Nonlinear Models

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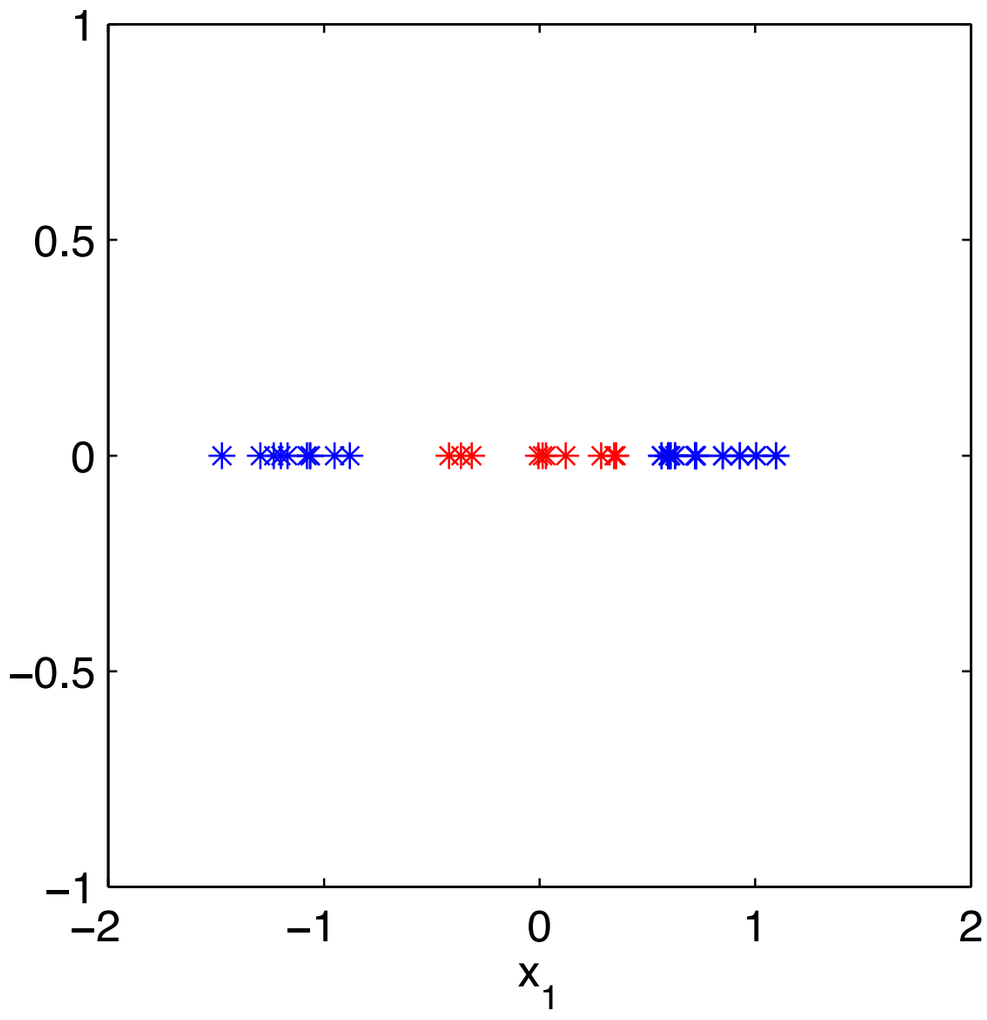
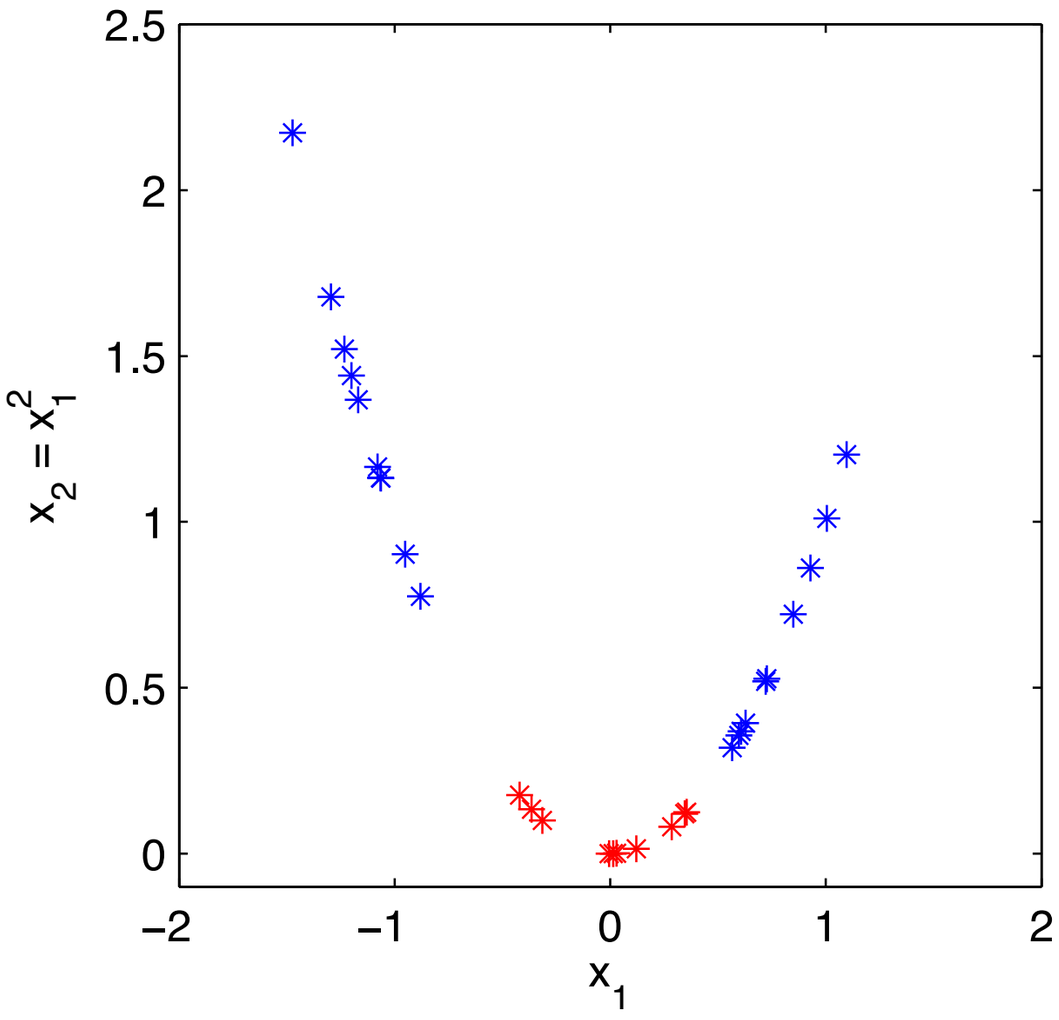
Nonlinearly separable data

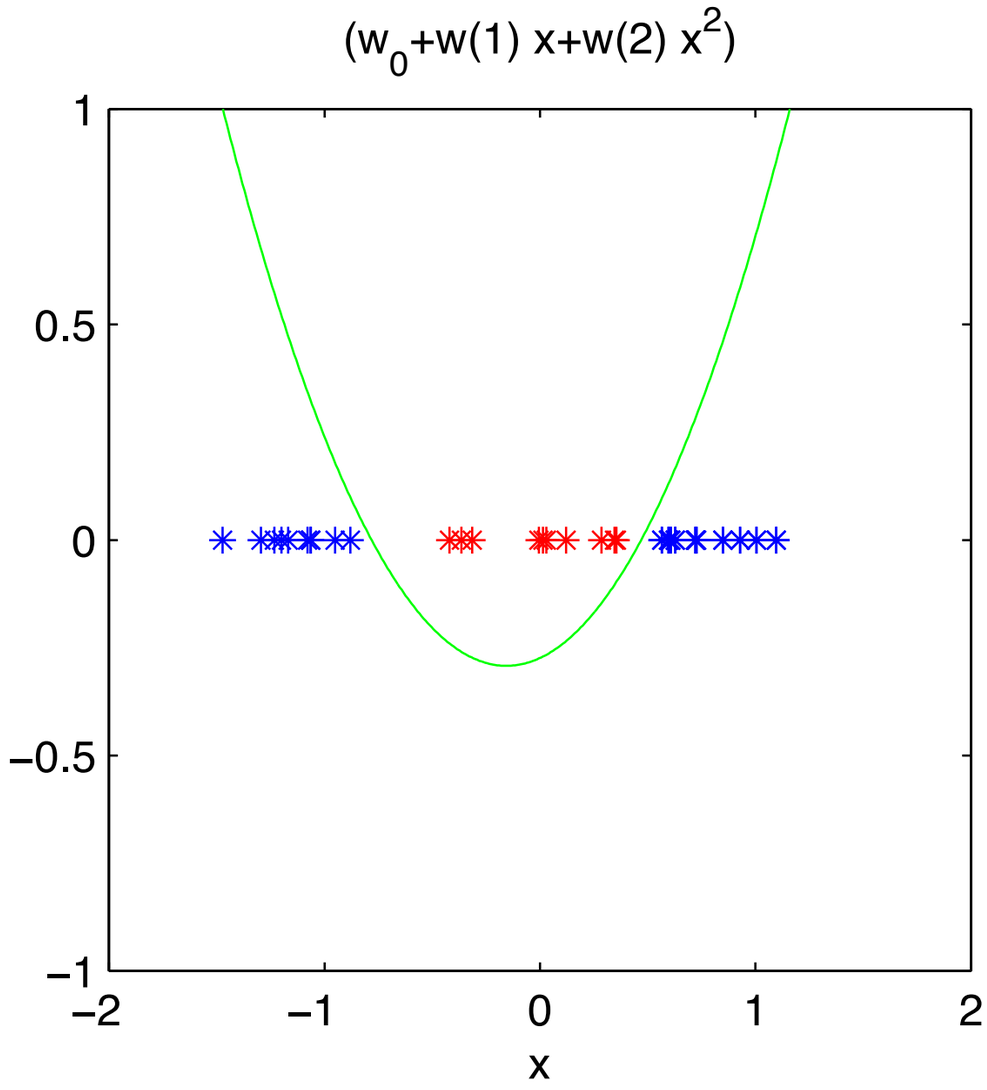
- A linear boundary might be too simple to capture the class structure.
- One way of getting a nonlinear decision boundary in the input space is to find a linear decision boundary in an expanded space (e.g., for polynomial regression.)
- Thus, $\mathbf{x}_i$ is replaced by $\phi(\mathbf{x}_i)$, where ϕ is called a *feature mapping*

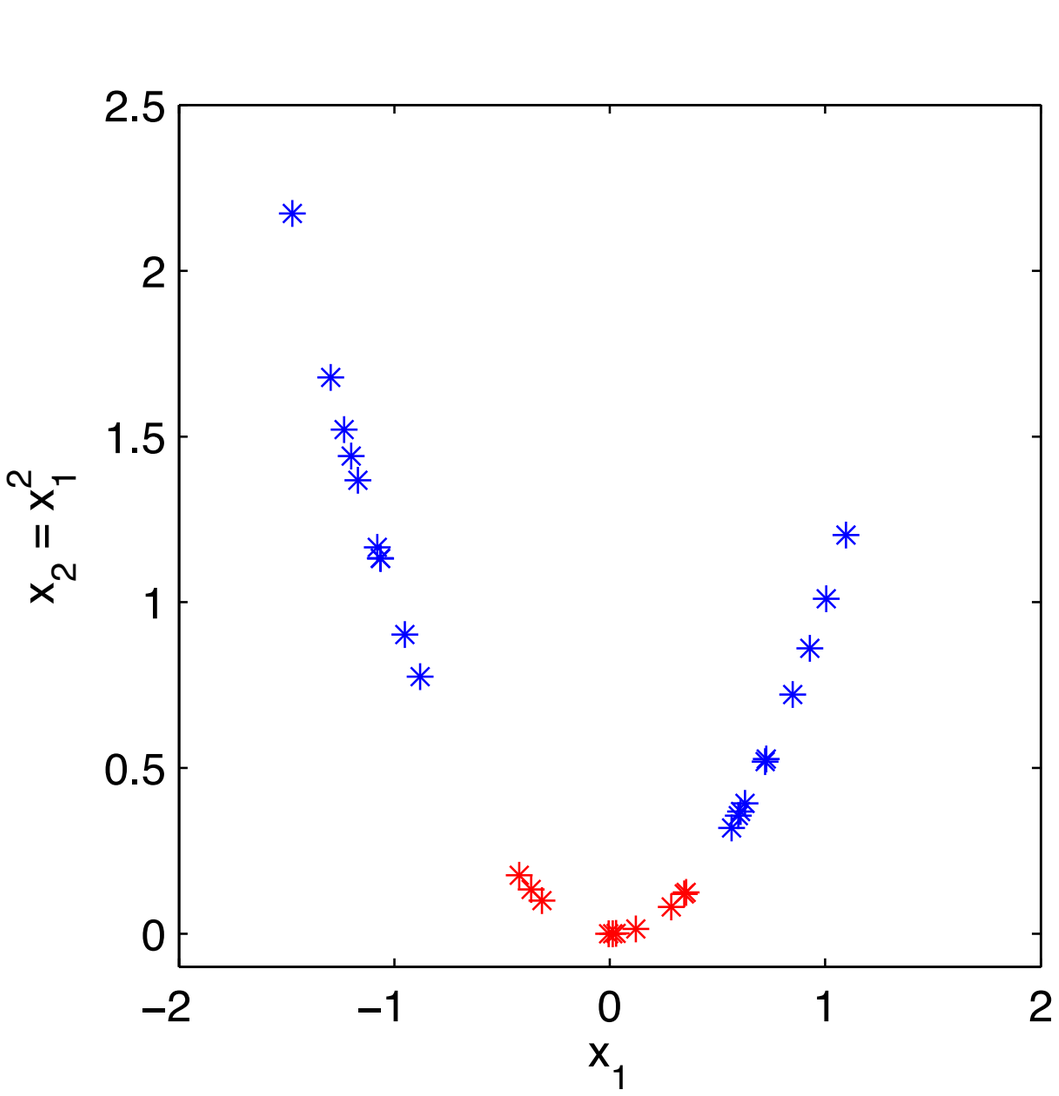
Separability by adding features



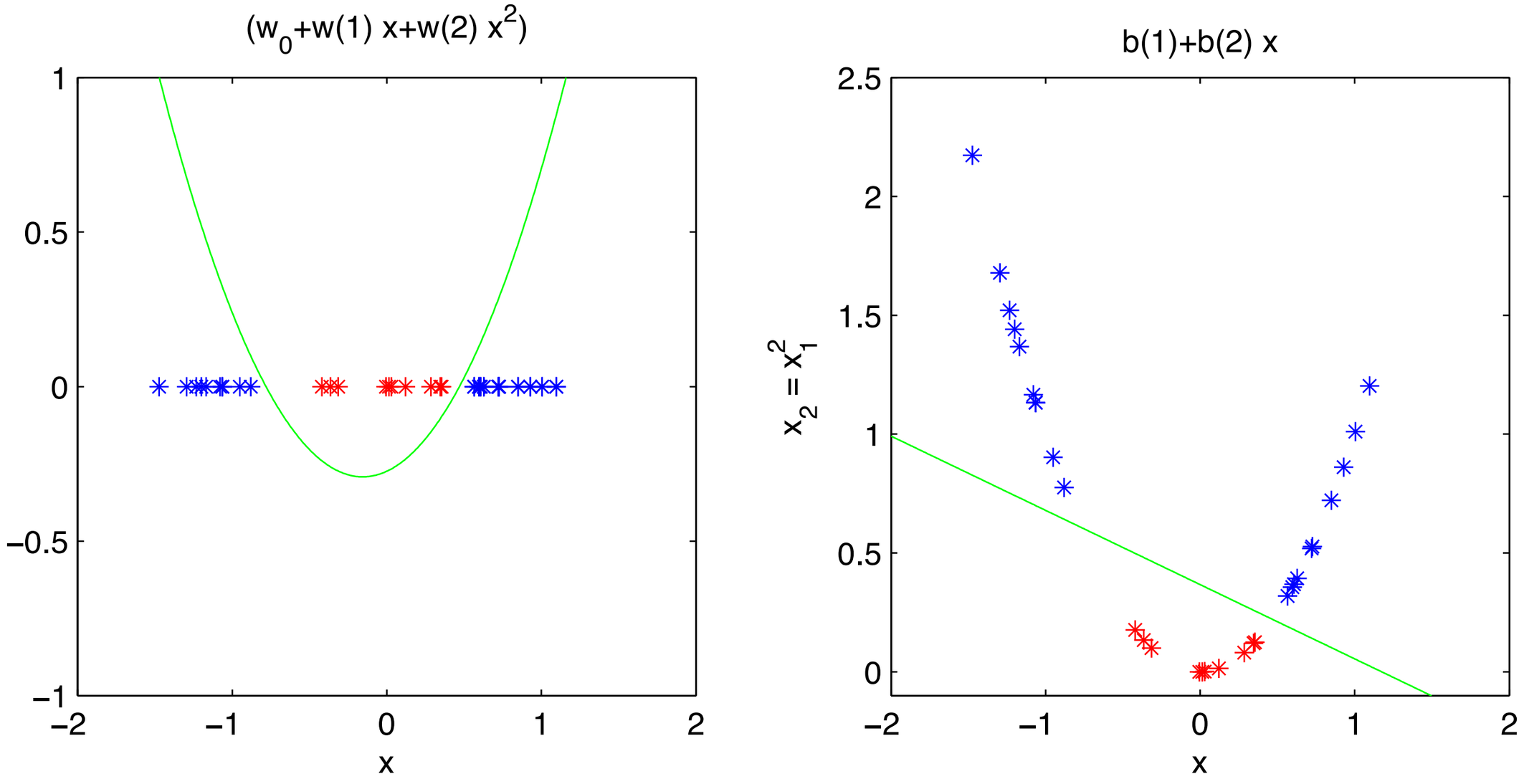


Separability by adding features





Separability by adding features



more flexible decision boundary ≈ enriched feature space

Margin optimization in feature space

- Replacing $\mathbf{x}_i$ with $\phi(\mathbf{x}_i)$, the dual form becomes:

$\max \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j))$
w.r.t. α_i
s.t. $0 \leq \alpha_i \leq C$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$

- Classification of an input $\mathbf{x}$ is given by:

$$h_{\mathbf{w},w_0}(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^{n} \alpha_i y_i (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x})) + w_0\right)$$

- Note that in the dual form, to do both SVM training and prediction, we only ever need to compute *dot-products of feature vectors*.

Kernel functions

- Whenever a learning algorithm (such as SVMs) can be written in terms of dot-products, it can be generalized to kernels.
- A *kernel* is any function $K : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ which corresponds to a dot product for some feature mapping ϕ:

$$K(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2) \text{ for some } \phi.$$

- Conversely, by choosing feature mapping ϕ, we implicitly choose a kernel function
- Recall that $\phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2) \propto \cos \angle(\mathbf{x}_1, \mathbf{x}_2)$ where $\angle$ denotes the angle between the vectors, so a kernel function can be thought of as a notion of *similarity*.

