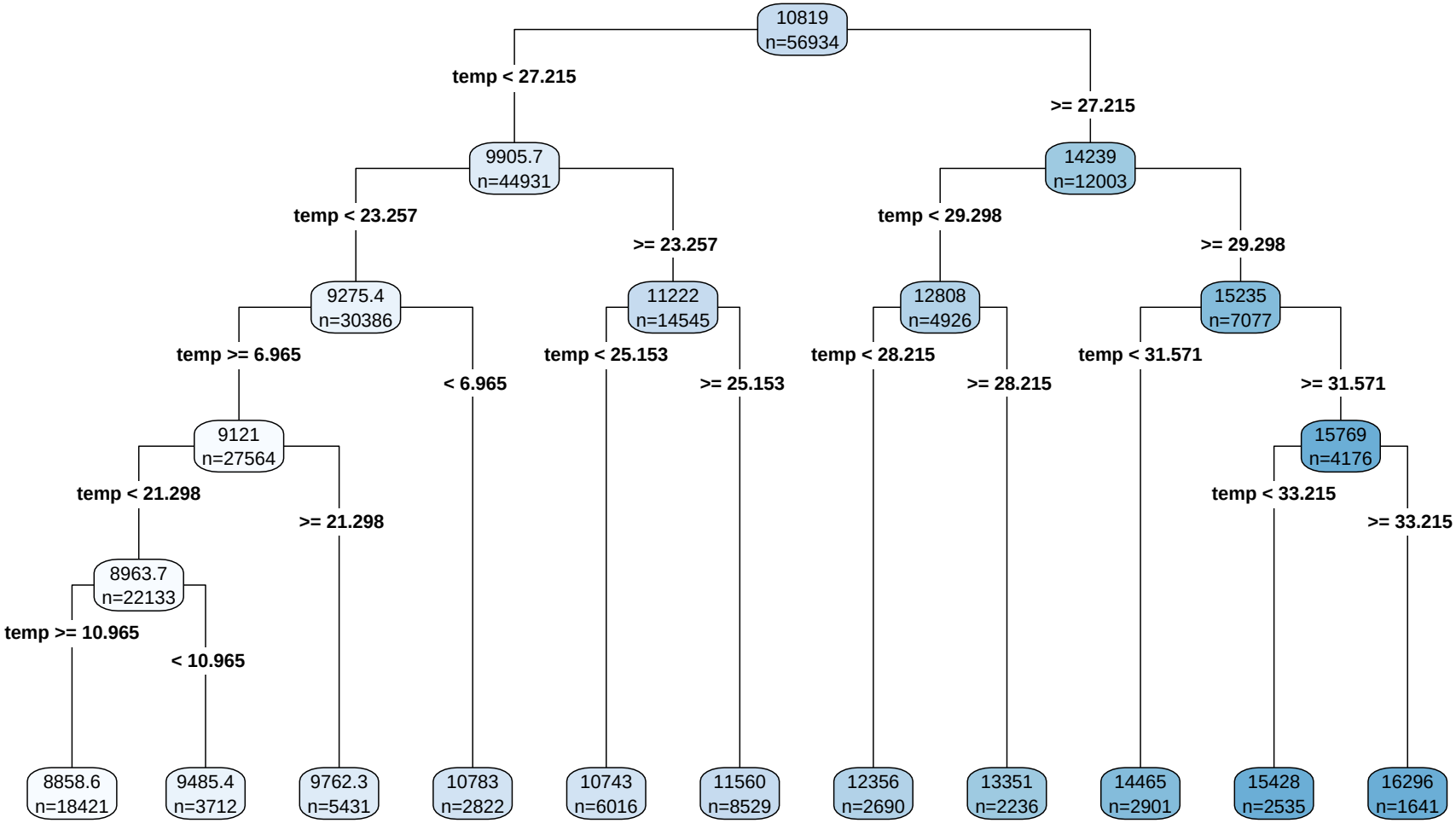
Goal: estimate $E(y \mid x)$

A regression tree



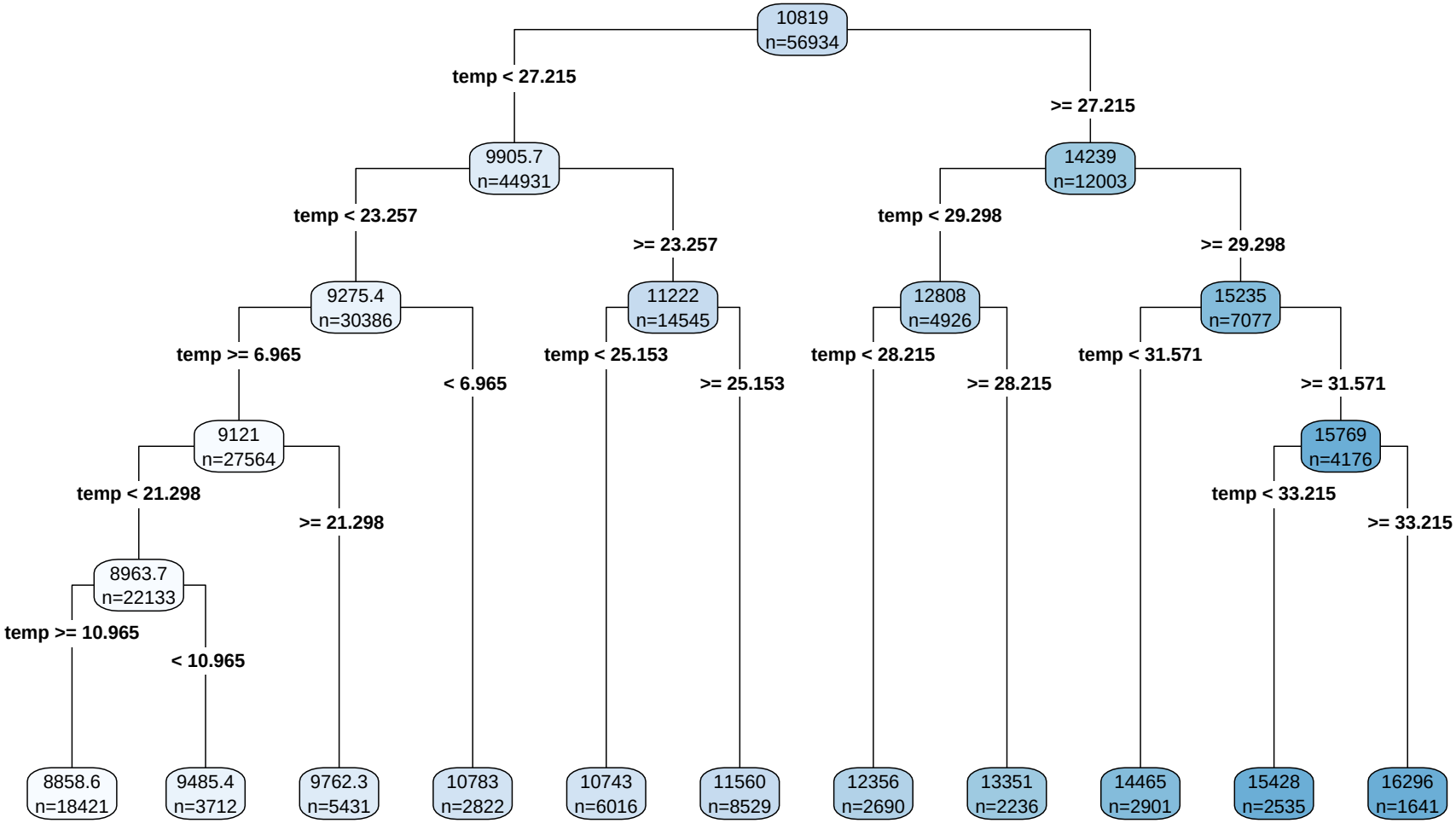
Now the leaf nodes show E(y | x), estimated by the average response (y) for the x's that "land" in that leaf.

A regression tree



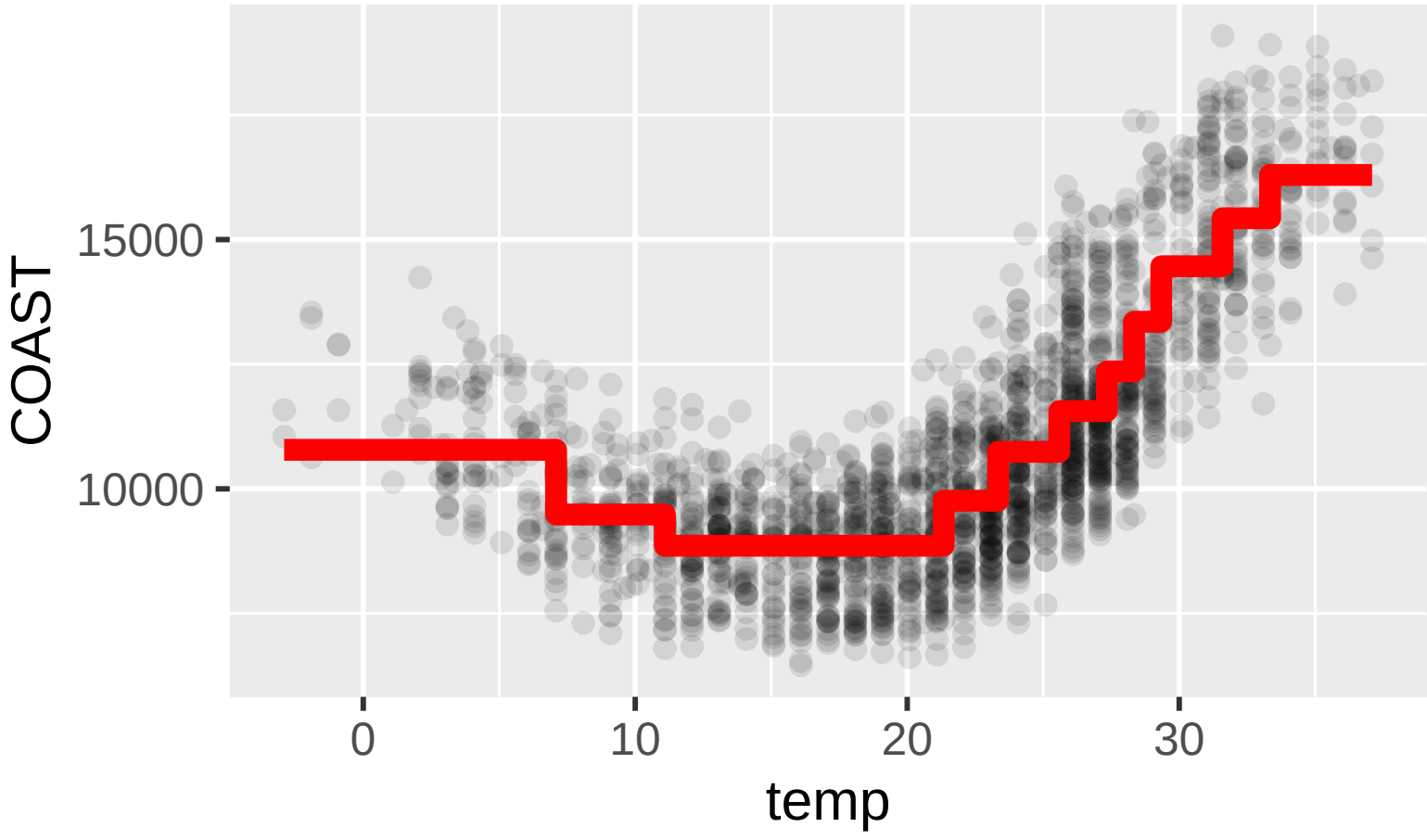
What does $f(x) = E(y \mid x)$ look like as a function of x?