Example: Quadratic kernel

- Let $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^2$.
- Is this a kernel?

$$K(\mathbf{x}, \mathbf{z}) = \left(\sum_{i=1}^{p} x_i z_i\right)\left(\sum_{j=1}^{p} x_j z_j\right) = \sum_{i,j \in \{1 \ldots p\}} \left(x_i x_j\right)\left(z_i z_j\right)$$

- Hence, it is a kernel, with feature mapping:

$$\phi(\mathbf{x}) = \langle x_1^2,\ x_1 x_2,\ \ \ldots,\ x_1 x_p,\ x_2 x_1,\ x_2^2,\ \ \ldots,\ x_p^2 \rangle$$

Feature vector includes all squares of elements and all cross terms.

- Note that computing ϕ takes $O(p^2)$ but *computing K takes only $O(p)$*!

Polynomial kernels

- More generally, $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^d$ is a kernel, for any positive integer d.

- If we expanded the product above, we get terms for all degrees up to and including d (in x_i and z_i).
- If we use the primal form of the SVM, each of these will have a weight associated with it!
- *Curse of dimensionality:* it is very expensive both to optimize and to predict with an SVM in primal form with many features.

The "kernel trick"

- If we work with the dual, we do not actually have to ever compute the feature mapping ϕ. We just have to compute the similarity K.
- That is, we can solve the dual for the α_i:

  $\max \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$ w.r.t. α_i
  s.t. $0 \leq \alpha_i \leq C$, $\sum_{i=1}^{n} \alpha_i y_i = 0$
- The class of a new input $\mathbf{x}$ is computed as:

$$h_{\mathbf{w},w_0}(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^{n} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + w_0\right)$$

- Often, $K(\cdot, \cdot)$ can be evaluated in $O(p)$ time—a big savings!

Some other (fairly generic) kernel functions

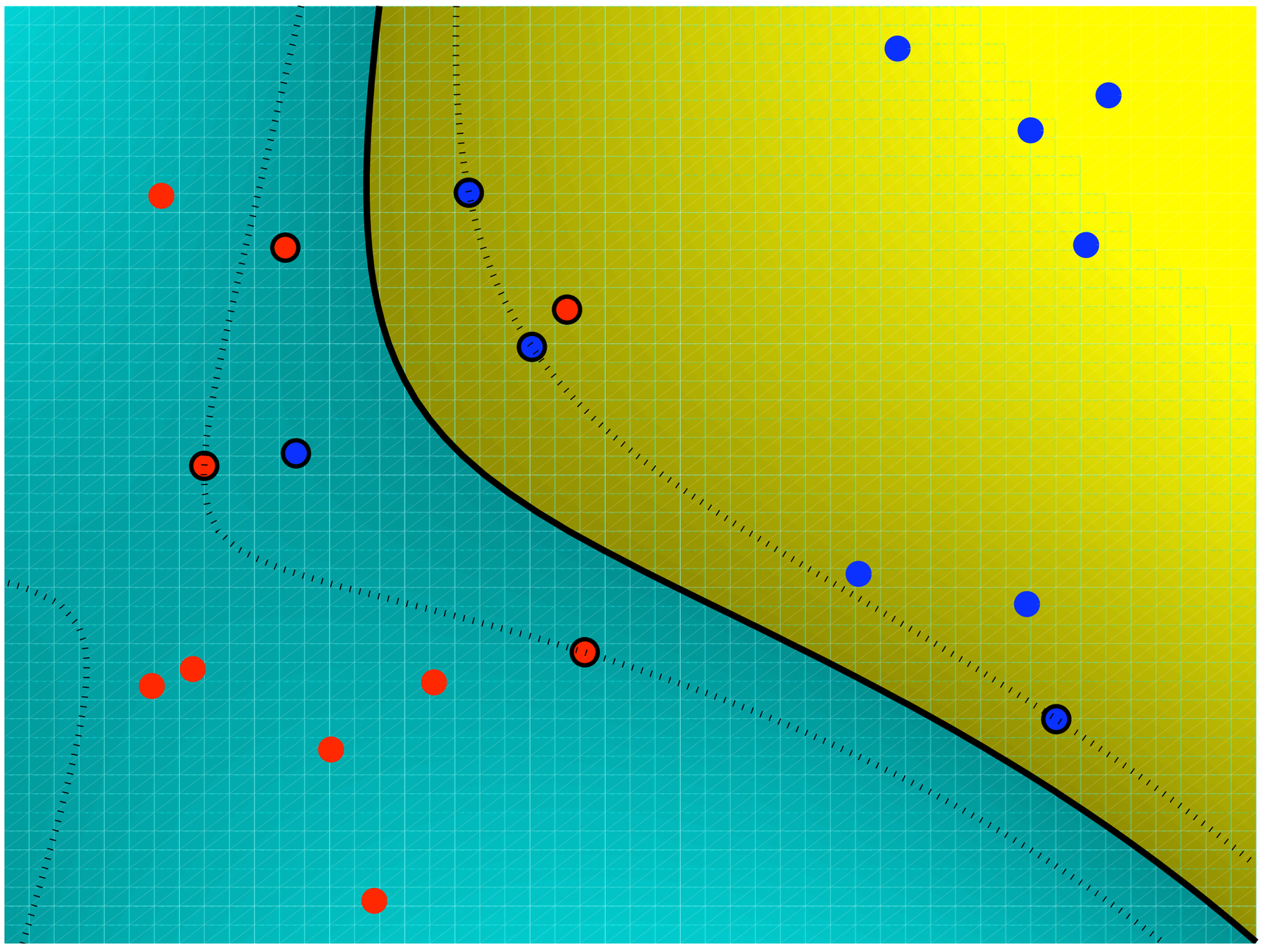
- $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^d$ – feature expansion has all monomial terms of degree $\leq d$.
- Radial basis/Gaussian kernel (**most popular**):

$$K(\mathbf{x}, \mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|^2 / 2\sigma^2)$$

  The kernel has an infinite-dimensional feature expansion, but dot-products can still be computed in $O(n)$!
- Sigmoid kernel:

$$K(\mathbf{x}, \mathbf{z}) = \tanh(c_1 \mathbf{x} \cdot \mathbf{z} + c_2)$$

Example: Gaussian kernel



Kernels beyond SVMs

- Remember, a kernel is a special kind of similarity measure
- A lot of research has to do with defining new kernel functions, suitable to particular tasks / kinds of input objects
- Many kernels are available:

- Information diffusion kernels (Lafferty and Lebanon, 2002)
- Diffusion kernels on graphs (Kondor and Jebara 2003)
- String kernels for text classification (Lodhi et al, 2002)
- String kernels for protein classification (e.g., Leslie et al, 2002)

… and others!

Example: String kernels

- Example: in DNA matching, we can use a sliding window of length k over the two strings that we want to compare
- The window is of a given size, and inside we can do various things:
  - Count exact matches, Weigh mismatches based on how bad they are, …
- The kernel is the sum of these similarities over the two sequences
- How do we prove this is a kernel? http://www.kernel-methods.net/ (http://www.kernel-methods.net/)
- Many other machine learning algorithms have a “dual formulation,” in which dot-products of features can be replaced with kernels.

Second brush with “feature construction”

- With polynomial regression, we saw how to construct features to increase the size of the hypothesis space
- This gave more flexible regression functions
- Kernels offer a similar function with SVMs: More flexible decision boundaries
- Often not clear what kernel is appropriate for the data at hand.

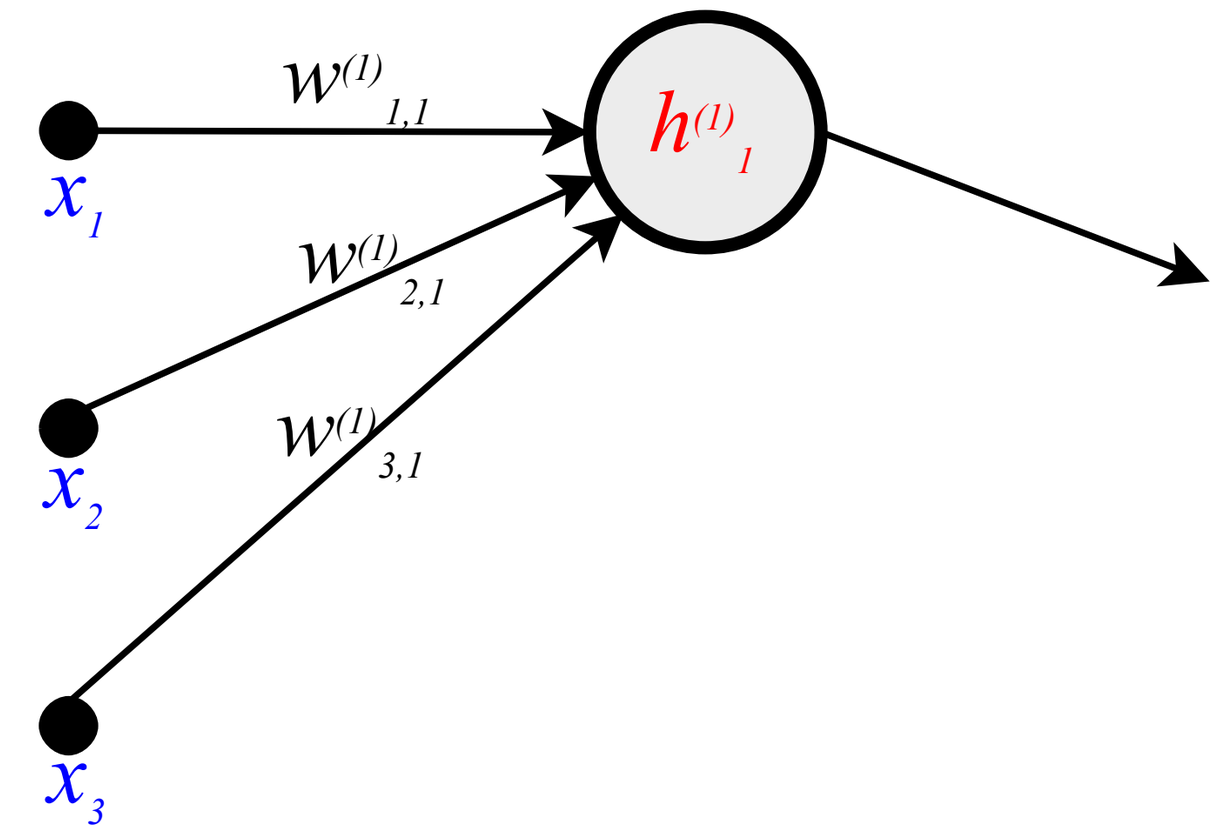
Getting SVMs to work in practice

- `libsvm` and `liblinear` are popular
- Scaling the inputs ($\mathbf{x}_i$) is very important. (E.g. make all mean zero variance 1.)
- Two important choices:
  - Kernel (and kernel parameters, e.g. γ for the RBF kernel)
  - Regularization parameter C
- The parameters may interact!
- Together, these control overfitting: always do a *within-fold parameter search, using a validation set*!
- Clues you might be overfitting: Low margin (large weights), Large fraction of instances are support vectors

Artificial Neural Networks (HTF Ch. 11)

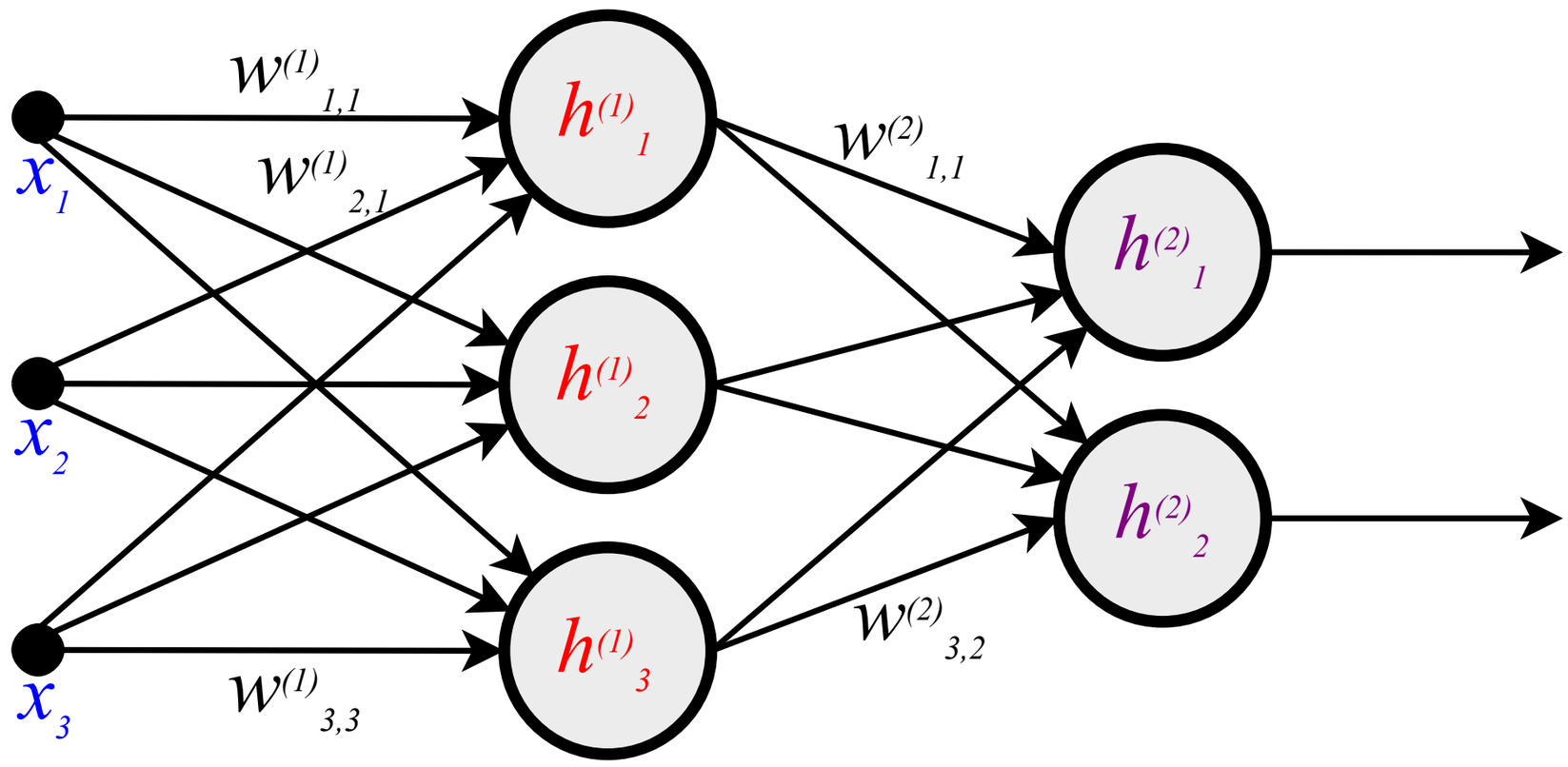
- Functional form + Training algorithm

Functional Form - Neuron



$$h_1^{(1)}(x_1, x_2, x_3) = \phi_1^{(1)}(w_{1,1}^{(1)}x_1 + w_{2,1}^{(1)}x_2, + w_{3,1}^{(1)}x_3 + w_{0,1}^{(1)})$$

Functional Form



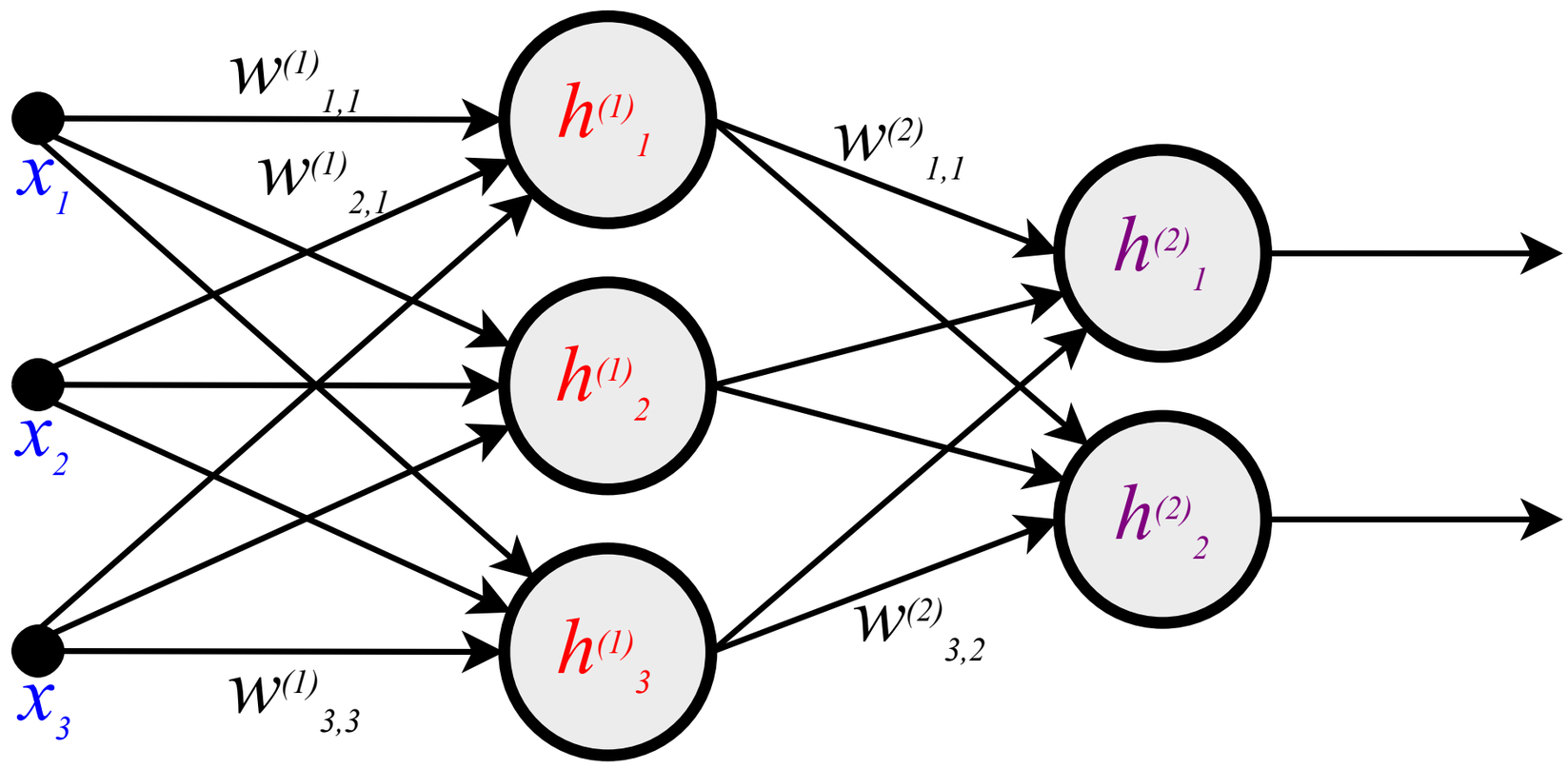
$$h_1^{(1)}(x_1, x_2, x_3) = \phi_1^{(1)}(w_{1,1}^{(1)} x_1 + w_{2,1}^{(1)} x_2, + w_{3,1}^{(1)} x_3 + w_{0,1}^{(1)}) \; h_2^{(1)}(x_1, x_2, x_3) = \phi_2^{(1)}(w_{1,2}^{(1)} x_1 + w_{2,2}^{(1)} x_2, + w_{3,2}^{(1)} x_3 + w_{0,2}^{(1)})$$
$$h_3^{(1)}(x_1, x_2, x_3) = \phi_3^{(1)}(w_{1,3}^{(1)} x_1 + w_{2,3}^{(1)} x_2, + w_{3,3}^{(1)} x_3 + w_{0,3}^{(1)})$$

$$h_1^{(2)}(x_1, x_2, x_3) = \phi_1^{(2)}(w_{1,1}^{(2)} h_1^{(1)} + w_{2,1}^{(2)} h_2^{(1)}, + w_{3,1}^{(2)} h_3^{(1)} + w_{0,1}^{(2)}) \; h_2^{(2)}(x_1, x_2, x_3) = \phi_2^{(2)}(w_{1,2}^{(2)} h_1^{(1)} + w_{2,2}^{(2)} h_2^{(1)}, + w_{3,2}^{(2)} h_3^{(1)} + w_{0,2}^{(2)})$$

“Activation” or “Transfer” Function ϕ

Name	Plot	Equation
Identity (https://en.wikipedia.org/wiki/Identity_function)	(https://en.wikipedia.org/wiki/File:Activation_identity.svg)	$f(x) = x$
Binary step (https://en.wikipedia.org/wiki/Heaviside_step_function)	(https://en.wikipedia.org/wiki/File:Activation_binary_step.svg)	$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Logistic (https://en.wikipedia.org/wiki/Logistic_function)	(https://en.wikipedia.org/wiki/File:Activation_logistic.svg)	$f(x) = \frac{1}{1 + e^{-x}}$
TanH (https://en.wikipedia.org/wiki/Hyperbolic_function#Hyperbolic_tangent)	(https://en.wikipedia.org/wiki/File:Activation_tanh.svg)	$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$
Rectified linear unit (/wiki/Rectifier_(neural_networks)) (ReLU)[9]	(/wiki/File:Activation_rectified_linear.svg)	$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$

Hidden Units are Features



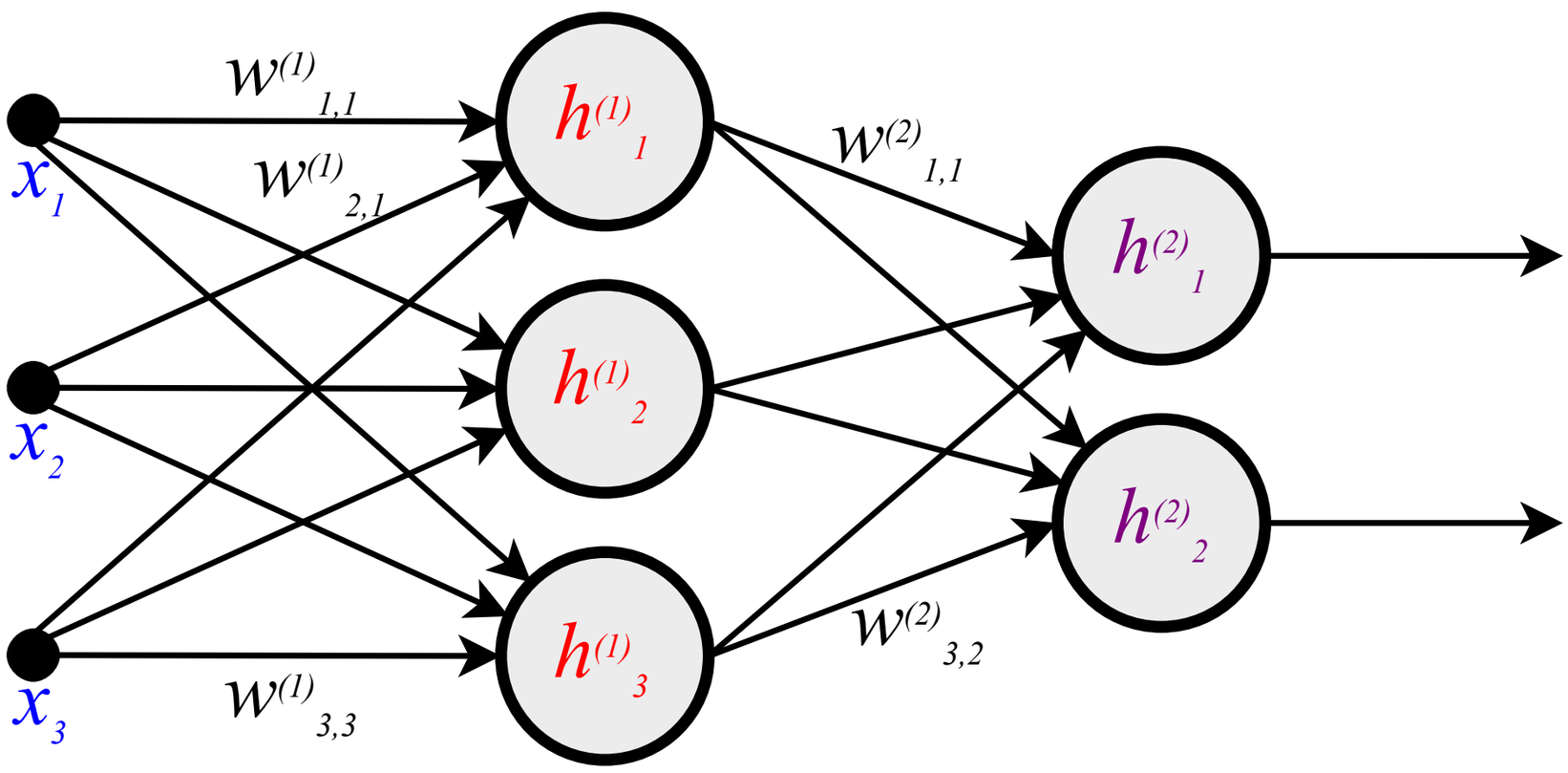
Aside: “One-Hot” Encoding

Sample	Human	Penguin	Octopus	Alien
1	1	0	0	0
2	1	0	0	0
3	0	1	0	0
4	0	0	1	0
5	0	0	0	1
6	0	0	1	0
7	0	0	0	1

Error Functions

$$J(\mathbf{w}) = \frac{1}{2}\sum_j \sum_{i=1}^{n} (h_j^{(L)}(\mathbf{x}_i) - y_i)^2$$

$$J(\mathbf{w}) = -\sum_j \sum_{i=1}^{n} y_i \log h_j^{(L)}(\mathbf{x}_i) + (1 - y_i)\log(1 - h_j^{(L)}(\mathbf{x}_i))$$



Training

Traditional ANN training is done by looping over examples (much like the perceptron) and taking a small step down the single-example gradient.

For a single output neuron:

$$\begin{aligned} J_j(\mathbf{w}) &= \frac{1}{2}(h_j^{(L)}(\mathbf{x}_i) - y_i)^2 \\ \nabla_{\mathbf{w}} J &= (h_j^{(L)}(\mathbf{x}_i) - y_i)\nabla_{\mathbf{w}} h_j^{(L)}(\mathbf{x}_i) \\ &= (\phi_j^{(L)}(\mathbf{x}_i^\top \mathbf{w}) - y_i) \cdot \phi_j'^{(L)}(\mathbf{x}_i^\top \mathbf{w}) \cdot \mathbf{x}_i \end{aligned}$$

Learning rule:

$$\mathbf{w}^{t+1} \leftarrow \mathbf{w}^t - \alpha \cdot (\phi_j^{(L)}(\mathbf{x}_i^\top \mathbf{w}) - y_i) \cdot \phi_j'^{(L)}\mathbf{x}_i^\top \mathbf{w}) \cdot \mathbf{x}_i$$

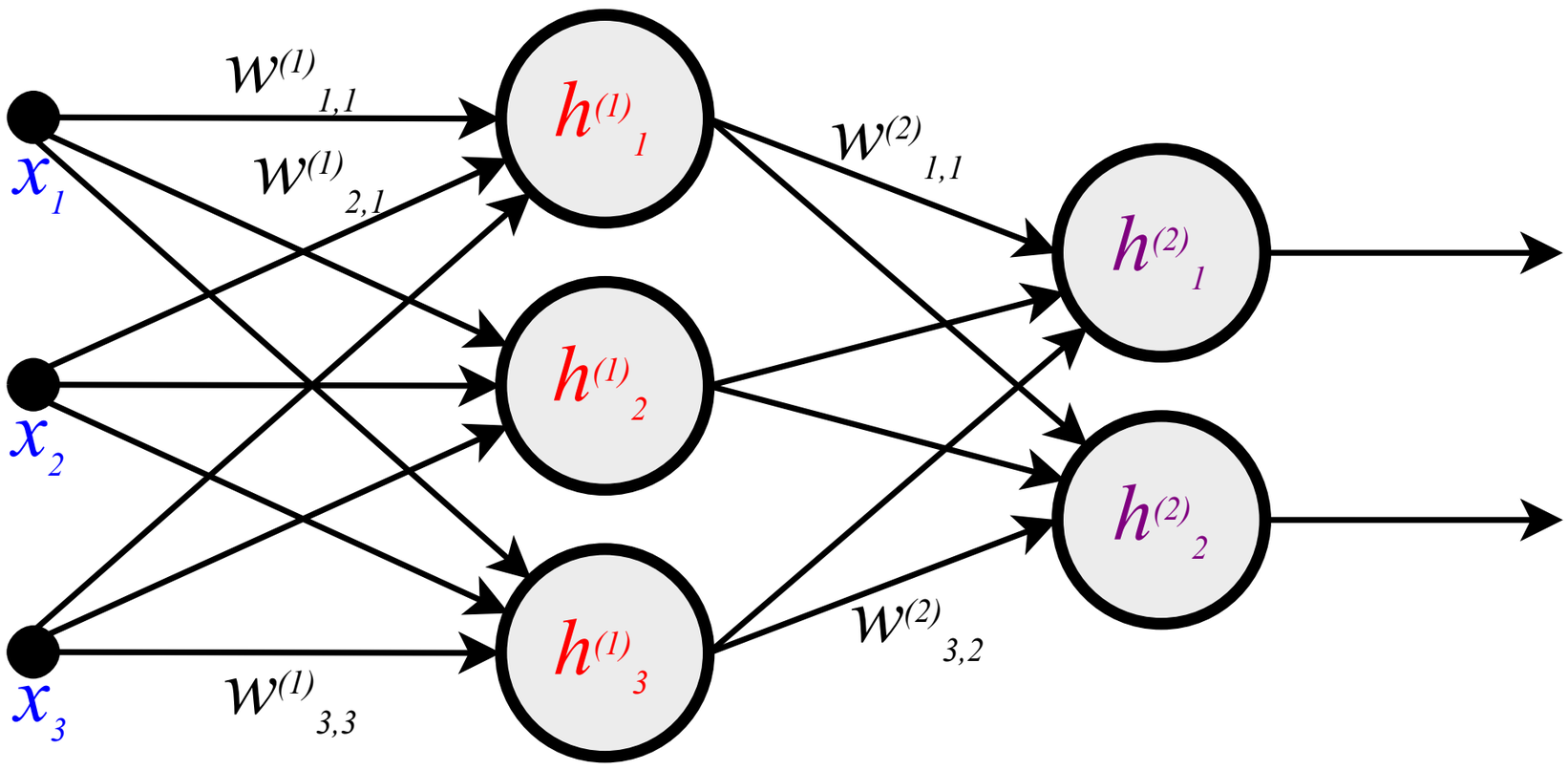
where α is a learning rate.

Backpropagation

$$\mathbf{w}_{\cdot,j}^{(\ell),t+1} \leftarrow \mathbf{w}_{\cdot,j}^{(\ell),t} - \alpha \cdot \delta_j^{(\ell)} \cdot \phi_j'^{(\ell)}(\mathbf{x}_i^\top \mathbf{w}_{\cdot,j}^{(\ell),t}) \cdot \mathbf{x}_i$$

where

$$\delta_j^{(\ell)} = \begin{cases} (\phi(\mathbf{x}_i^\top \mathbf{w}) - y_i) & \text{if } (\ell) \text{ is the output layer} \\ \sum_k w_{j,k}^{(\ell)} \delta_k^{(\ell+1)} & \text{otherwise} \end{cases}$$



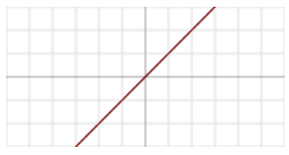
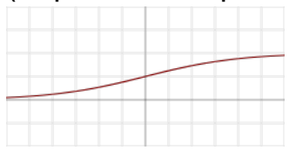
Variants of Backpropagation

- Adaptive learning rate
- “Momentum” or “inertia” - if weights keep changing in the same direction, change them faster.

Neural Net Design Decisions

- How many layers?
- How many nodes in each layer?
- What should ϕ be?
- What should the cost function be?
- What version of backprop should I use?
- What should my learning rates be?

Derivatives of ϕ

Name	Plot	Derivative (https://en.wikipedia.org/wi (with respect to x
Identity (https://en.wikipedia.org/wiki/Identity_function)	 (https://en.wikipedia.org/wiki/File:Activation_identity.svg)	$f'(x) = 1$
Binary step (https://en.wikipedia.org/wiki/Heaviside_step_function)	 (https://en.wikipedia.org/wiki/File:Activation_binary_step.svg)	$f'(x) = \begin{cases} 0 & \text{for} \quad x \neq 0 \\ ? & \text{for} \quad x = 0 \end{cases}$
Logistic (https://en.wikipedia.org/wiki/Logistic_function)	 (https://en.wikipedia.org/wiki/File:Activation_logistic.svg)	$f'(x) = f(x)(1 - f(x))$
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Rectified linear unit (/wiki/Rectifier_(neural_networks)) (ReLU)[9]	 (/wiki/File:Activation_rectified_linear.svg)	$f'(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$

Backprop “Conventional Wisdom”

- Small derivatives -> weights go nowhere
- In very deep networks, error gets “diluted” -> weights go nowhere
- Gets trapped in local optima

Deep Learning: “Unconventional Wisdom”

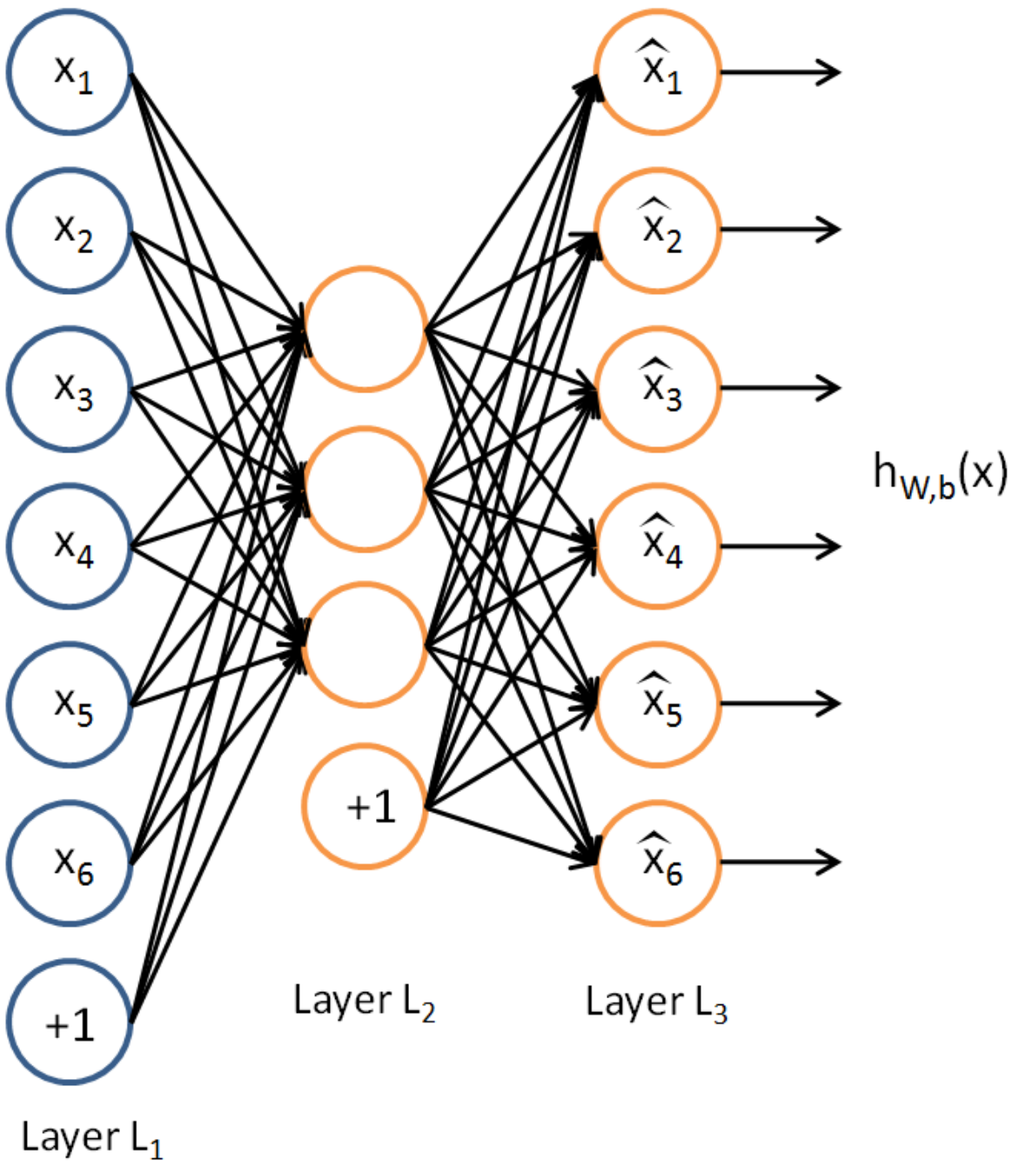
- Many layers (e.g. 10-20)
- Billions of connections
- Hundreds of millions of weights

http://www.nature.com/nature/journal/v521/n7553/full/nature14539.html (http://www.nature.com/nature/journal/v521/n7553/full/nature14539.html)

What changed?