A regression tree



Hint: the tree partitions the x space into disjoint regions. Within each region, E(y | x) is constant.

A regression tree



This is the fitted regression function $f(x) \approx E(y \mid x)$. It's a **step function** (always the case with tree models).

A regression tree (two x's)

What if we consider the same problem, but with an additional feature?

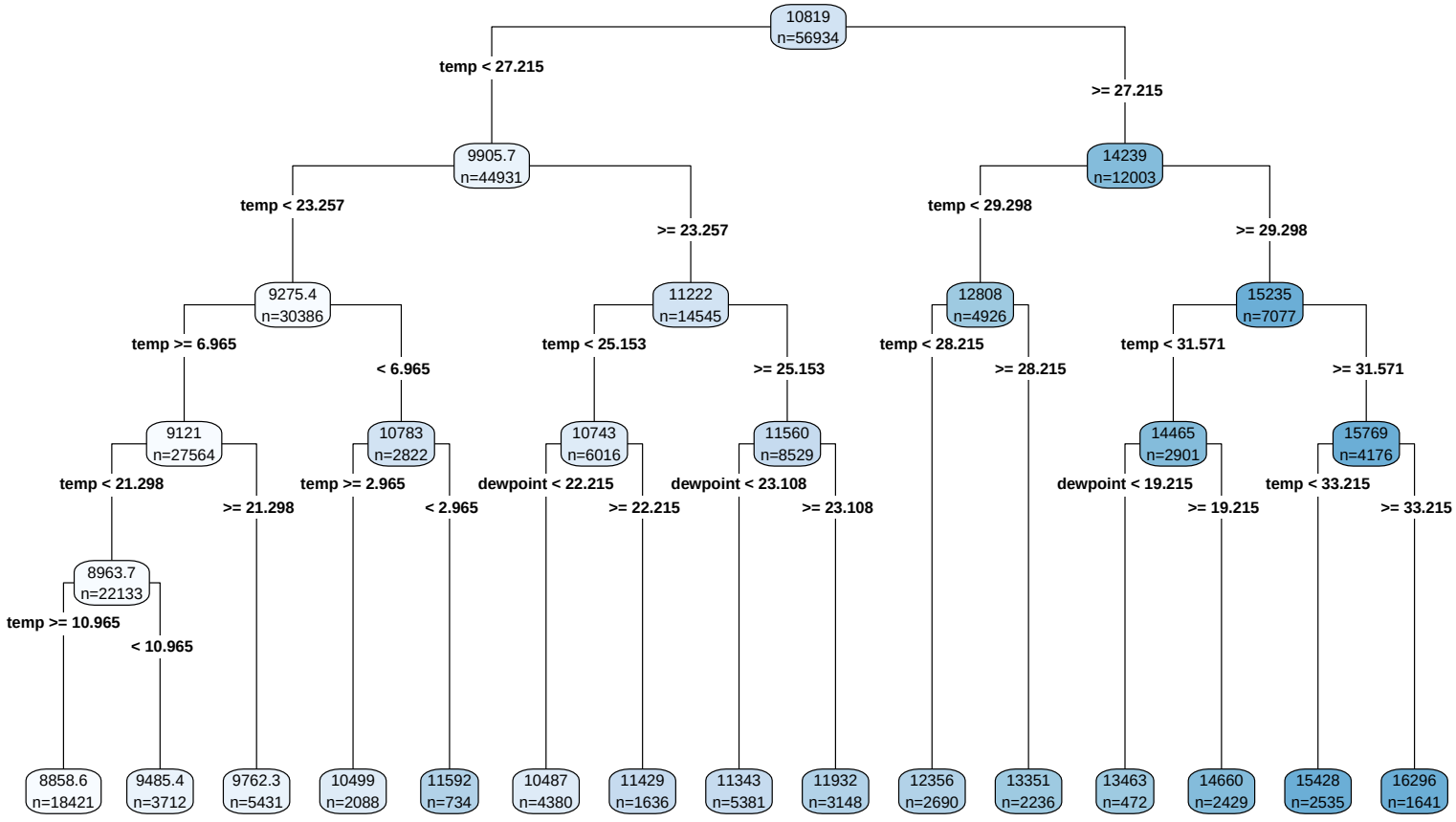
- x_1 = temperature at Houston's Hobby airport in degrees C
- x_2 = dewpoint at Houston's Hobby airport in degrees C
- y = peak power consumption in the ERCOT coast region

The linear model equivalent would look like

$$E(y \mid x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

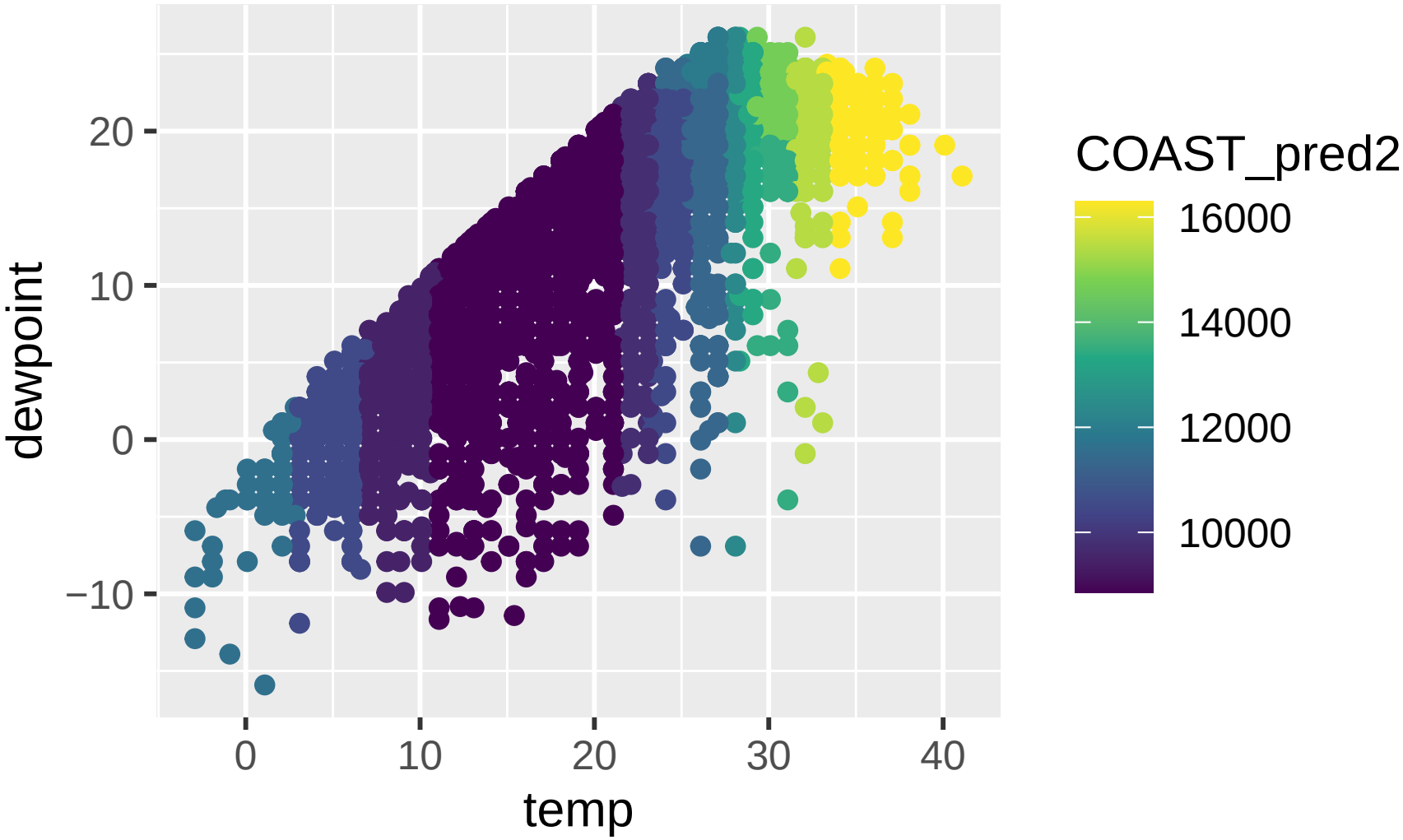
What does the tree look like?

A regression tree (two x's)



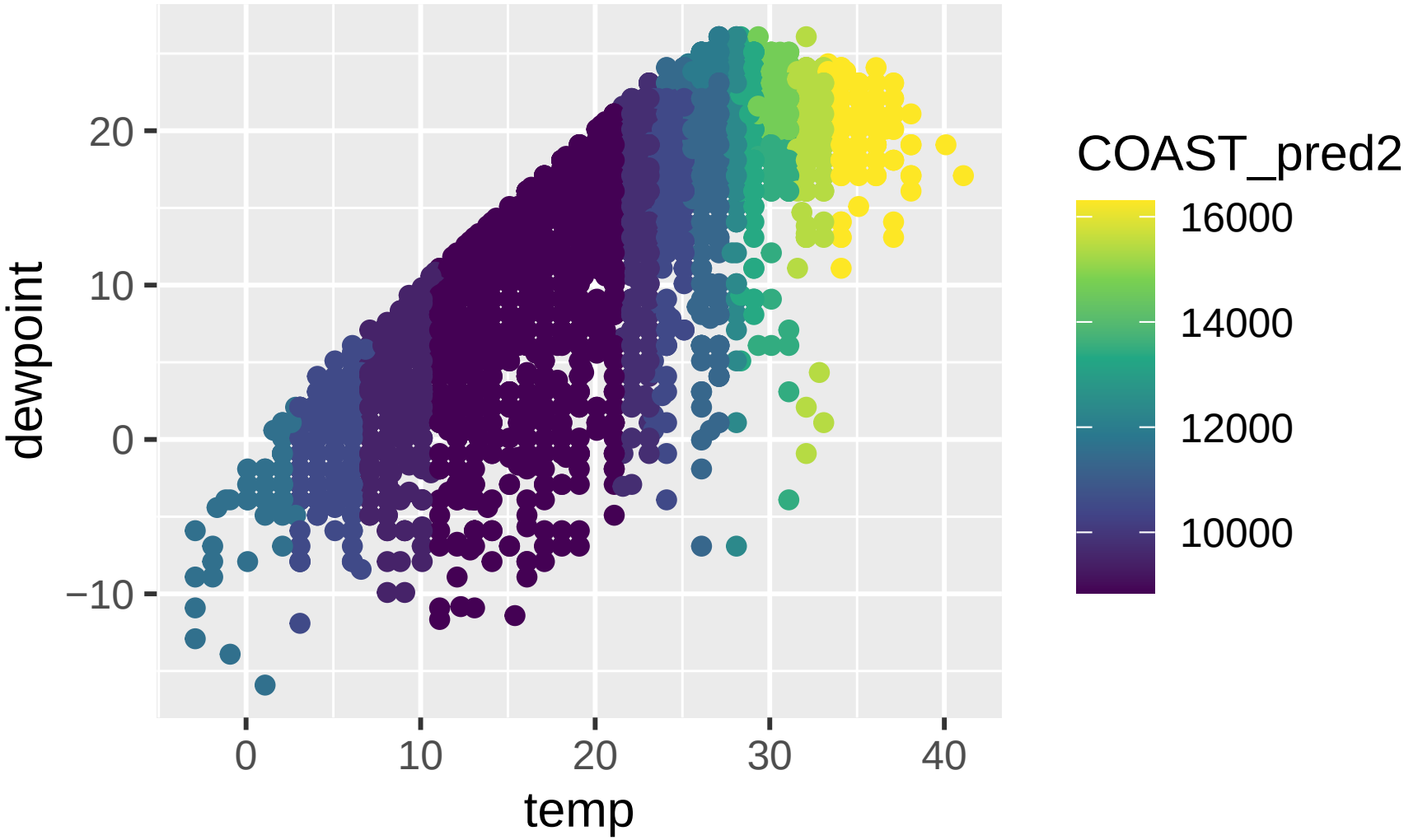
Now each mini-decision can split on temperature or dewpoint (but not both).

A regression tree (two x's)



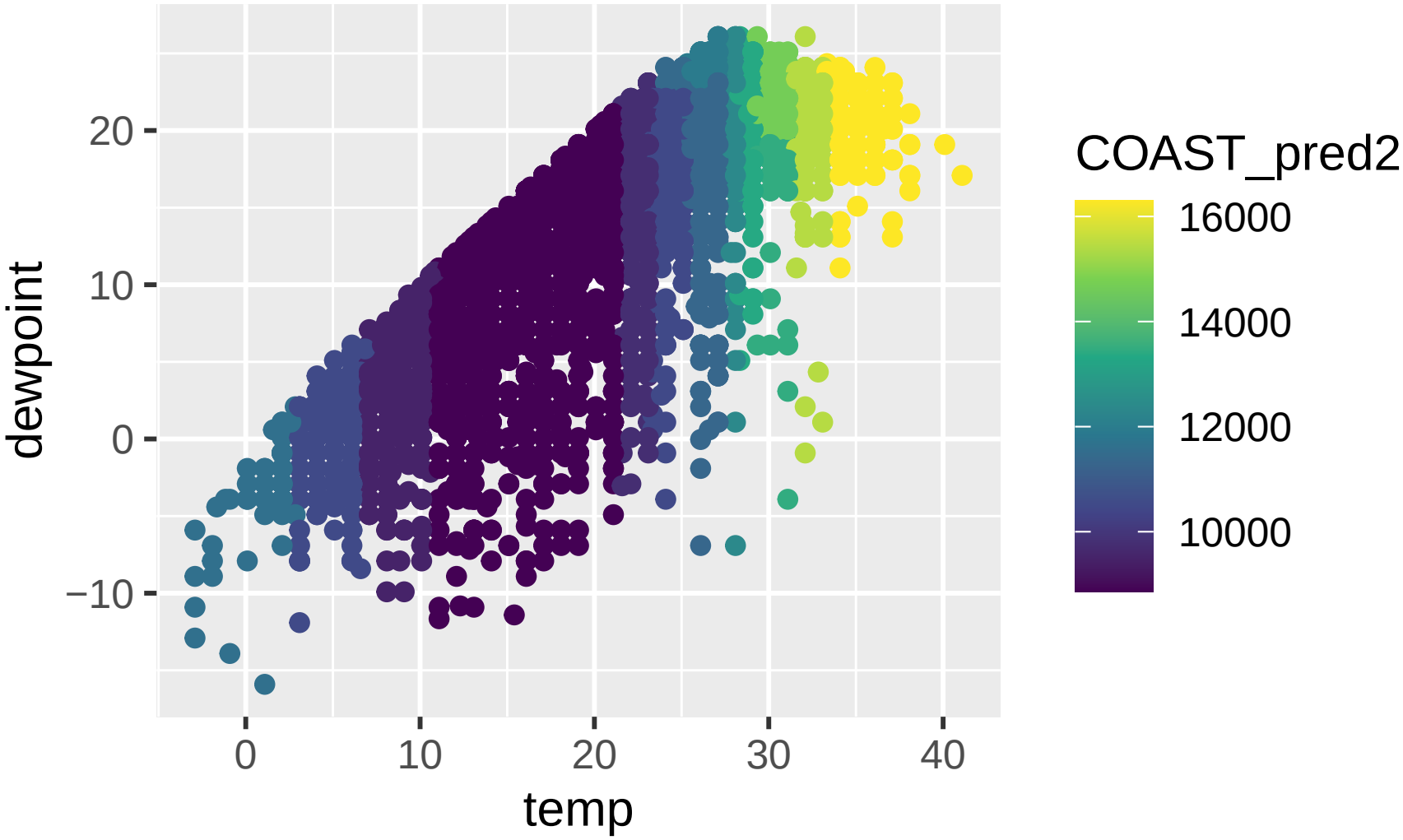
The tree partitions (x1, x2) space into rectangles. Within each rectangle, the fitted value E(y | x1, x2) is constant.

A regression tree (two x's)



The resulting fit is a step function in the 2D plane. The regions of constant color show the steps.

A regression tree (two x's)



Key point: **notice the interaction!** Do you see it?

Trees: interactions

Trees provide automatic interaction detection (AID). For example:

- Effect of age on survival different for male and female passengers.
- Effect of dewpoint on power consumption is different at low vs. high temperatures.

AID was an original motivation for building decision trees. (Older algorithms have it in their name: CHAID, US-AID, . . .)

This is pretty powerful technology:

- automatic adaptation to nonlinearity and interaction, without having to specify it in advance! (compare with `lm`. . .)
- Moreover, nonconstant variance is no problem.

Trees: a summary

- Trees use recursive binary splits to partition the feature space.
- Each binary split is a rule that sends x left or right.
- For numeric x, the decision rule is of the form if $x < c$.
- For categorical x, the rule lists the set of categories sent left.
- The set of bottom nodes (or leaves) give a partition of the x space.
- To predict, we drop x down the tree until it lands in a leaf node.
  - For numeric y, we predict using that leaf's average y value from the training data.
  - For categorical y, predict using that leaf's category proportions from the training data.

Tree models: pros and cons

Pros:

- Flexible fitters that can automatically detect nonlinearities and interactions.
- Invariant to transformations of the x variables.
- Handles categorical and numeric variables easily.
- Fast to fit.
- Interpretable (when small).

Tree models: pros and cons

Cons:

- Inherently non-smooth (step functions).
- Don't scale to very large feature sets.
  - Trees can bog down with hundreds or thousands of features.
  - But can often fix this with dimension-reduction techniques.
- Not the best at out-of-sample performance.
  - Generally must be deep to predict well (and thus less interpretable).
  - But still not bad at prediction!
  - And by *ensembling*, or averaging multiple trees, we can get excellent off-the-shelf predictions.

Fitting trees

As usual, we'll maximize data log-likelihood (minimize deviance)—here by fiddling with the tree's decision nodes.

- How many?
- What order?
- What feature and how to split that feature?

Two common loss functions:

- Regression deviance: $\sum_{i=1}^{n}(y_i - \hat{y}_i(x_i))^2$
- Classification deviance: $-\sum_{i=1}^{n} \log \hat{p}_{y_i}(x_i)$

Instead of being based on $x \cdot \beta$, predicted $\hat{y}$ and $\hat{p}$ are functions of x passed through the tree's decision nodes, just like we've seen.

Fitting trees

How do we do the minimization?

Now we have a problem.

- While trees are simple in some sense, once we view them as variables in an optimization, they are large and complex.
- A key to tree modeling is the success of the following algorithm for fitting trees to training data: **grow big, prune back.**
- This algorithm is *greedy* and *recursive*. Let's unpack those terms.