- Data explosion (Google and others)
- Computational power (GPGPUs)

Deep Learning “Trick”: Pre-training



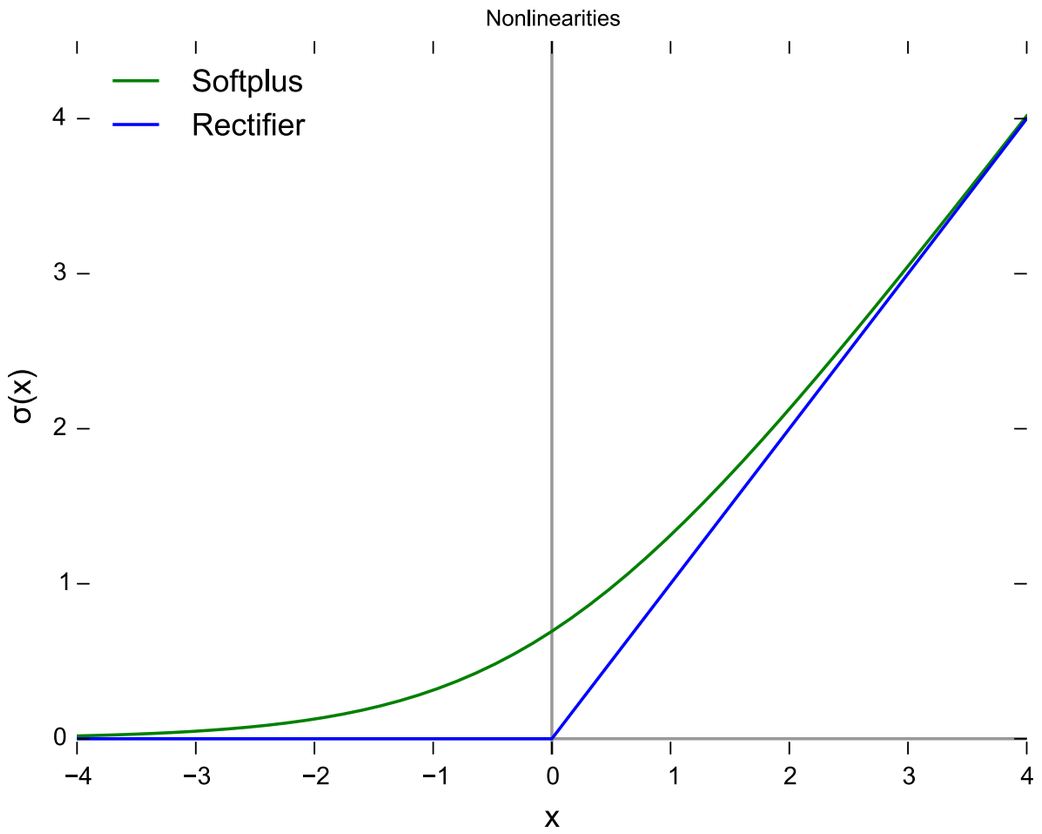
Deep Learning “Trick”: Dropout

Before presenting each training example and performing backprop, randomly ignore 50% of the nodes in your network.

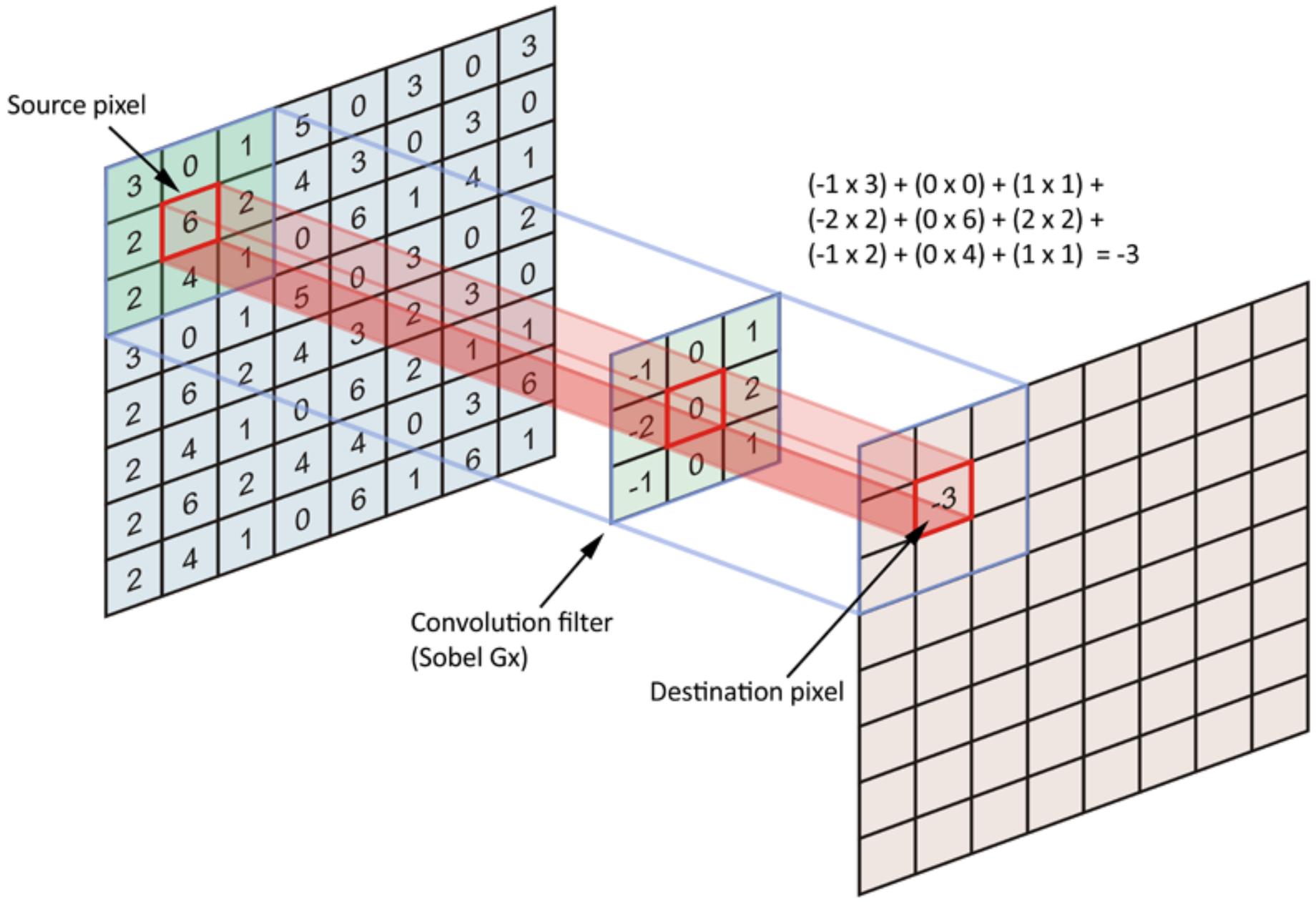
http://www.jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf (http://www.jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf)

Deep Learning “Trick”: ReLUs

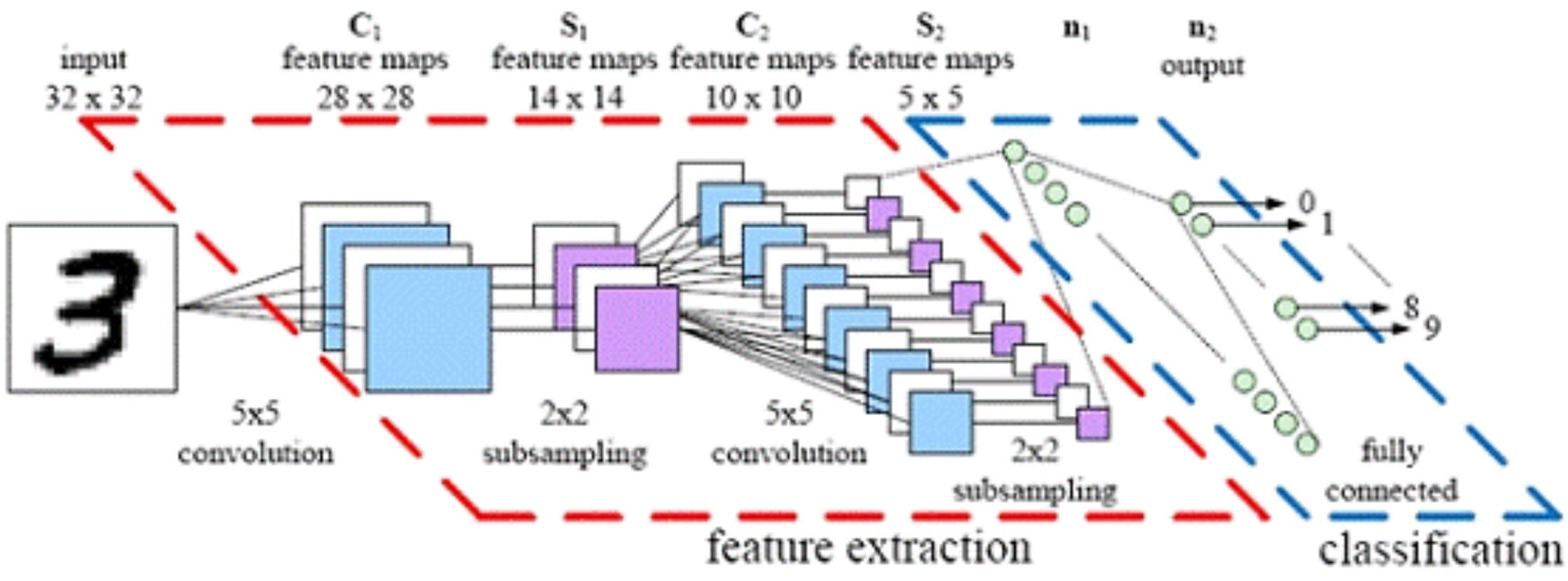
- May not need pre-training or dropout.



Aside: Convolution



Convolutional Neural Network (HTF 11.7)



http://cs231n.github.io/convolutional-networks/ (http://cs231n.github.io/convolutional-networks/)

Want to give it a try?

https://www.tensorflow.org (https://www.tensorflow.org)

(Other packages available.)

- Be prepared to:
  - Search for and read papers
  - Try different architectures
  - Try different training methods
  - Wait (depending on your network size/training set size)

Instance-based learning, Decision Trees

- Non-parametric learning
- k-nearest neighbour
- Efficient implementations
- Variations

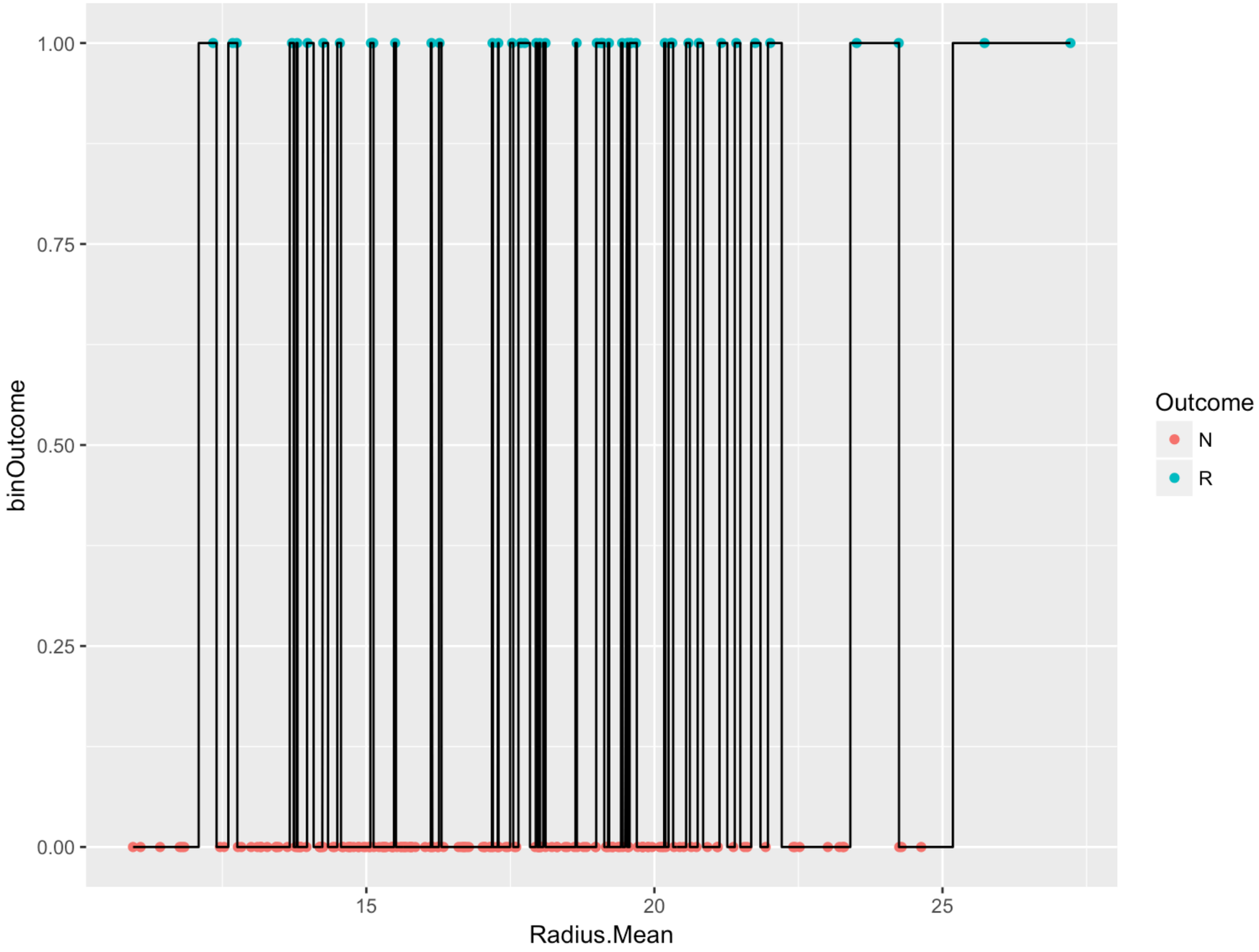
Parametric supervised learning

- So far, we have assumed that we have a data set D of labeled examples
- From this, we learn a *parameter vector* of a *fixed size* such that some error measure based on the training data is minimized
- These methods are called *parametric*, and their main goal is to summarize the data using the parameters
- Parametric methods are typically global, i.e. have one set of parameters for the entire data space
- But what if we just remembered the data?
- When new instances arrive, we will compare them with what we know, and determine the answer

Non-parametric (memory-based) learning methods

- Key idea: just store all training examples $\langle \mathbf{x}_i, y_i \rangle$
- When a query is made, compute the value of the new instance based on the values of the *closest (most similar) points*
- Requirements:
  - A distance function
  - How many closest points (neighbors) to look at?
  - How do we compute the value of the new point based on the existing values?

Simple idea: Connect the dots!



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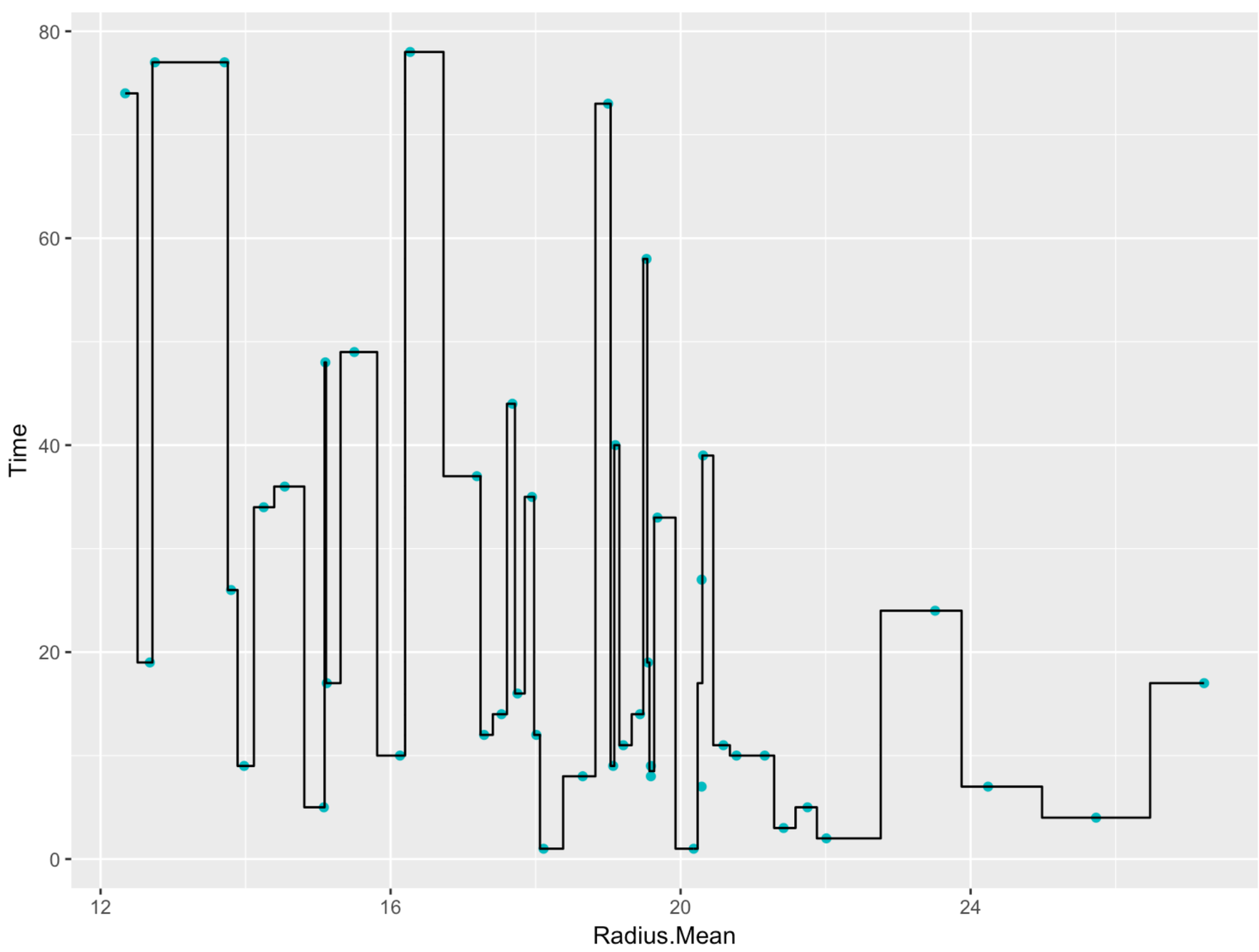


One-nearest neighbor

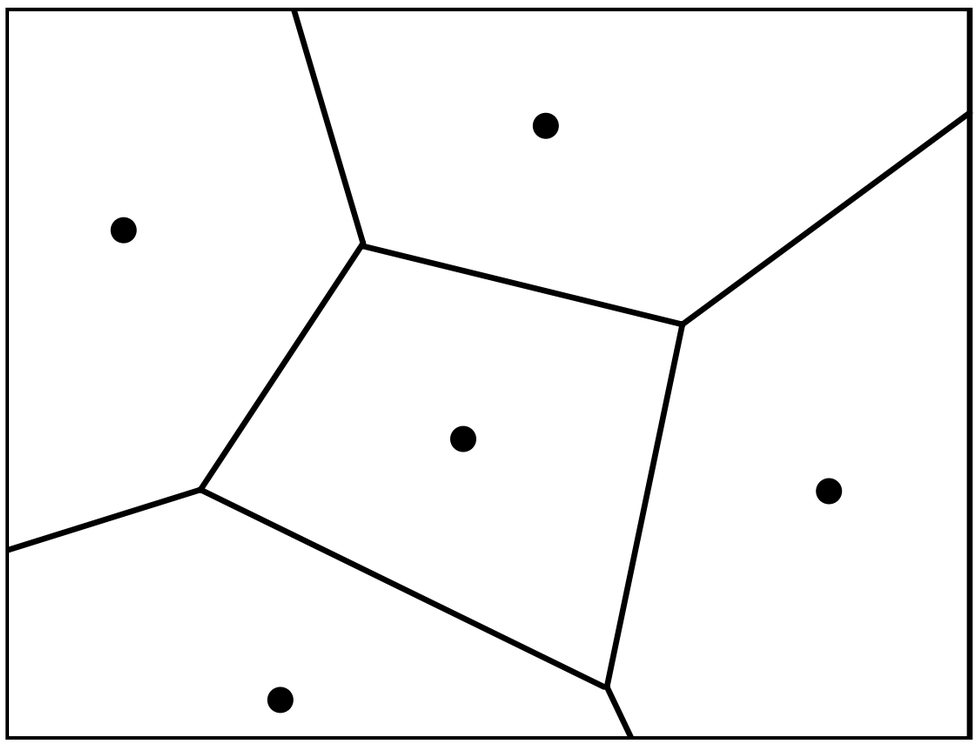
- Given: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, distance metric d on $\mathcal{X}$.
- Training: Nothing to do! (just store data)
- Prediction: for $\mathbf{x} \in \mathcal{X}$
    - Find nearest training sample to $\mathbf{x}$.

$$i^* \in \arg\min_i d(\mathbf{x}_i, \mathbf{x})$$

    - Predict $y = y_{i^*}$.