Grow big

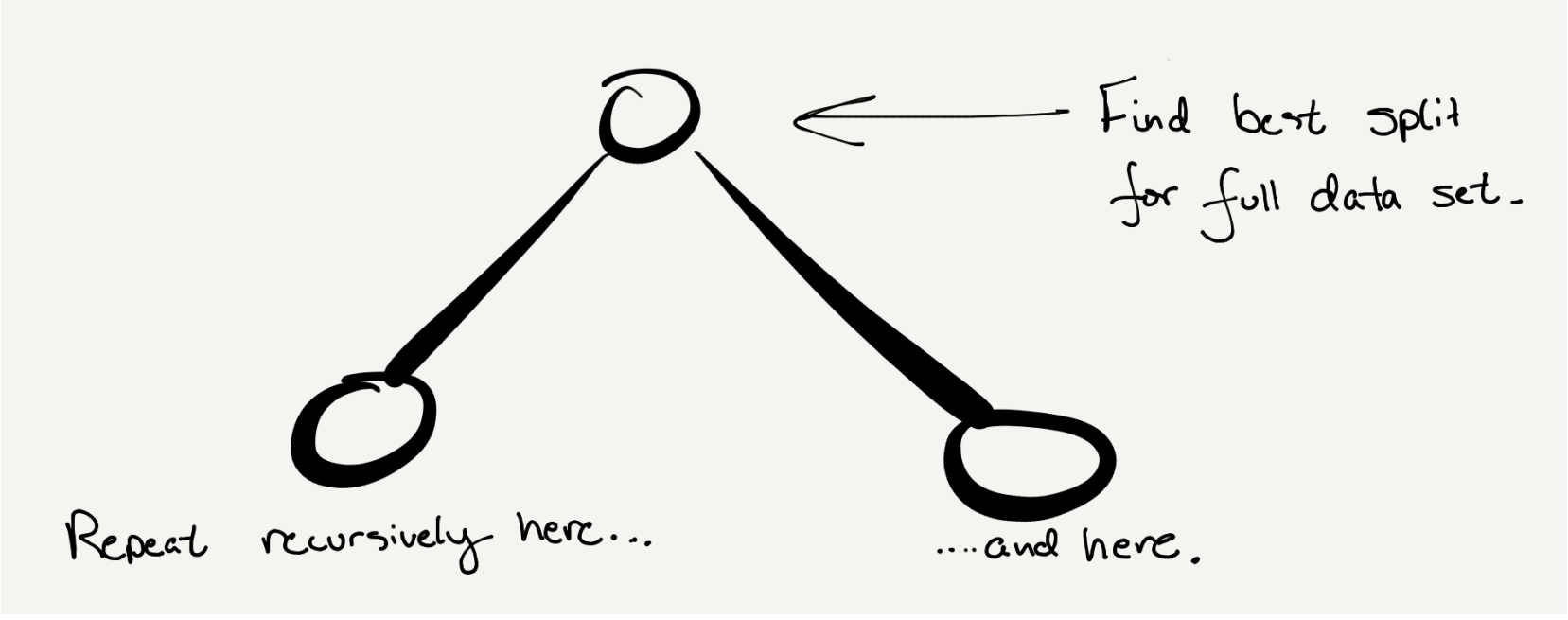
Use a greedy, recursive forward search to build a big tree, starting with all data in a single node (one leaf).

For each leaf node, *get greedy*:

1. Search over all possible splitting rules to find the single split that gives the biggest decrease in loss (increase in fit). This can be done very quickly.
2. Using this optimal rule, split this "parent" into two "children".

Then *repeat recursively*, treating each child as a new parent. You typically stop splitting and growing when the size of the leaf node hits some minimum threshold (e.g., 10 obs. per leaf).

Grow big



The key word is *recursive*—like how trees grow in the real world!

Prune back

Given a current tree with D leaf nodes:

1. Examine every pair of "sibling" leaf nodes (i.e. leaf nodes of the tree having the same parent) and check the increase in loss (decease in fit) from "pruning" that split.
2. Prune the "least useful" split, i.e. the prune that yields the smallest increase in loss (decrease in fit).

Repeat recursively on the newly pruned tree having D-1 leaf nodes. Stop when you've pruned all the way down to a single node.

Let's see this process on the board.

Prune back

Prune back

Why grow, then prune? To **generate a sequence of trees** of sizes $D, D-1, D-2, \ldots, 2, 1$, each tree locally optimal for its size.

A good analogy is the lasso solution path:

- The big trees fit best, but have lots of splits and fewer data points in each leaf node. (Lower bias, higher variance).
- The small trees fit less well, but are simpler and have more data points in each leaf node. (Higher bias, lower variance.)

Grow-then-prune yields candidate trees that (hopefully) span the bias-variance trade-off. We can then use cross-validation to choose.

CART

This basic fitting algorithm is called CART, for "classification and regression trees."

CART is also sometimes called "recursive partitioning" and this is reflected in the R syntax:

```
load.tree = rpart(COAST~temp + dewpoint, data=load,
                  control = rpart.control(cp = 0.002, minsplit=30))
```

`control` gives the "stopping points" for controlling tree growth. You'll often want to change these from their defaults. Here we split a node only if:

- it has at least 30 observations. . .
- AND if the split improves the deviance by a factor of 0.002 (0.2%).

CART

So to recap, CART:

- Grow the tree greedily and recursively to make deviance as small as possible.
- Stop growing when you hit your minimum size or complexity stopping points.
- Prune back from there to generate candidate trees.
- Choose by cross validation (min or 1SE).

Let's go see some examples in `tree_examples.R`.

CART: what we learned

From our examples, we learned a few things:

1. As tree complexity increases, CV error generally goes down quickly, levels off, and goes back up really s-l-o-w-l-y.
2. A sensible way to pick a tree is to use the "1SE rule":
   - Choose the smallest tree whose cross-validated error is within one standard error of the minimum.
   - This gives a simpler model whose performance is not discernibly different from the best performer.
3. Trees that perform well tend to be pretty deep. (This is often true even on simple problems—but still worth trying, you might be surprised.)

CART: what we learned

This last point—that good trees tend to be deep trees—is especially concerning.

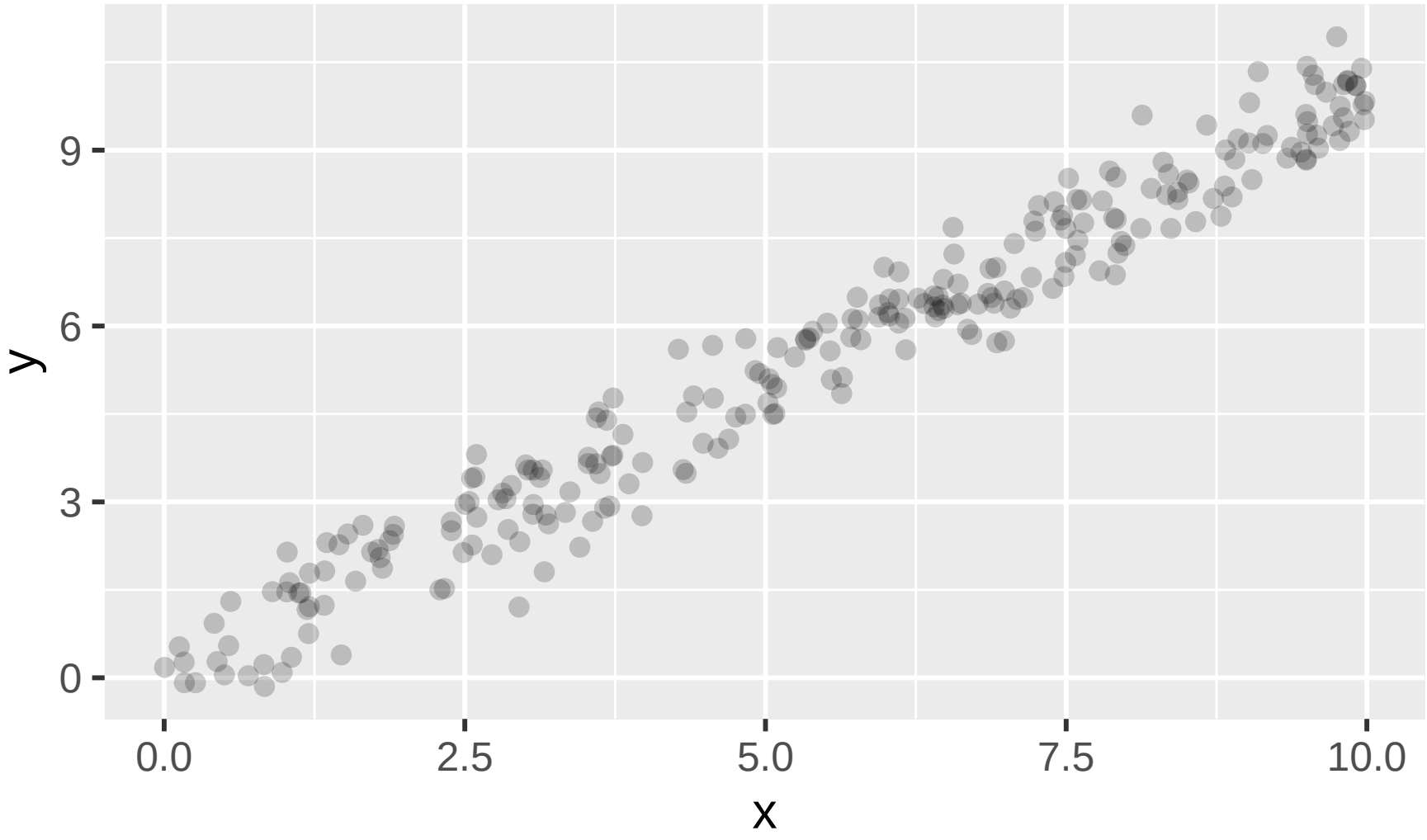
In deep trees, at least some (and perhaps most) of the leaf nodes have very few observations in them.

- This deep structure makes trees inherently prone to overfitting.
- They tend to find mini-decisions that memorize random noise, in addition to the underlying signal.

Deep trees also ruin interpretability:

- a small tree with a handful of mini-decisions can be interpreted by a person...
- but probably not hundreds or thousands of mini-decisions in a deep tree.

A toy example



True model: $y = x + e,\ e \sim N(0, 1))$

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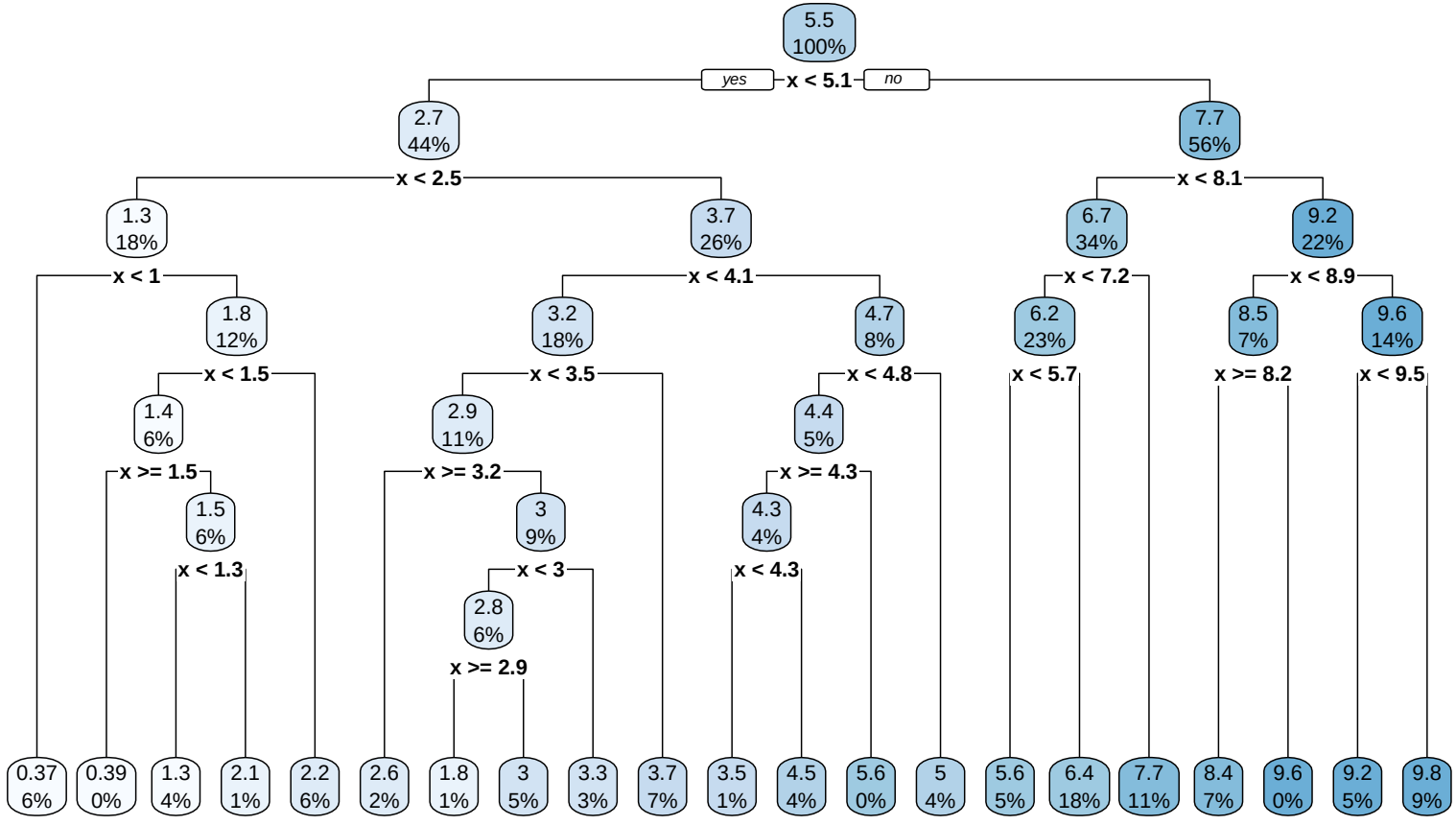

A single tree fit using the 1SE rule.

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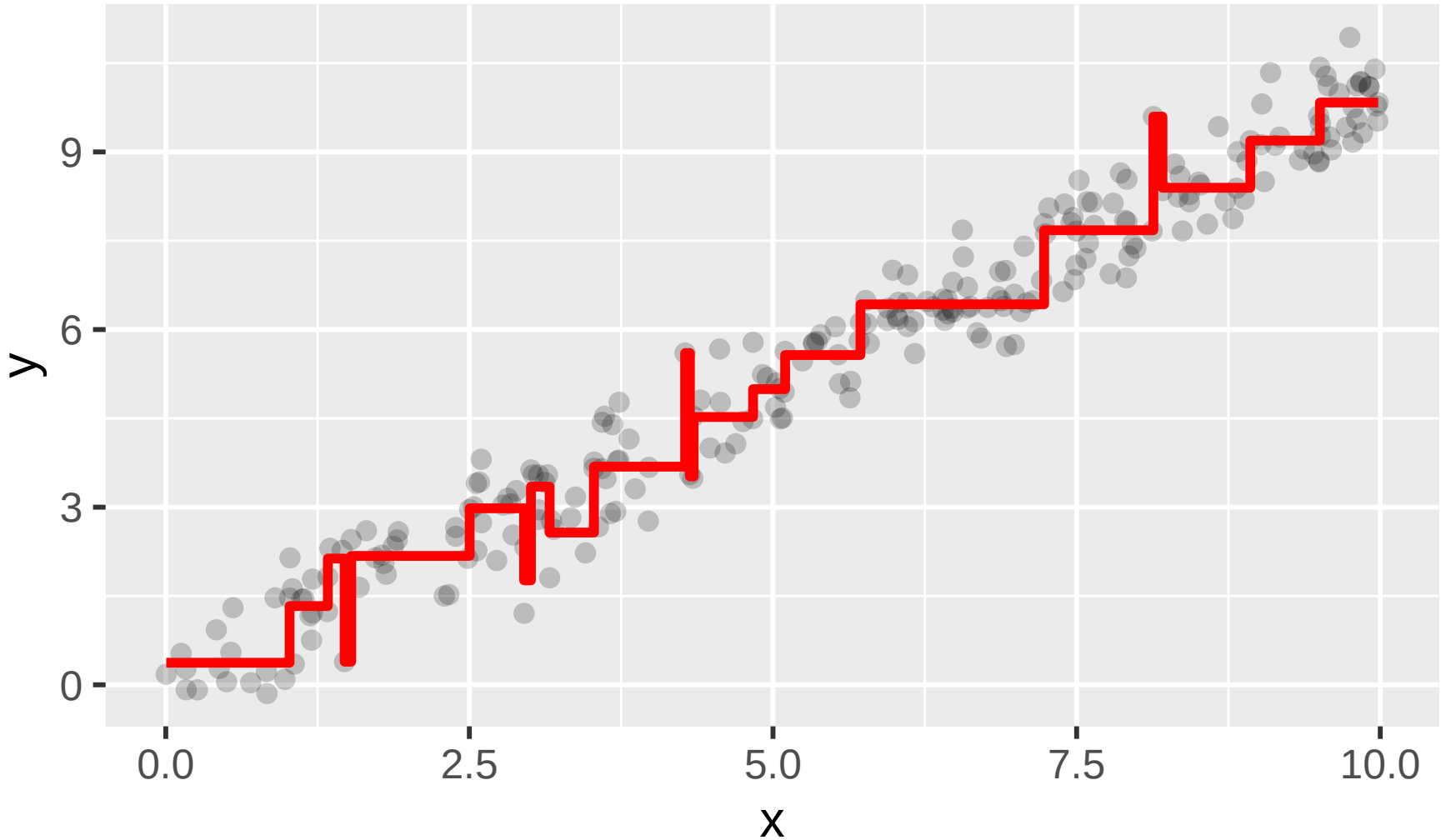

A single tree fit using the 1SE rule.

Bagging: bootstrap aggregating

Bagging—or Bootstrap Aggregating:

- involves averaging the predictions from multiple trees.
- is a way to *reduce estimation variance without adding bias*, thereby preventing trees from overfitting quite so badly.
- doesn't address interpretability (but hey, deep trees are hard to interpret anyway!)

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Let's see *how* bagging works, before we consider *why* it works:

- **Bootstrap**: resample the data with replacement B times, to get B "jittered" versions of your original data set (each size n).
- **Fit**: for each bootstrapped data set, fit a deep tree by CART.
- **Aggregate**: when you want to predict y for some x, average the predictions from this "forest" of B trees.

Why on earth would this work?

Remember our basic intuition for why averaging works in the most basic problem of all: estimating a mean.

$$y_i = \mu + e_i$$

- Think of μ as the signal and e_i as the noise.
- We take a bunch of IID samples y_i, $i = 1, \ldots, n$.
- We estimate μ as $\hat{\mu} = (1/n) \sum_i x_i$.
- When you take a bunch of samples and average them, the individual noise terms "wash out" in the averaging.
- But μ is there in each sample and doesn't wash out.

Why on earth would this work?

It's kind of the same in bagging, where we think $y_i = f(x) + e_i$:

- We take bootstrapped samples $b = 1, \ldots, B$ and build lots of big trees to give an estimate $\hat{f}^{(b)}(x)$.
- We estimate $f(x)$ as the average

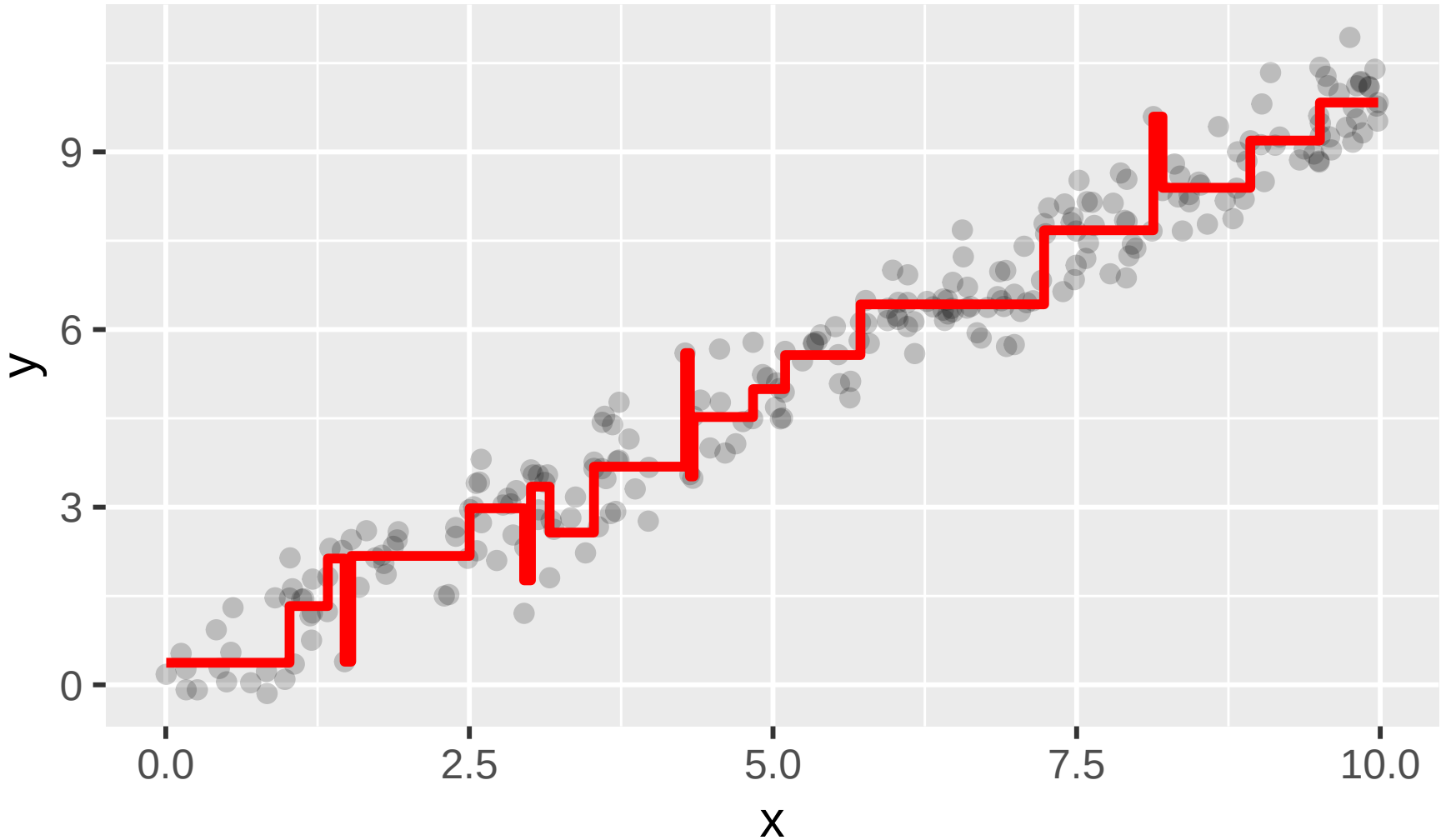
$$f(x) = \frac{1}{B} \sum_b \hat{f}^{(b)}(x)$$