What does the approximator look like?

- Nearest-neighbor does not explicitly compute decision boundaries
- But the effective decision boundaries are a subset of the *Voronoi diagram* for the training data



Each line segment is equidistant between two points of opposite classes.

What kind of distance metric?

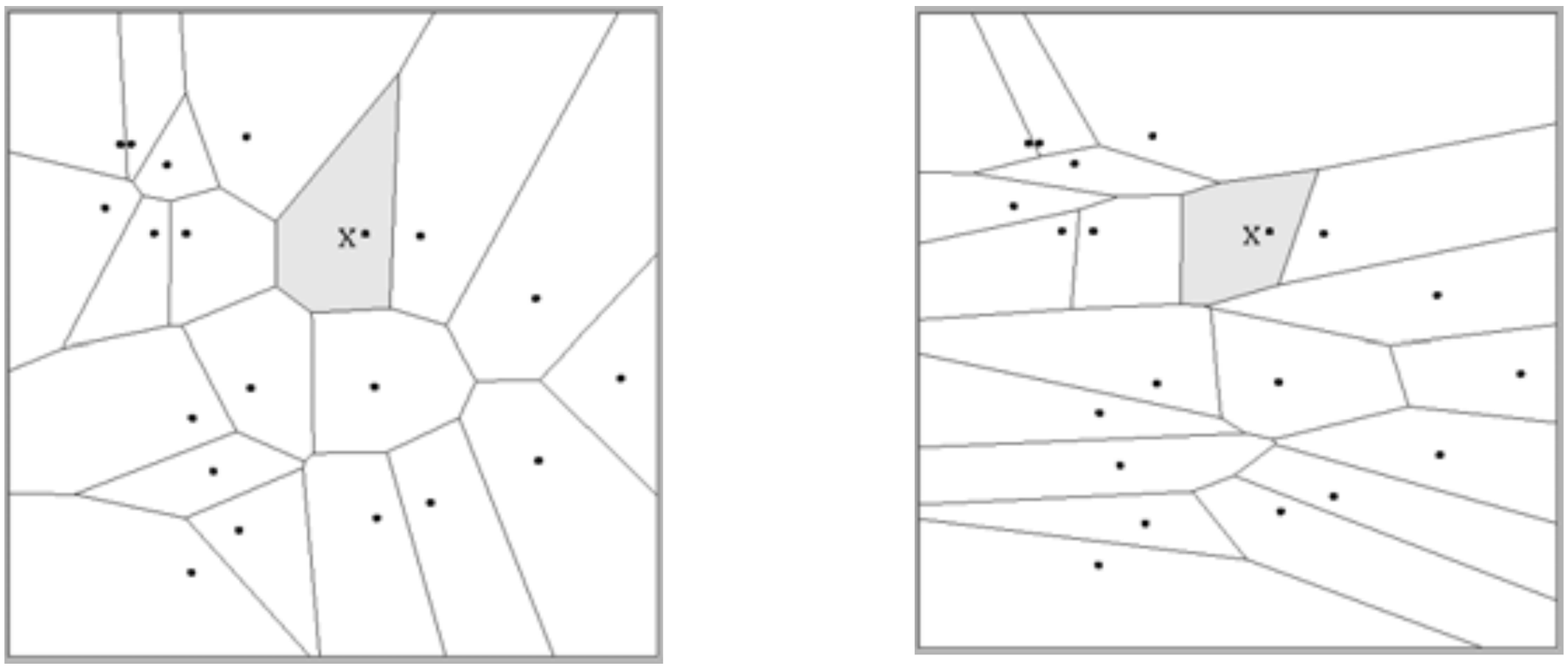
- Euclidian distance
- Maximum/minimum difference along any axis

- Weighted Euclidian distance (with weights based on domain knowledge)

$$d(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{p} u_j (x_j - x'_j)^2$$

- An arbitrary distance or similarity function d, specific for the application at hand (works best, if you have one)

Distance metric is really important!



Left: attributes weighted equally Right: unequal weighting

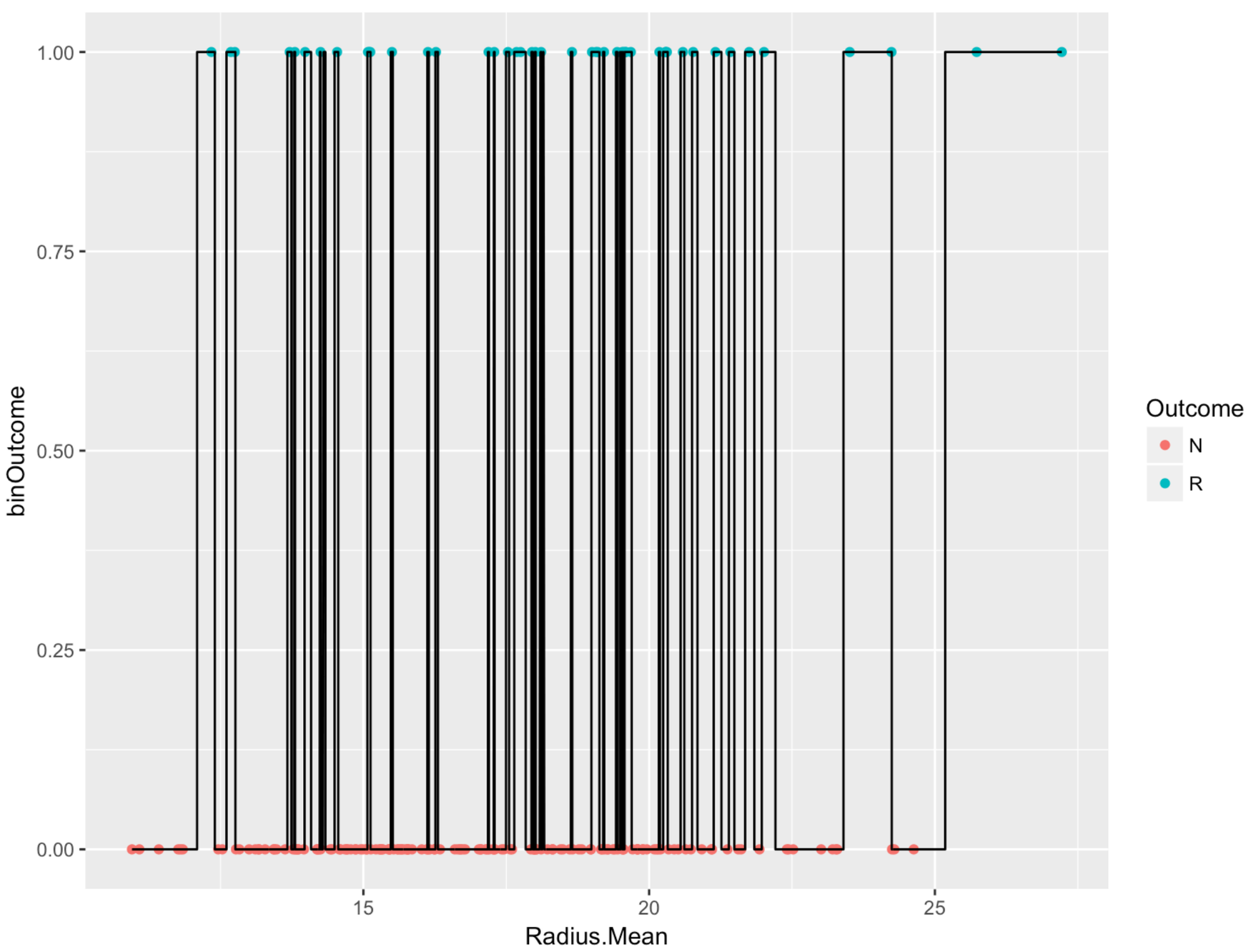
Distance metric tricks

- You may need to do preprocessing:
    - *Scale* the input dimensions (or normalize them)
    - Remove noisy inputs
    - Determine weights for attributes based on cross-validation (or information-theoretic methods)
- Distance metric is often domain-specific
    - E.g. string edit distance in bioinformatics
    - E.g. trajectory distance in time series models for walking data
- Distance metric can be learned sometimes (more on this later)

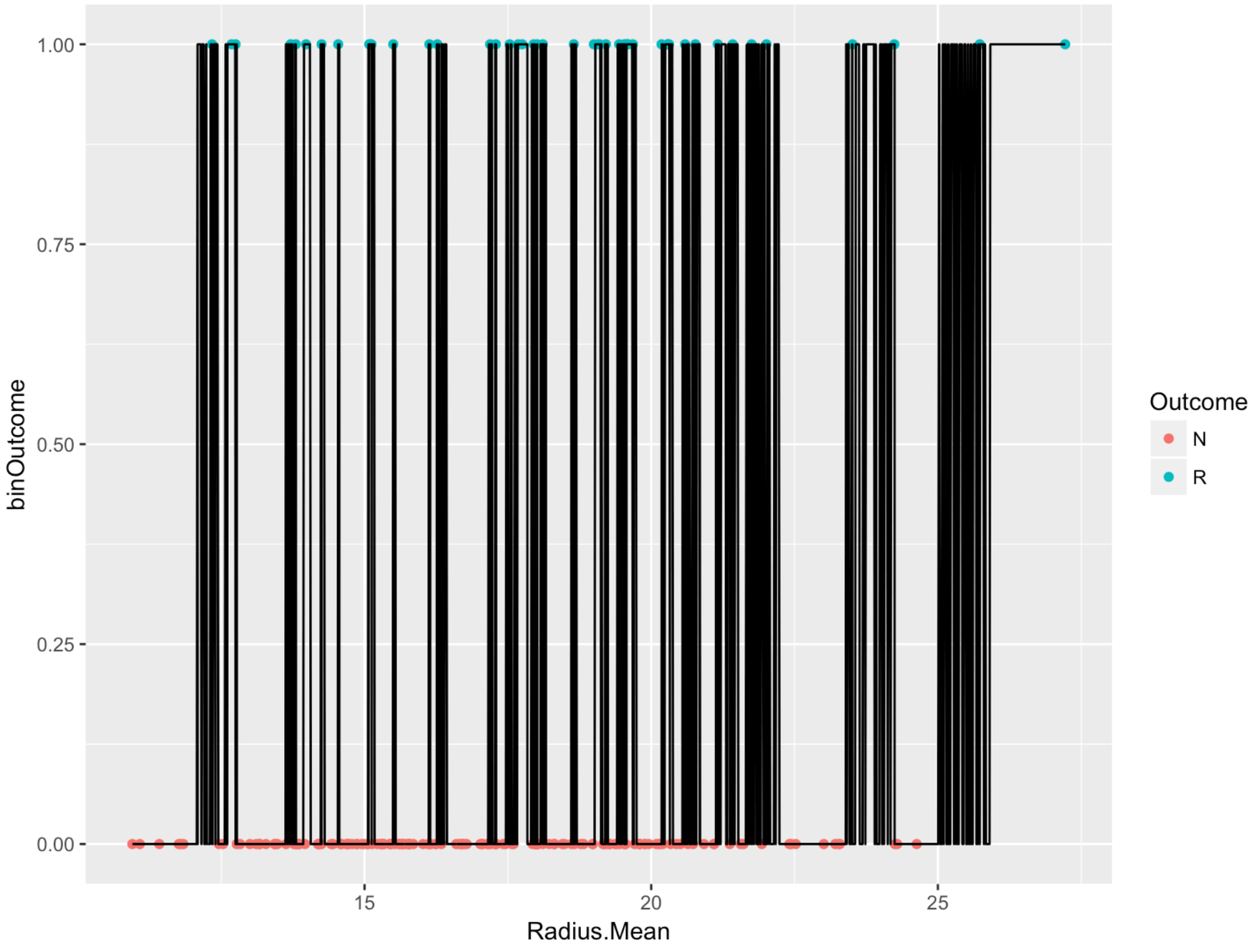
k-nearest neighbor

- Given: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, distance metric d on $\mathcal{X}$.
- Learning: Nothing to do!
- Prediction: for $\mathbf{x} \in \mathcal{X}$
    - Find the k nearest training samples to $\mathbf{x}$.
      Let their indices be $i_1, i_2, \ldots, i_k$.
    - Predict
        - $y =$ mean/median of $\{y_{i_1}, y_{i_2}, \ldots, y_{i_k}\}$ for regression
        - $y =$ majority of $\{y_{i_1}, y_{i_2}, \ldots, y_{i_k}\}$ for classification, or empirical probability of each class