- Wiggles in $f(x)$ that are real captured in most or all of the bootstrapped estimates.
- Wiggles that are over-fit to a few data points, "by chance," are idiosyncratic to only a few estimates, and get "washed out" in the averaging.[1]

Leo Breiman. **Brilliant.**

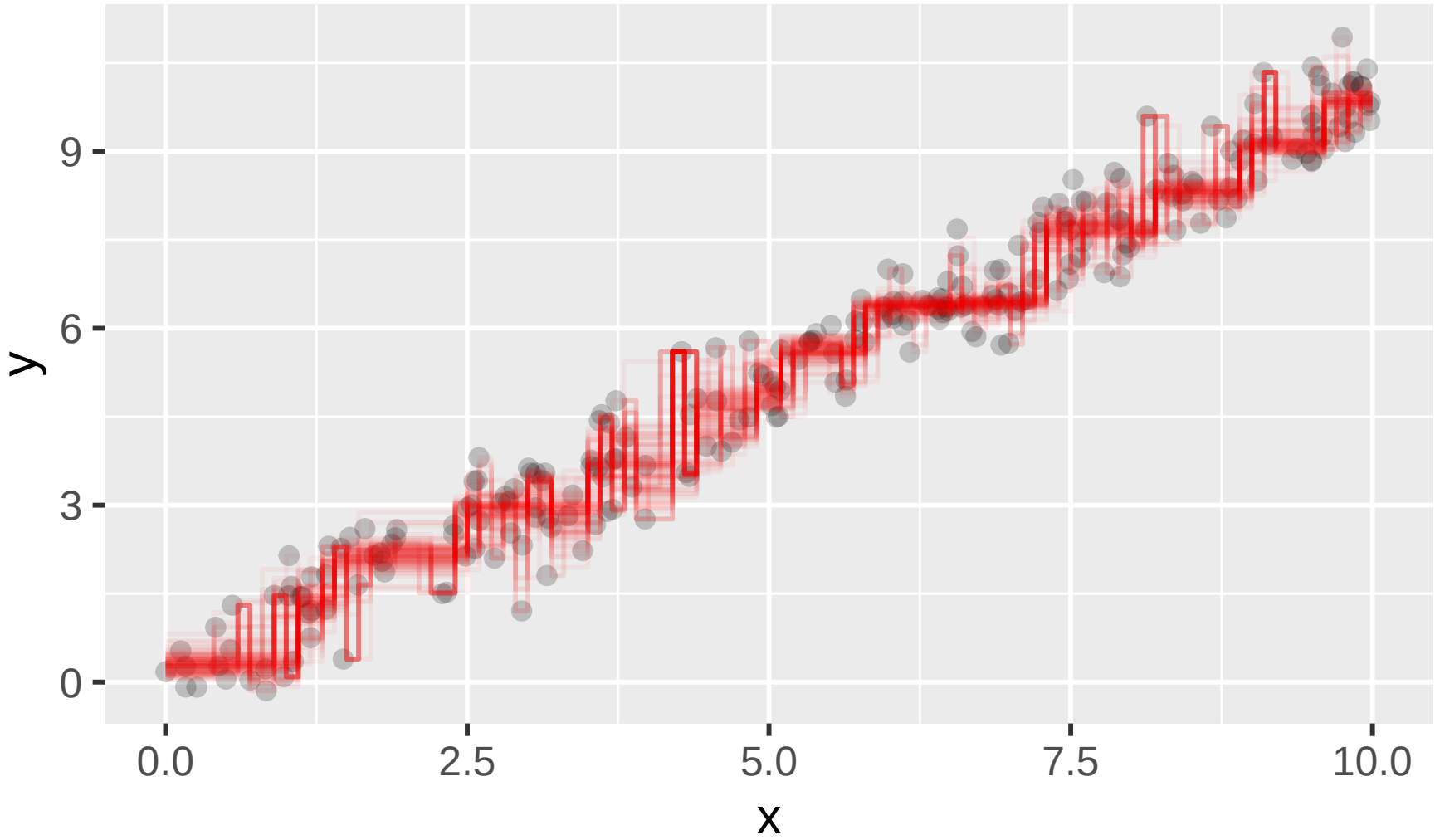
[1] The math is a bit more complicated than on the previous slide, because the bootstrapped estimates are correlated with each other. But they're not perfectly correlated, which is the source of variance reduction.

Let's see it work.



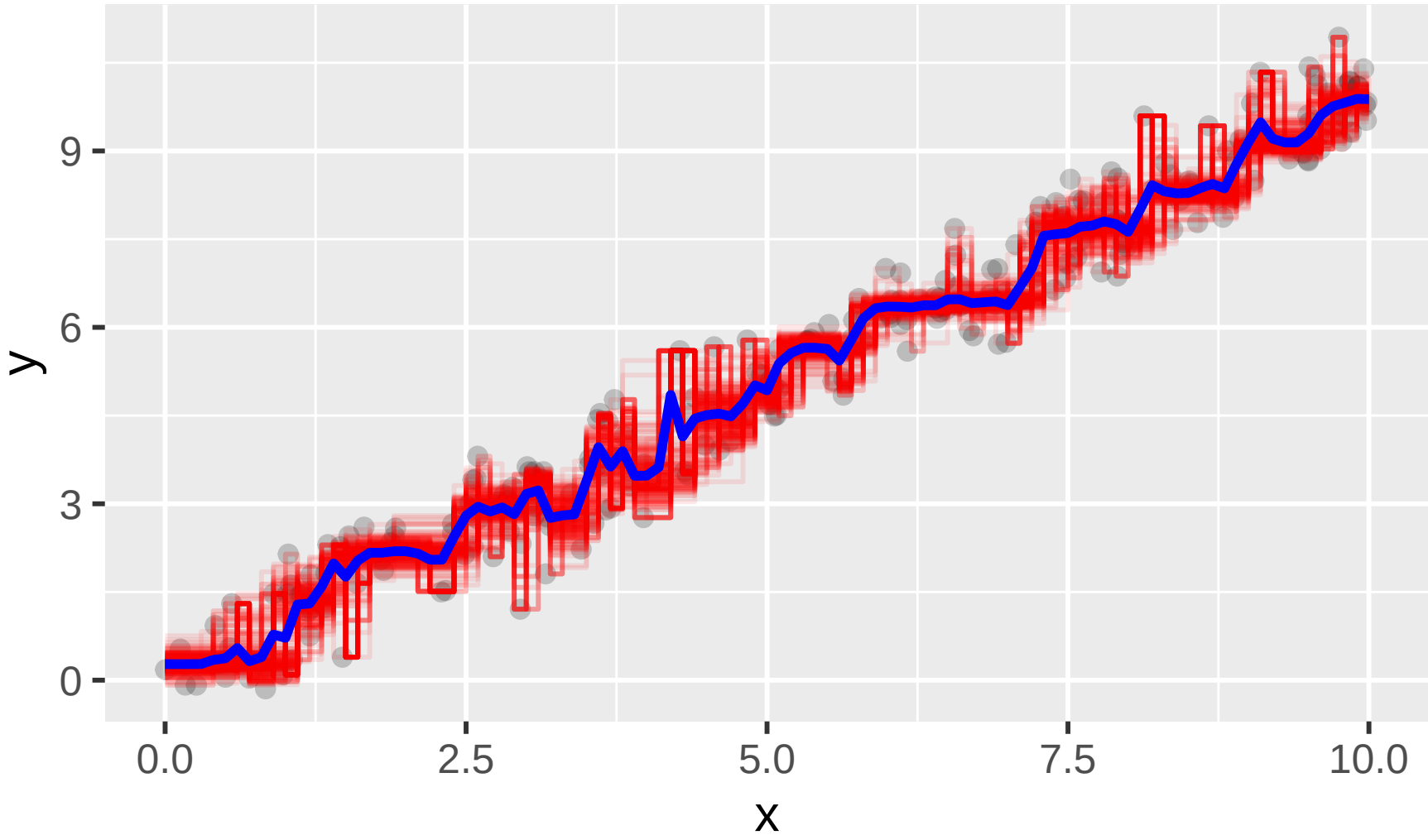
Original fit.

Let's see it work.



Fits from 100 bootstrapped samples.

Let's see it work.



Average of fits from 100 bootstrapped samples. OK, still overfit, but not nearly so badly!

Bagging: a summary

Fit trees to B bootstrapped samples of the original data.

- For numerical y, average the predictions.
- For categorical y, let each tree vote, or average the trees' predicted class probabilities.

You need B large enough to enjoy the effect of averaging.

- 100 is a decent starting point, 500 is better if your machine has the flops and memory.
- It doesn't seem to hurt if you make B even larger.
- The only real cost of a large B is computational time.

Bagging: a summary

Bagging "works" because it usually gives you a smoother (lower-variance) fit than a single tree. This is quite a general phenomenon:

- we can often improve a high-variance nonparametric regression model by bagging it. This is the simplest form of "ensembling" or "model averaging"—a super useful, very general idea.
- the corrollary is that a stable, low-variance estimator (e.g. a linear model) usually won't be improved by bagging.
- trees are ideal candidates for bagging because they're high-variance, flexible fitters than are also quite fast to fit.

The downside:

- when we bag a model, any simple structure is lost.
- this is because a bagged tree is no longer a tree, but a forest!

Random forests

A "random forest" starts from bagging...

- We still take B bootstrapped samples of the original data and fit a tree to each one.
- We still average the predictions of the B different trees.

But it adds **more randomness.** Within each bootstrapped sample:

- We don't search over **all** the features in x when we do our greedy build of a big tree.
- Instead, we randomly choose a subset of $m < p$ features to use in building that tree.

Why would using fewer features in each tree actually help!?

- it simplifies each tree, reducing its variance
- it diversifies the B trees, decorrelating their predictions

Random forests

A maybe-useful analogy: evolutionary co-adaptation.

- Co-adaptation occurs when two or more traits/genes/organisms undergo mutual adaptation together as a group. Classic example: flowering plants and pollinating insects.
- But if the environmental conditions change, heavily co-adapted organisms can suffer. They're "overfit" to conditions that no longer exist.

Random forests

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A common way that trees overfit is by learning heavily "co-adapted" sets of features, i.e. deep interactions that explain noise.

- Example: "No Democratic presidential incumbent without military service has ever beaten a challenger whose last name is worth more in Scrabble."
- By forcing each tree to rely on only a few features, we prevent its features from "co-adapting" with each other in brittle, non-generalizable ways.

Random forests

In random forests, you must choose:

- B: number of bootstrapped samples. Use hundreds, or thousands if possible!
- m: number of features to sample within each bootstrapped sample. A common choice is $m \approx \sqrt{p}$.

Some notes:

- bagging is just random forests with $m = p$, but you'll typically see better performance with $m < p$.
- there is no explicit regularization parameter, as in the lasso and single-tree models.
- random forests might be the most popular "off the shelf" nonparametric regression technique. They're effective, fast, and require little or no tuning via CV (default settings do well).

"Out-of-bag" error estimation

With random forests, there's a nice built-in way to estimate the generalization error of the model.

- In each bootstrap sample ("bag"), some of your original observations are "in the bag" (math says: about $1 - 1/e \approx 2/3$, on average).
- The rest are "out of bag."

By carefully keeping track of which trees use which observations, you can get "out-of-bag" predictions.

- This is a decent way to estimate out-of-sample performance.
- We typically use this to reassure ourselves we've used enough trees in the forest.

Random forests: example

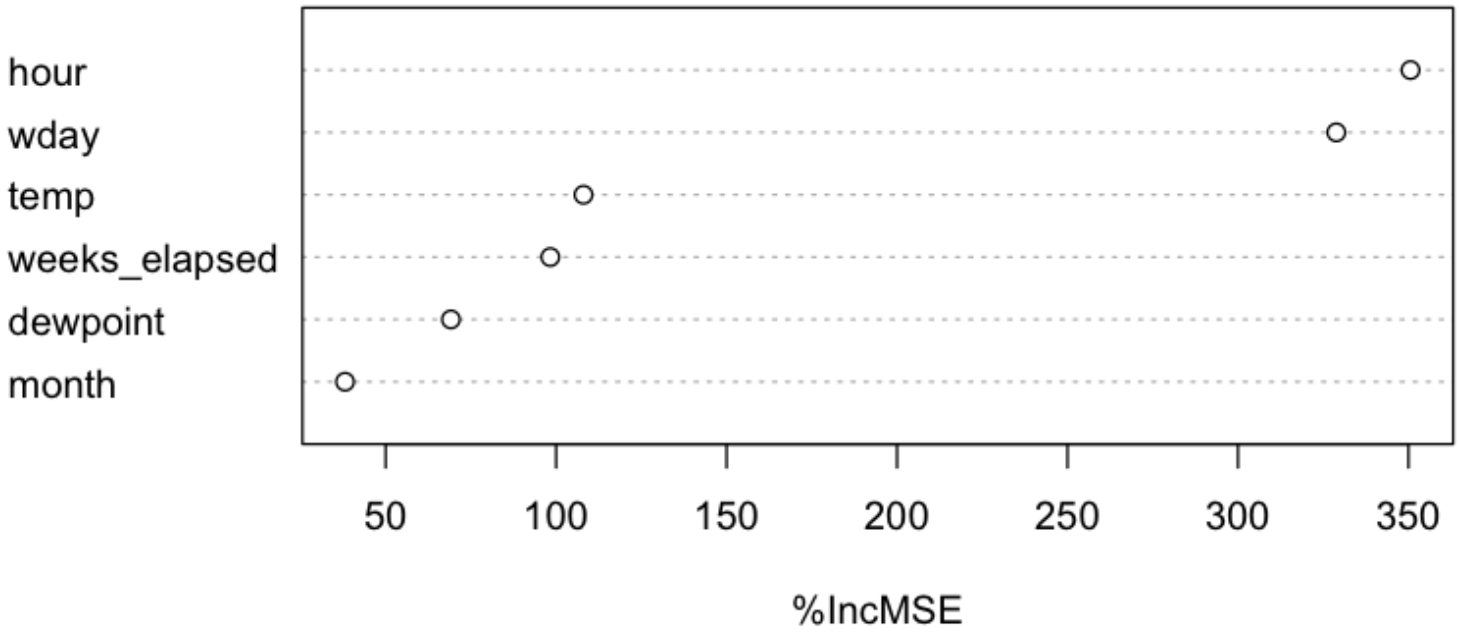
Let's go to `random_forest_example.R`.

Then we'll come back to discuss a couple of follow-up topics:

- variable importance plots
- partial dependence functions

Variable importance plots

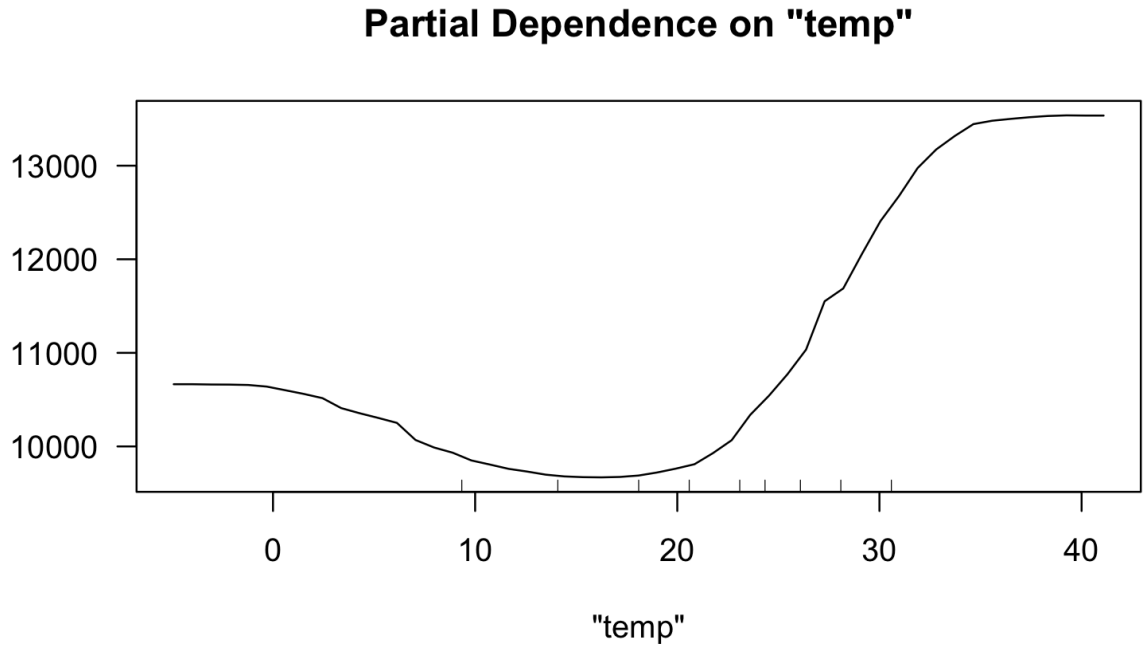
We've seen on our example how random forests can give us a variable importance measure, like this:



This is calculated by procedure similar to a permutation test: we compare out-of-bag performance of the model, versus the same model with a "shuffled" version of the predictor.

Partial dependence functions

Our RF model also gave us a "partial dependence plot":



This shows the relationship between power load and temperature, taking account of the joint effect of other features.

It seems to make sense, but it's a bit mysterious at first how R computes this. **What, exactly, is this thing?**

Partial dependence functions

The partial dependence (PD) function attempts to represent the marginal effect that one (or maybe two) features have on the predicted outcome of a model.

- A PD function can be defined for any model, not just random forests. It is chiefly a tool for visualizing and understanding a model, rather than direct prediction.
- A PD function is focused on a specific variable x_j, or maybe two variables. (More than 2 gets unwieldy.)
- Plotting the PD function can show whether the relationship between the target y and feature x_j is linear, monotonic, or more complex.

Partial dependence functions

Suppose that x_S is a "subset of interest" of your model's features, and that x_C is all the other features in the model.

- Usually, there are only one or two features in the set S.
- The feature(s) in S are those whose effect on the prediction $\hat{y} = \hat{f}(x)$ we wish to understand.
- Together, x_S and x_C contain all the features: $f(x) = f(x_S, x_C)$.

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The partial dependence function is defined pointwise over x_S by marginalizing out the features in x_C:

$$r_S(x_S) = E_{x_C}(f(x_S, x_C)) \approx \frac{1}{N} \sum_{i=1}^{N} f\left(x_S, x_C^{(i)}\right)$$

This expected value is taken under the true probability distribution that generated features x_C.