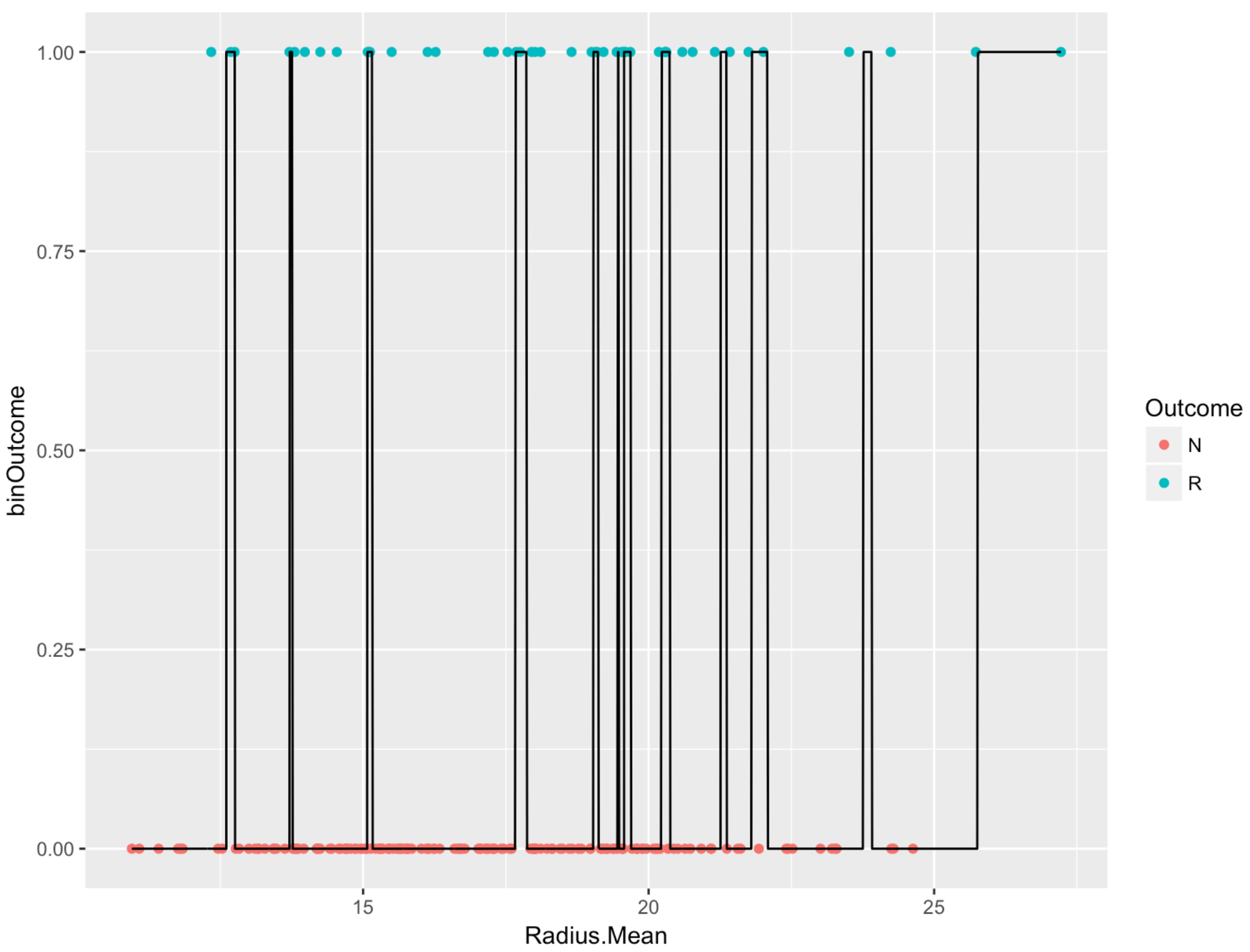
k-NN classification, Majority, k=1



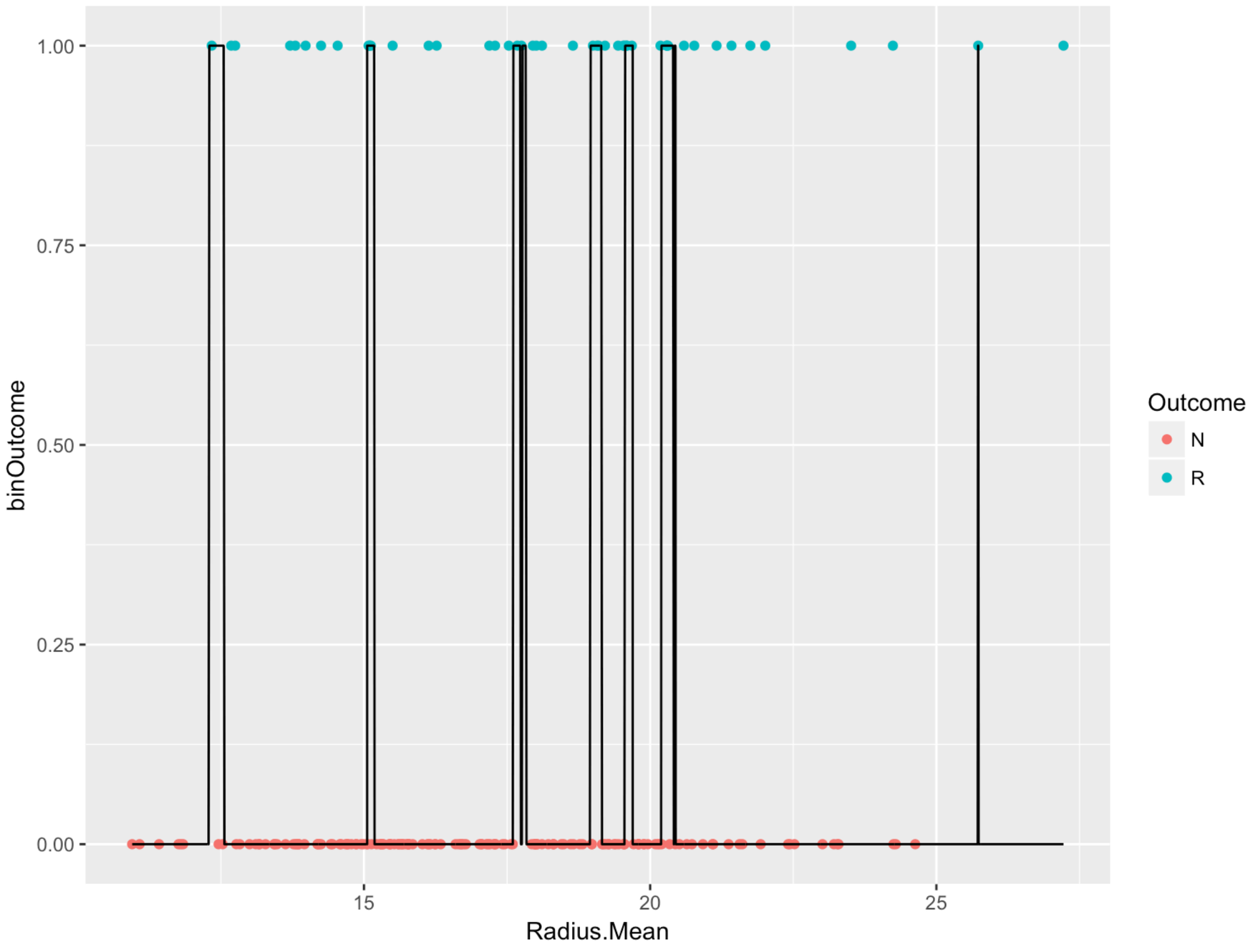
k-NN classification, Majority, k=2



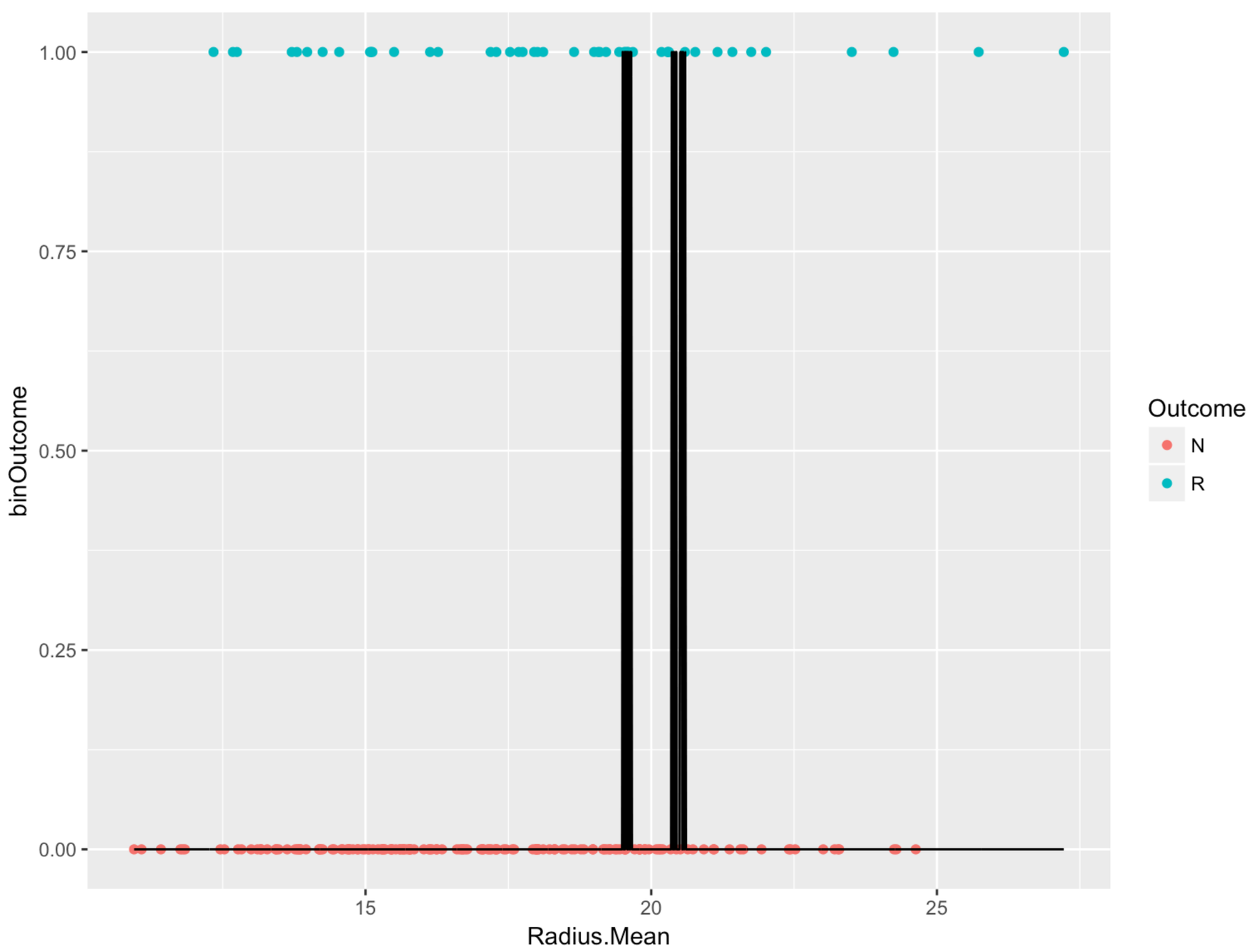
k-NN classification, Majority, k=3



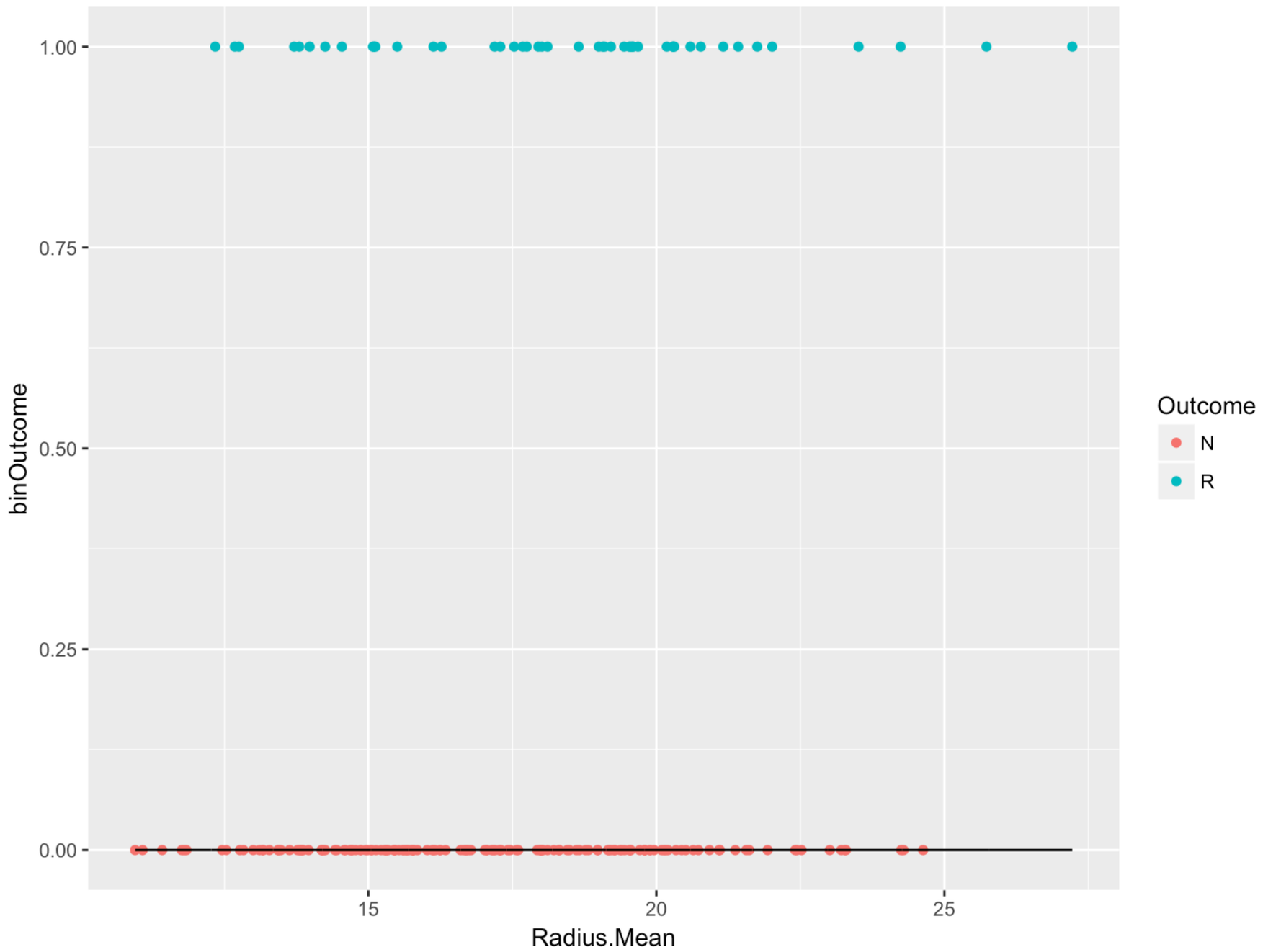
k-NN classification, Majority, k=5



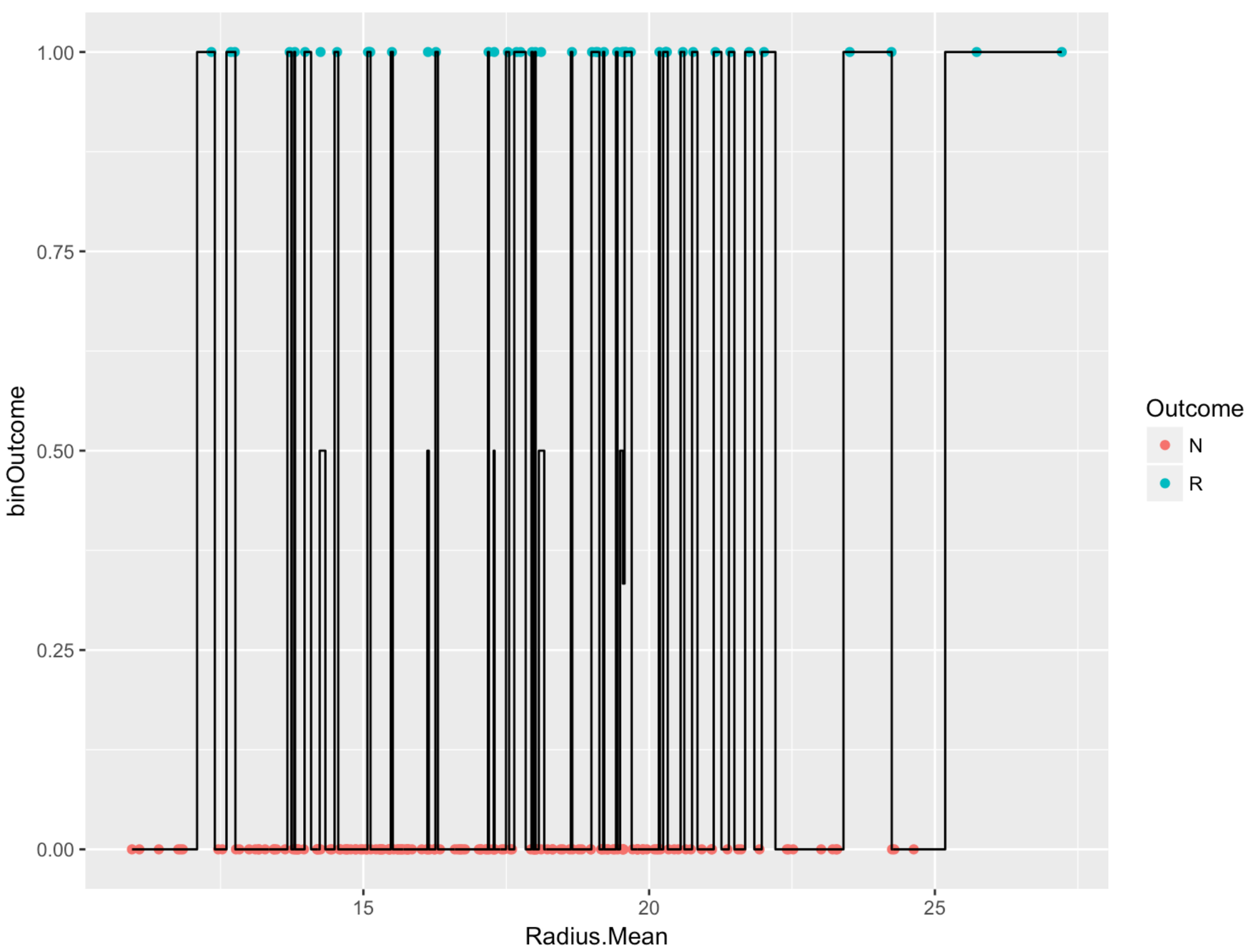
k-NN classification, Majority, k=10



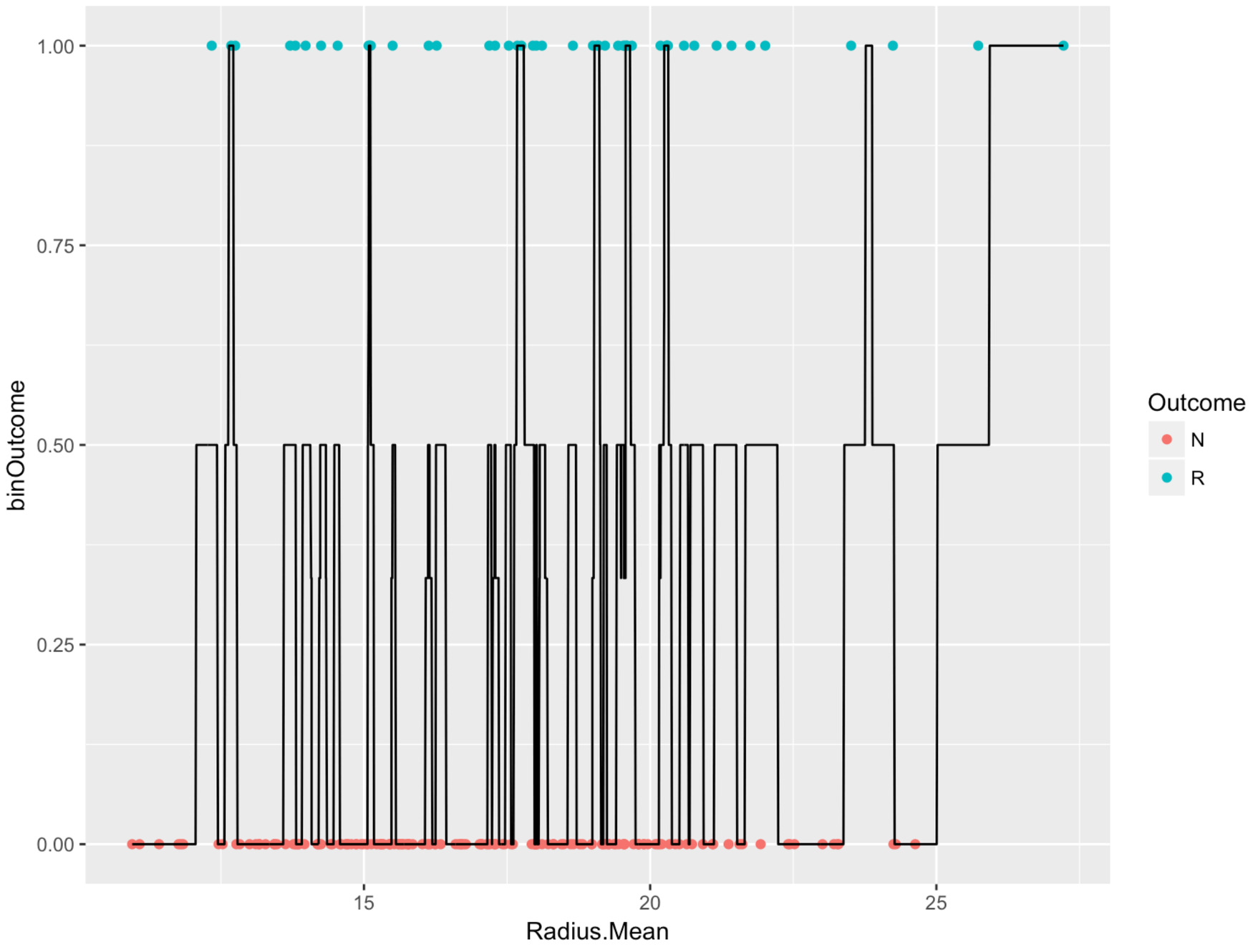
k-NN classification, Majority, k=15



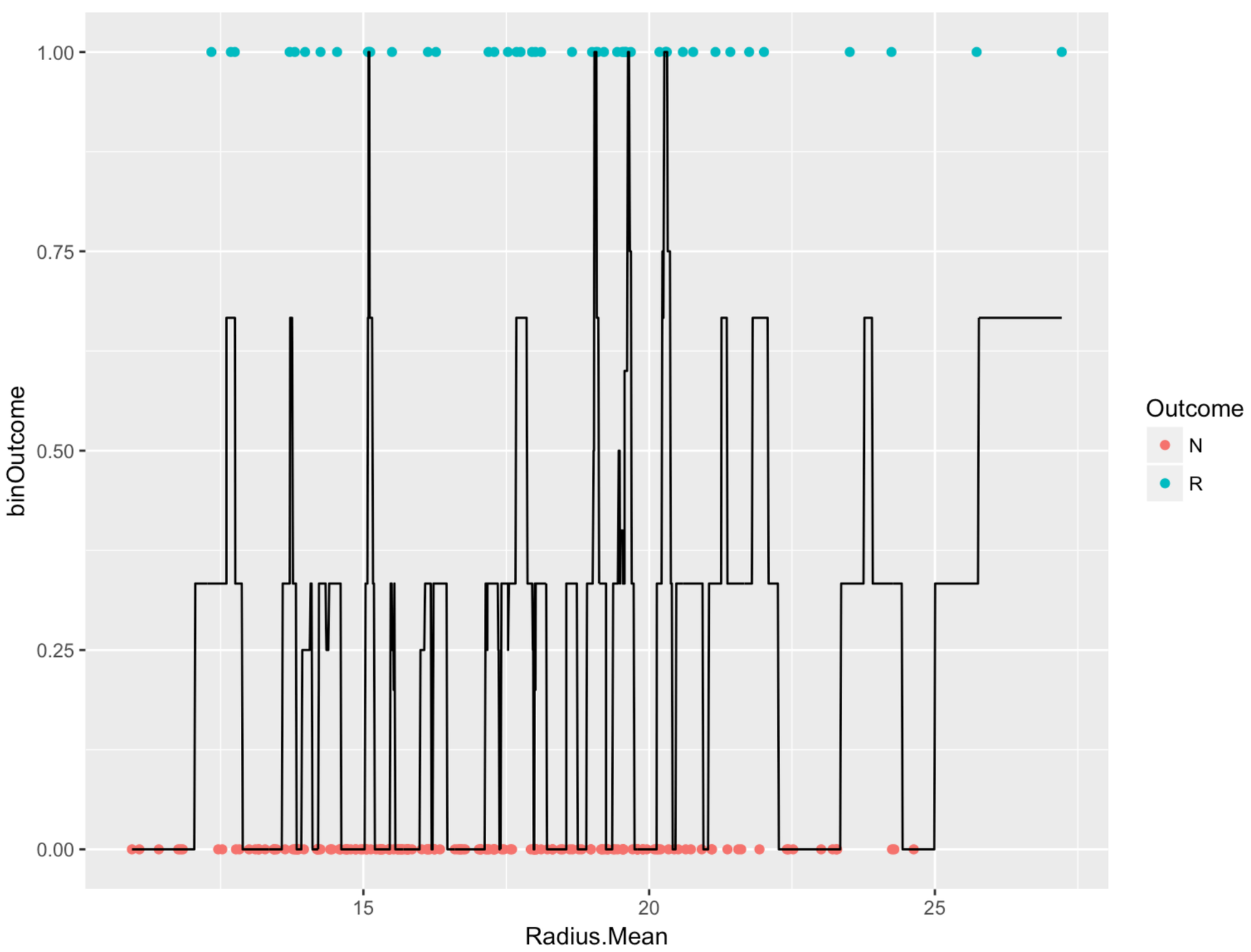
k-NN classification, Mean (prob), k=1



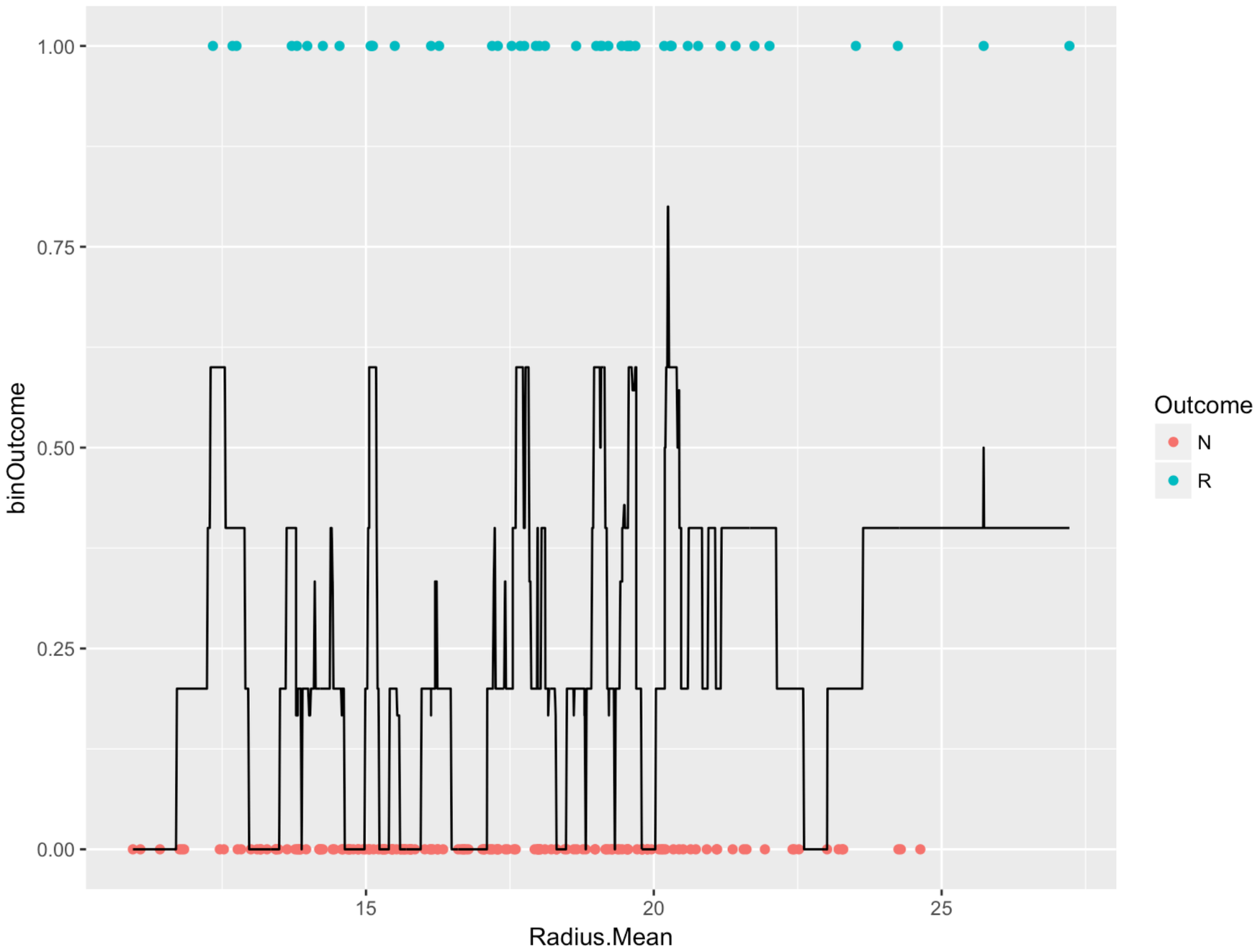
k-NN classification, Mean (prob), k=2



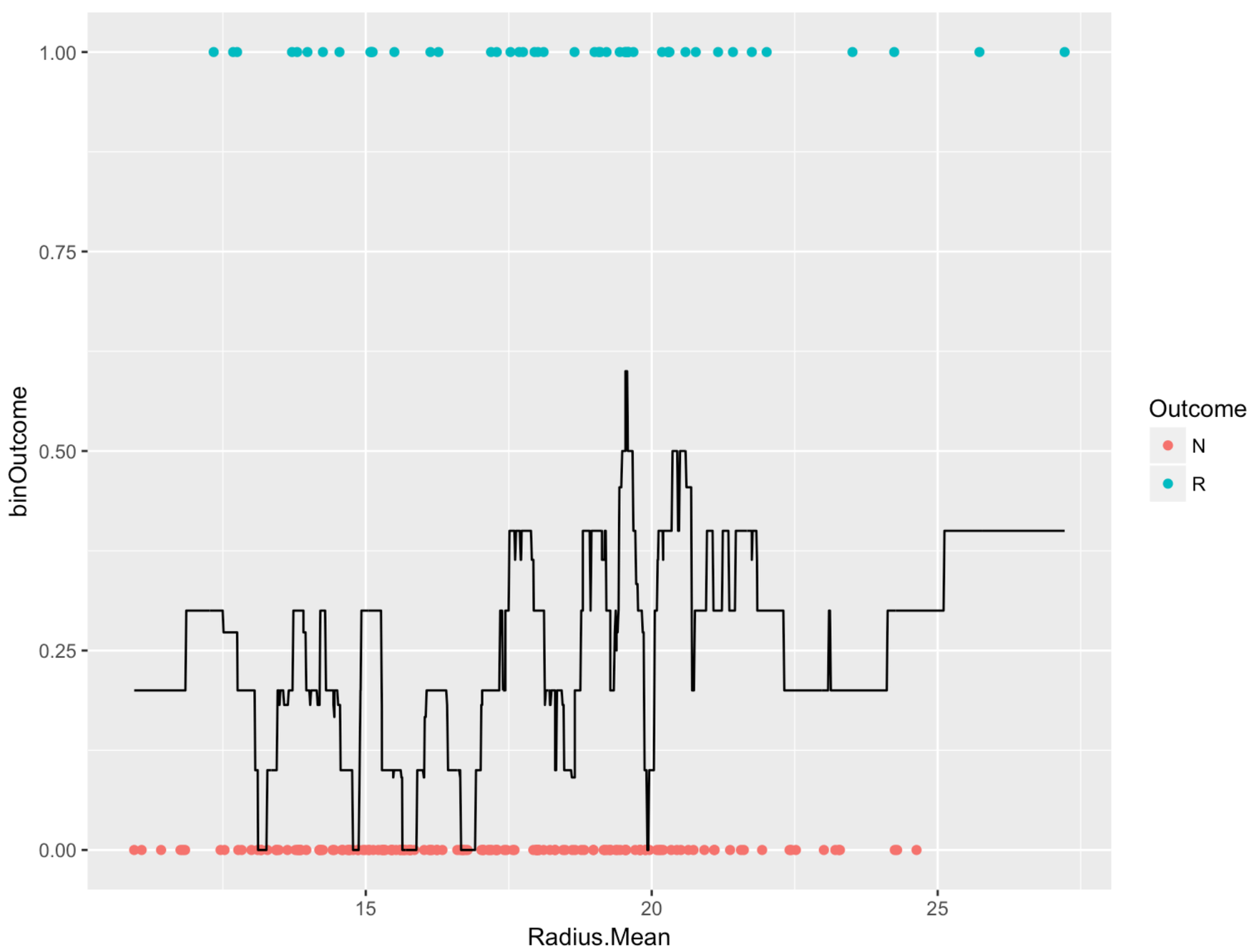
k-NN classification, Mean (prob), k=3



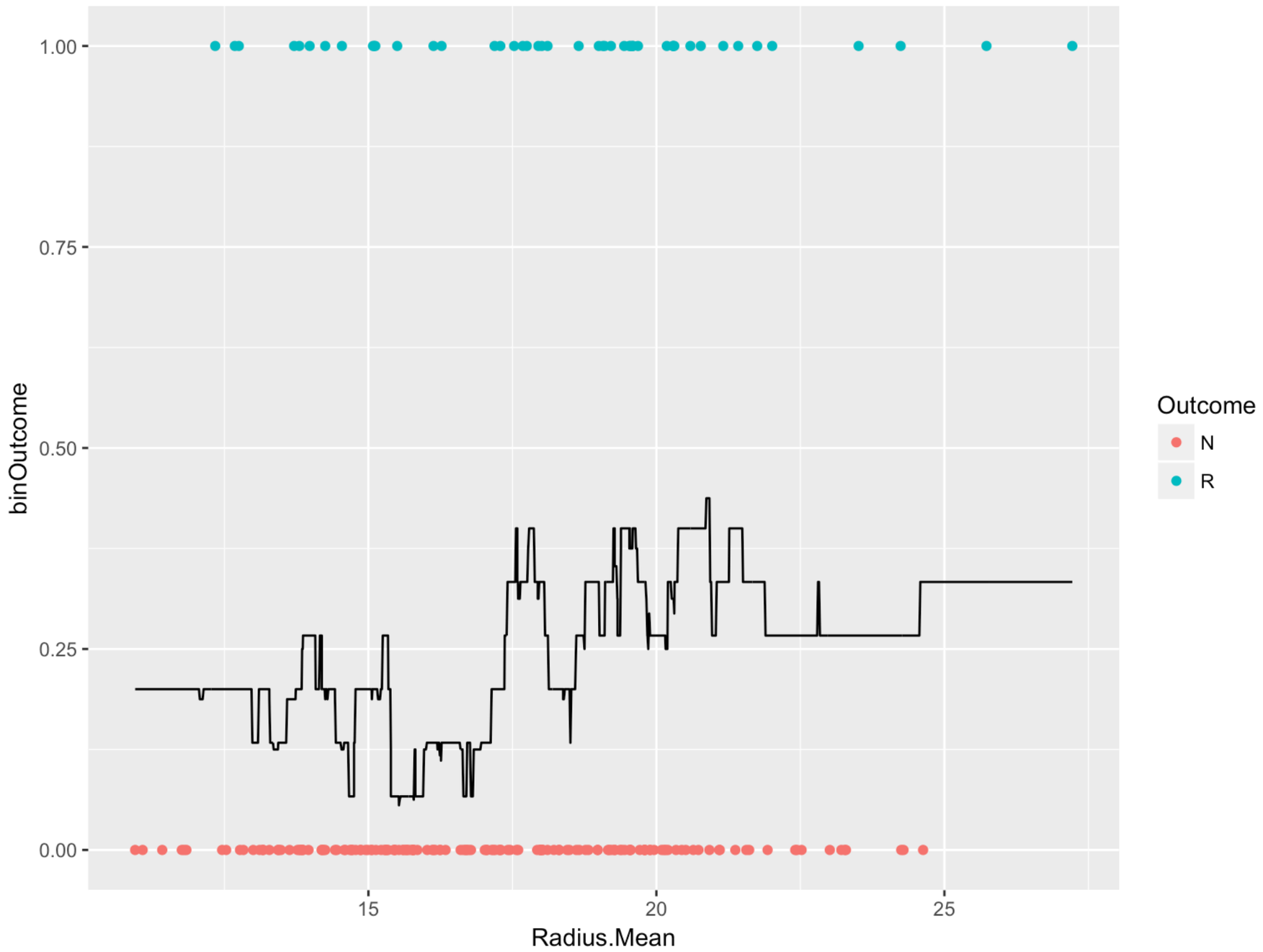
k-NN classification, Mean (prob), k=5



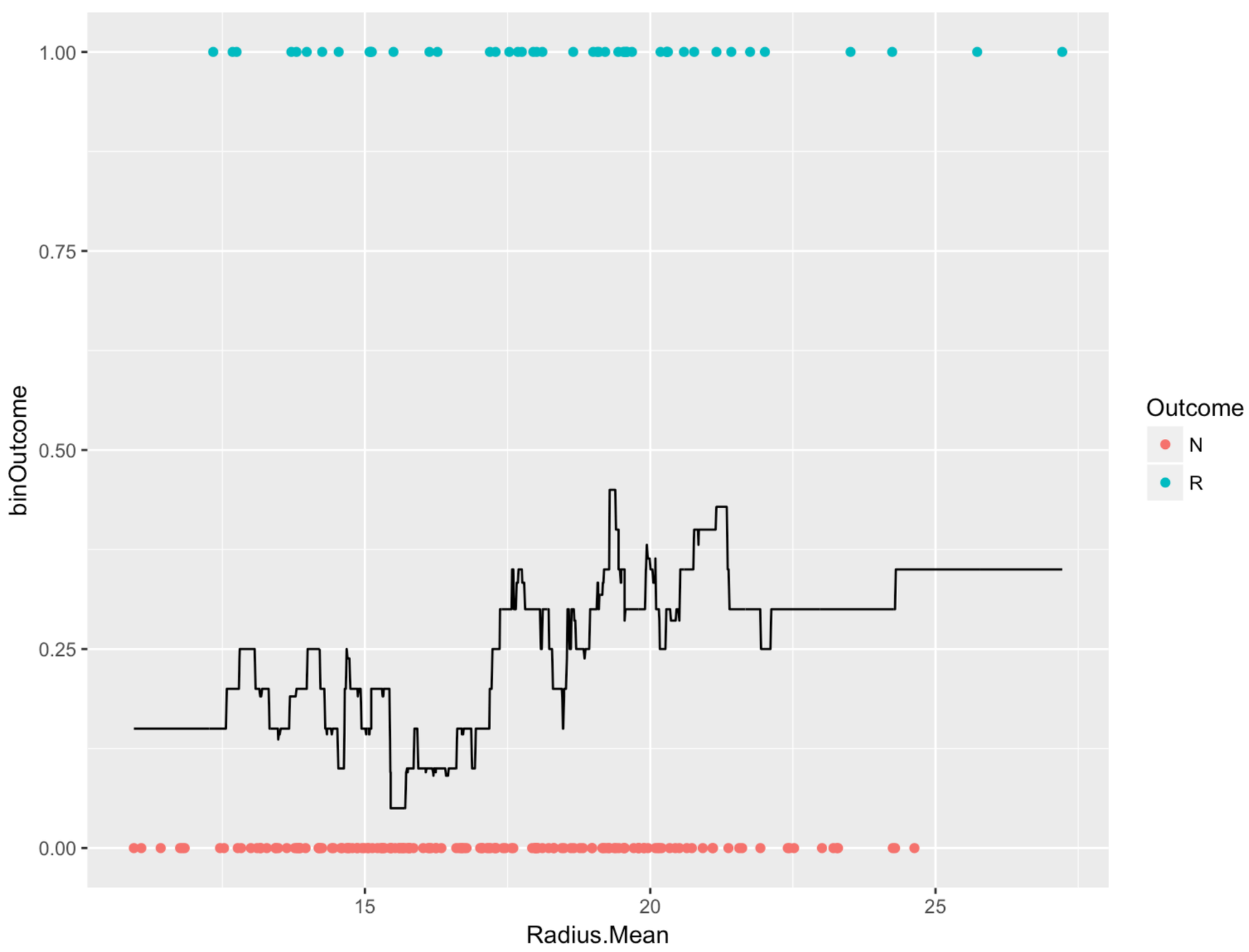