Partial dependence functions

Let's unpack that formula a bit:

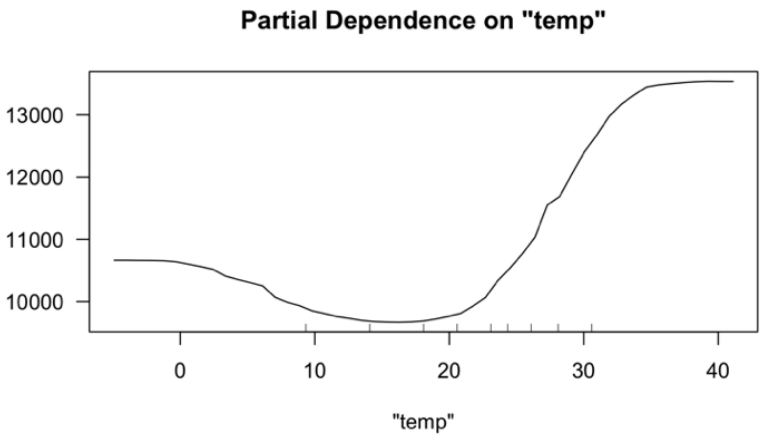
$$r_S(x_S) = E_{x_C}(f(x_S, x_C)) \approx \frac{1}{N}\sum_{i=1}^{N} f\left(x_S, x_C^{(i)}\right)$$

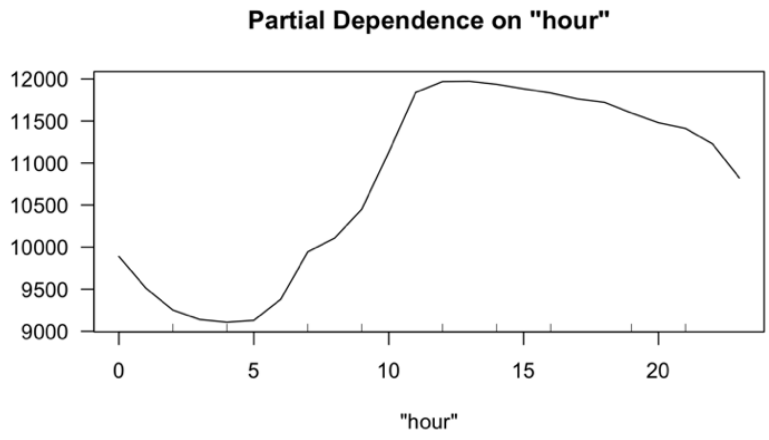
In words, to estimate the PD function, you:

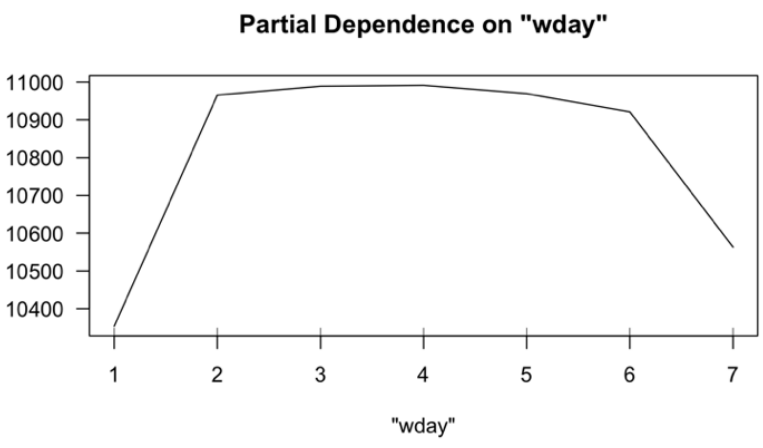
- pick a target value of x_S where you want to evaluate $r_S(x_S)$
- evaluate $f\left(x_S, x_C^{(i)}\right)$ at all points $x_C^{(i)}$ in your training set.
- average these function evaluations
- Keep repeating for across a grid of target values of x_S, and you build up the PD function one point $(x_S, r_S(x_S))$ at a time.

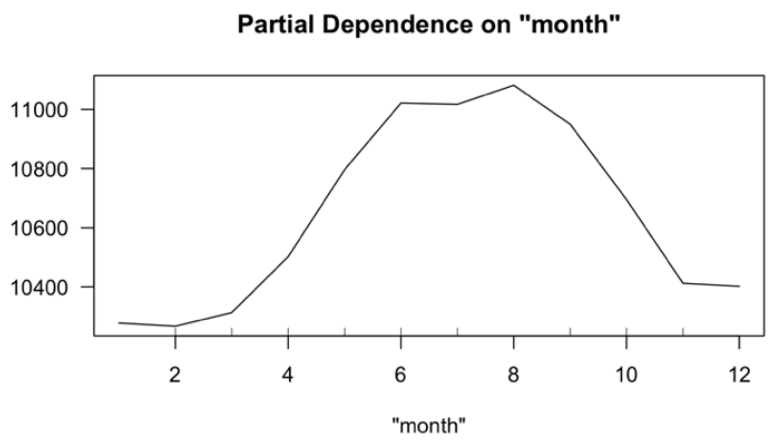
The partial dependence function at a particular feature value x_S represents **the average prediction if we force all data points to assume that feature value.**

Partial dependence functions









Partial dependence functions: disadvantages

Realistic max number of features in a PD function is two; hard to overcome, it's just a limitation of our screens and brains.

PD functions are easy to over-interpret in regions of x_S space with little data.

- But this problem is mitigated by showing the distribution of the x_S points in the training data.
- Example: a rug on the x axis, or histogram.

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PD functions **implicitly assume independence of x_S and x_C.** Remember, the PD at x_S is the average prediction if we force all data points to assume that feature value.

- E.g. suppose we calculate r_S at `temp=5` (41 degrees F).
- So we fixing `temp=5` and average across the other features.
- But this average includes points where `temp=5`, `month=August` (umm, not in Houston!)

Partial dependence functions: disadvantages

The assumption of independence is by far the biggest downside to PD functions: when the features are correlated, we hallucinate new data points in areas of the feature distribution with low probability:

- `temp=5, month=August` for Houston weather
- `height=200cm, weight=50kg` for an adult human.
- etc.

There's a cottage industry in machine learning of proposing alternatives to PD plots. E.g.

- Individual Conditional Expectation, or ICE, plots.
- Accumulated Local Effect, or ALE, plots.

This topic broadly falls under the area of interpretable machine learning. Lots of papers and R packages (e.g. `ICEbox`) if you're interested!

Boosting

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Like Random Forests, boosting is an ensemble method in that the overall fit is produced from many trees.

The idea however, is totally different. In Boosting we:

- Fit the data with a single tree.
- Crush the fit so that it does not work very well. (Huh?!)
- Look at the part of y not captured by the crushed tree and fit a new tree to what is "left over."
- Crush the new tree. Your new fit is the sum of the two trees.
- Repeat the above steps iteratively. At each iteration you fit "what is left over" with a tree, crush the tree, and then add the new crushed tree into the fit.
- Your final fit is the sum of many trees.

Boosting

Unlike many ideas, this one is actually much clearer when you write it out as an algorithm. This assumes a numeric y:

1. Set $\hat{f}^{(0)}(x) = 0$ and set $r_i = y_i$ for every training-data point.
2. For $b = 1, 2, \ldots, B$, repeat:
   - Fit a tree $\hat{g}^{(b)}$ with D splits to the training-data pairs (x_i, r_i).
   - Update $\hat{f}^{(b)}$ as

$$\hat{f}^{(b)} \longleftarrow \hat{f}^{(b-1)} + \lambda \hat{g}^{(b)}(x) \quad \text{where} \quad \lambda \in (0, 1)$$

   - Update r_i as

$$r_i \longleftarrow r_i - \lambda \hat{g}^{(b)}(x_i)$$

3. Output the final boosted model as

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{g}^{(b)}(x)$$

Boosting

What's going on here? Let's examine the core loop.

For $b = 1, 2, \ldots, B$, repeat:

- Fit a tree $\hat{g}^{(b)}$ with D splits to the training-data pairs (x_i, r_i). This fits a "simple" tree to the current working residuals r_i, i.e. what the current working model cannot explain.

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- Update the working residuals:

$$r_i \longleftarrow r_i - \lambda \hat{g}^{(b)}(x_i)$$

Boosting

Boosting represents $f(x)$ as the sum of many "weak learners." In this respect, it's like two techniques we've already met:

- Linear regression: sum of weighted features.

$$\hat{f}(x) = \sum_{j=1}^{P} \beta_j x_j$$

- Random forests: sum of simple bootstrapped tree fits

$$\hat{f}(x) = \sum_{b=1}^{B} \frac{1}{B} \hat{f}^{(b)}(x)$$

- Boosting: sum of "shrunken" tree fits to partial residuals

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{g}^{(b)}(x)$$

Boosting

Boosting has three main tuning parameters:

- B, the number of boosting steps.
- D, the depth of each tree.
- λ, the "shrinkage" or "crush" factor. Typically small, e.g. 0.05.

Boosting can work great, but it tends to be pretty sensitive to these tuning parameters.

- Because each tree is "guided" by knowledge of what the prior trees missed, you'd expect boosting to do a little better than random forests.
- And indeed, it is often possible outperform random forests with careful tuning.
- But boosting is more brittle! Random forests work pretty well on most problems "out of the box," with no tuning.

Boosting

Let's see an example in `capmetro.R`.

Boosting for categorical y

Boosting for categorical y works in an analogous manner, but it is messier how you define "the part left over" at each stage. You can't just use residuals. Also you can't just add up the fit.

But it is the same idea:

- fit what is left over
- crush fit
- repeat many times
- aggregate crushed fits at the end

Round-up

We've seen three techniques for building tree models.

- CART: recursive partitions, pruned back, tree chosen by CV.
- randomForest: average many simple CART trees. Pretty robust, basically eliminates need for CV.
- Boosted Trees: repeatedly fit simple trees to residuals. Fast, but it is tough to avoid over-fitting (requires full CV). "Should" work better than random forests, but it's more sensitive to tuning parameters.

There are many other tree-based algorithms. For example:

- Bayesian Additive Regression Trees: mix many simple trees. Robust prediction, comes with Bayesian error bars, but suffers with non-constant variance.

Trees are poor in high dimension, but fitting them to low dimensional summaries (e.g. principal components) is a good option.

Round-up

There are also many other nonparametric learning algorithms.

- Neural Networks (and deep learning): many recursive logistic regressions.
- Support Vector Machines: move from Low-D to High-D, then classify.
- Gaussian Processes, splines, wavelets, etc: use sums of curvy "basis" functions in regression.

Some of these are great, but all take a ton of tuning.

- **Nothing's better out-of-the-box than trees**, at least with modest-dimensional feature.
- But: when the (simpler) linear model fits, it will do better. This is often the case in very high dimensions.