k-NN classification, Mean (prob), k=10



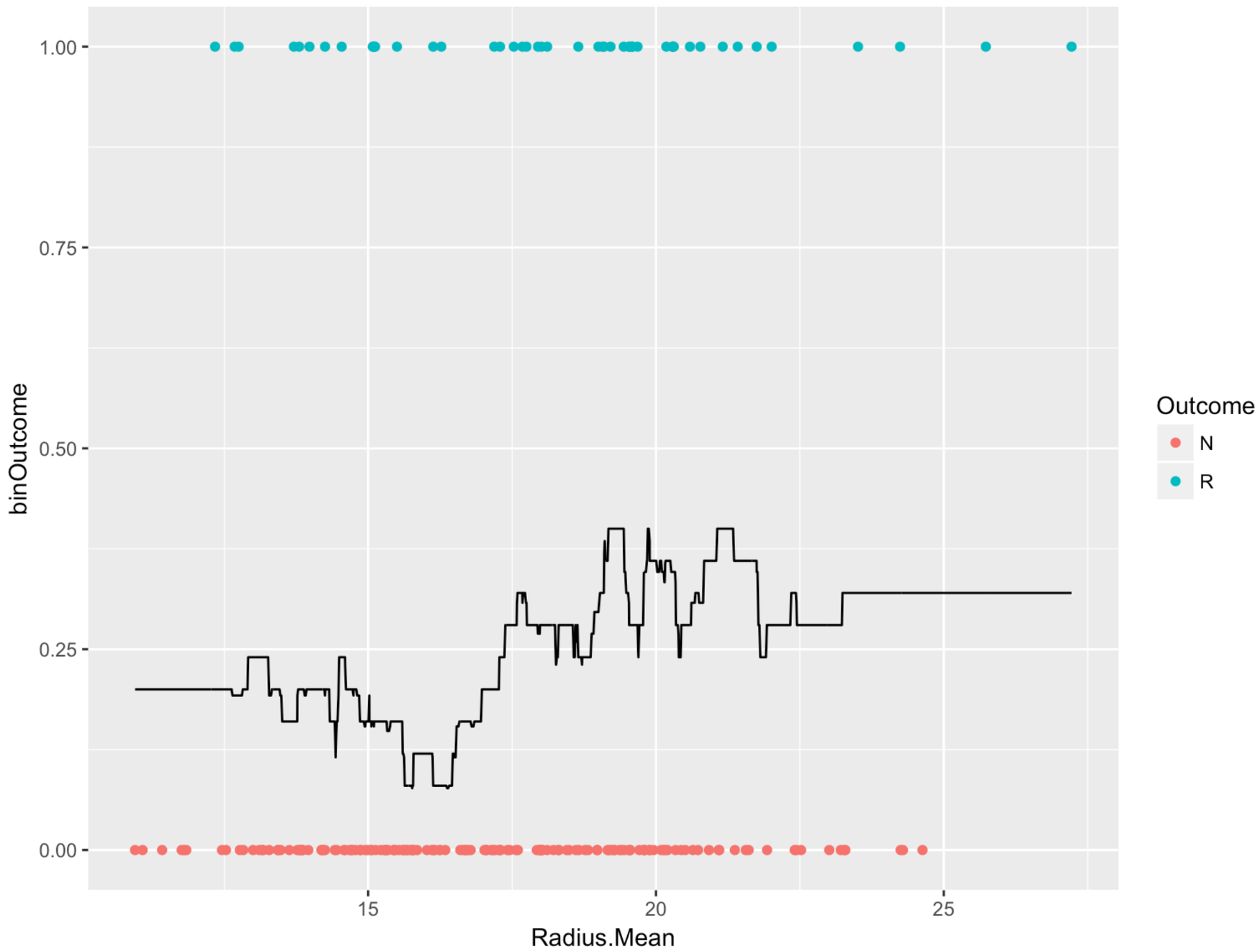
k-NN classification, Mean (prob), k=15



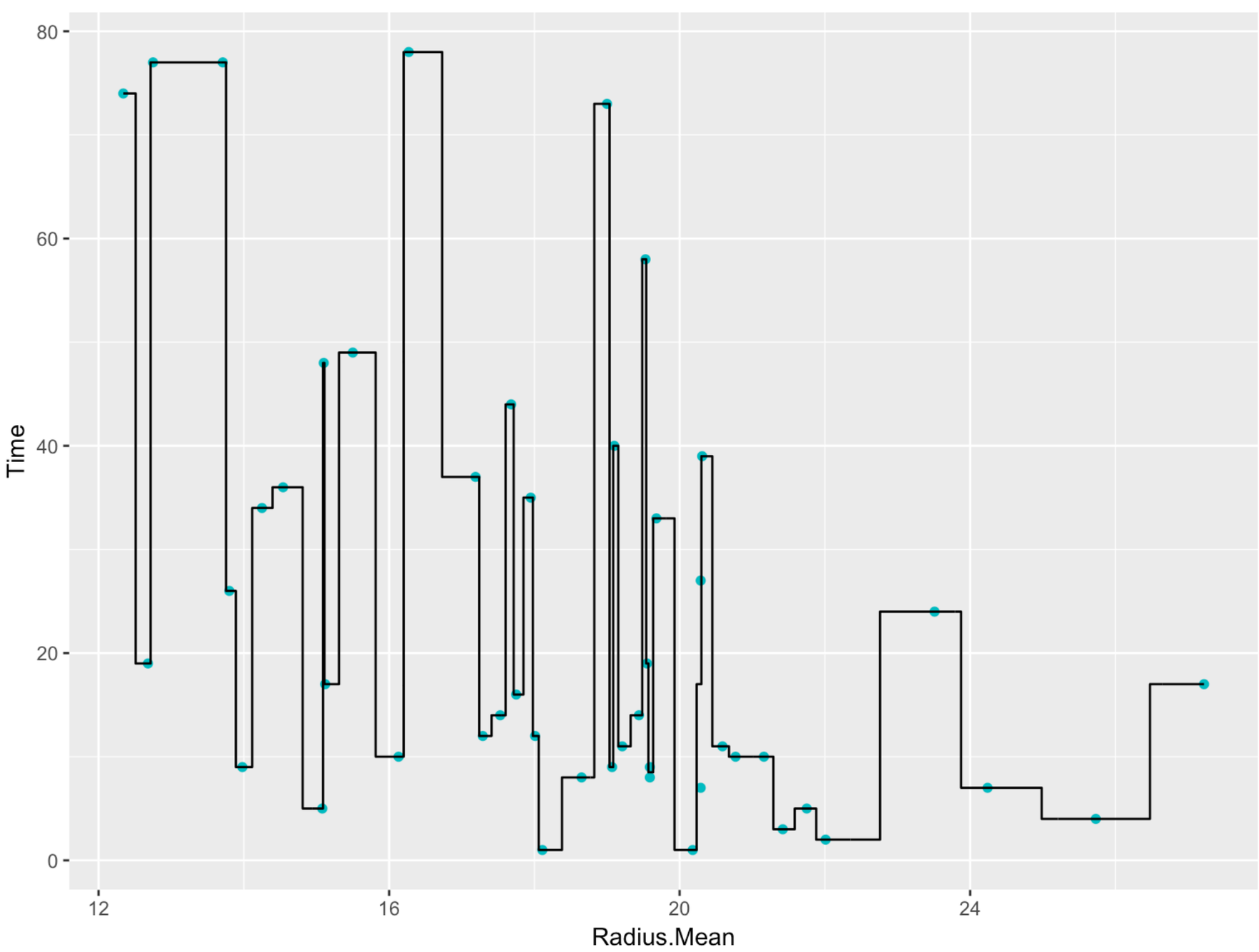
k-NN classification, Mean (prob), k=20



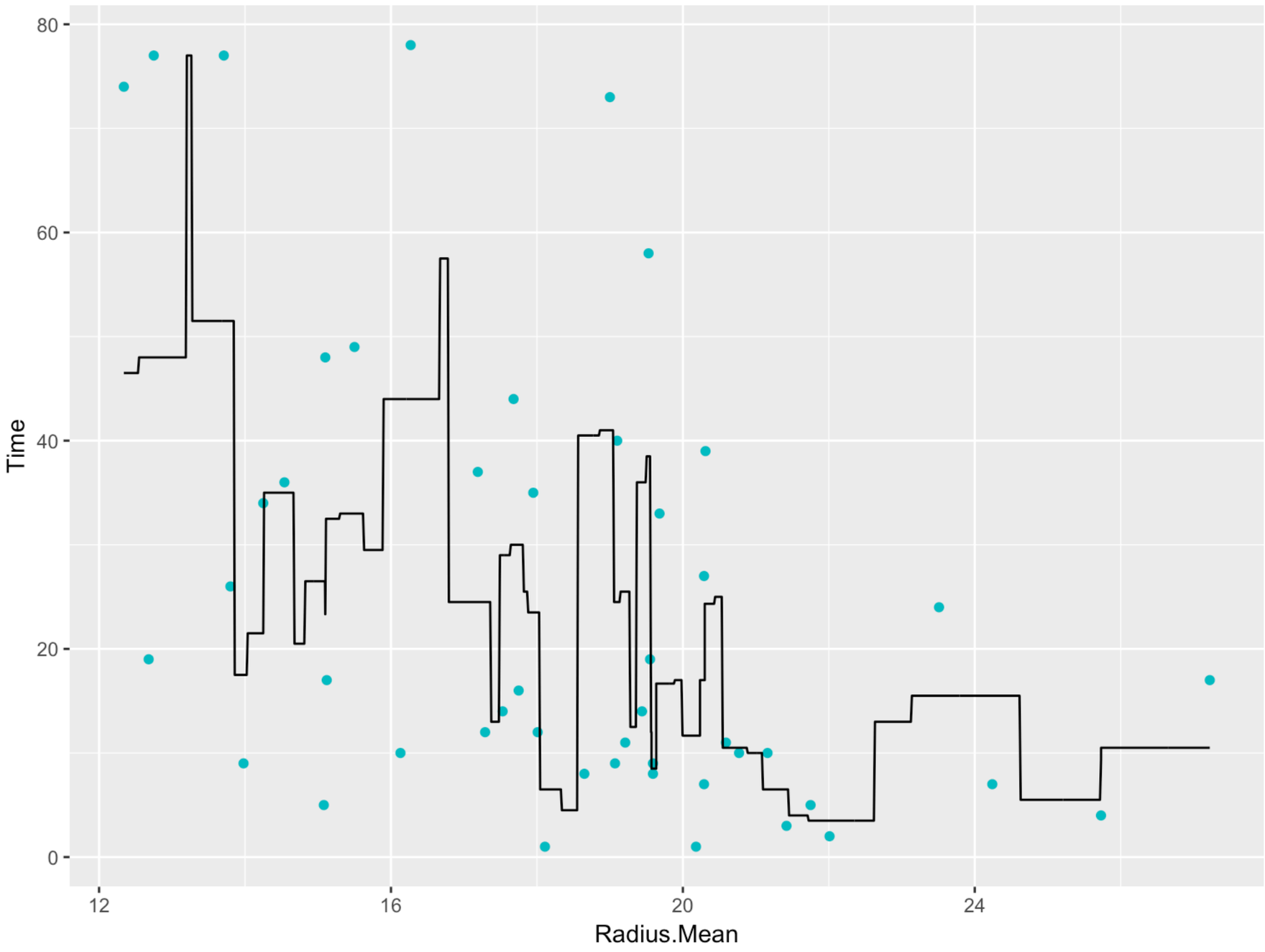
k-NN classification, Mean (prob), k=25



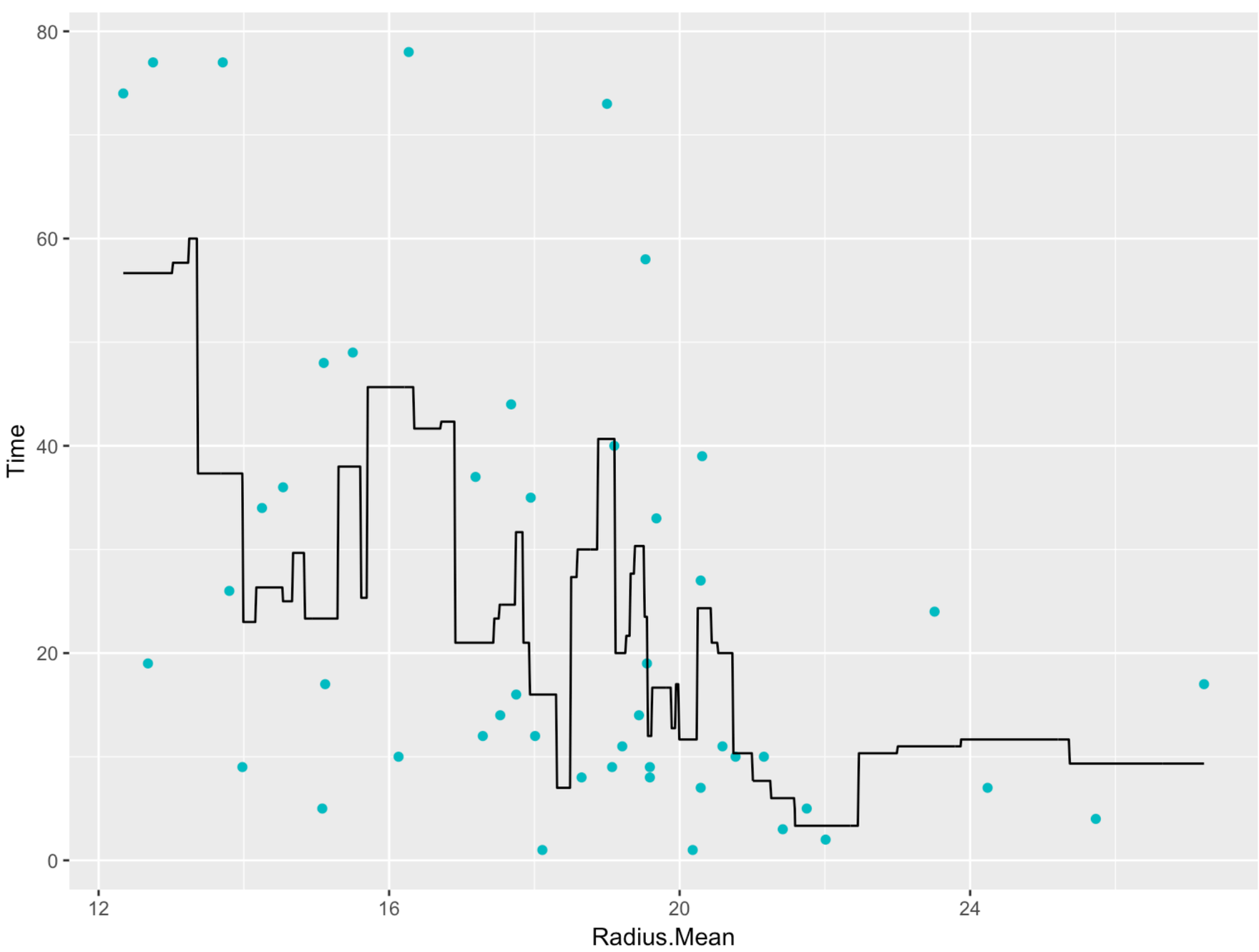
k-NN regression, Mean, k=1



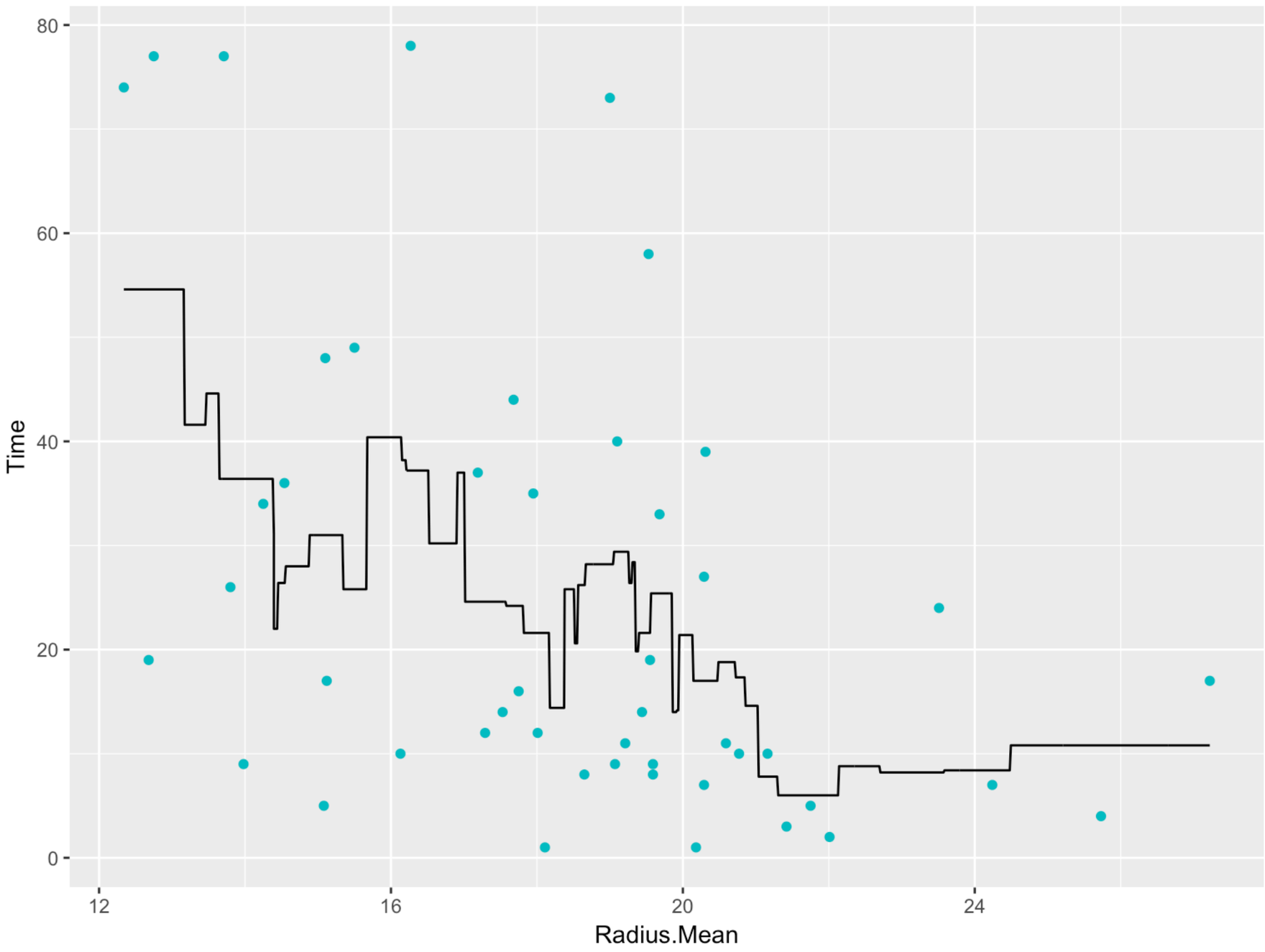
k-NN regression, Mean, k=2



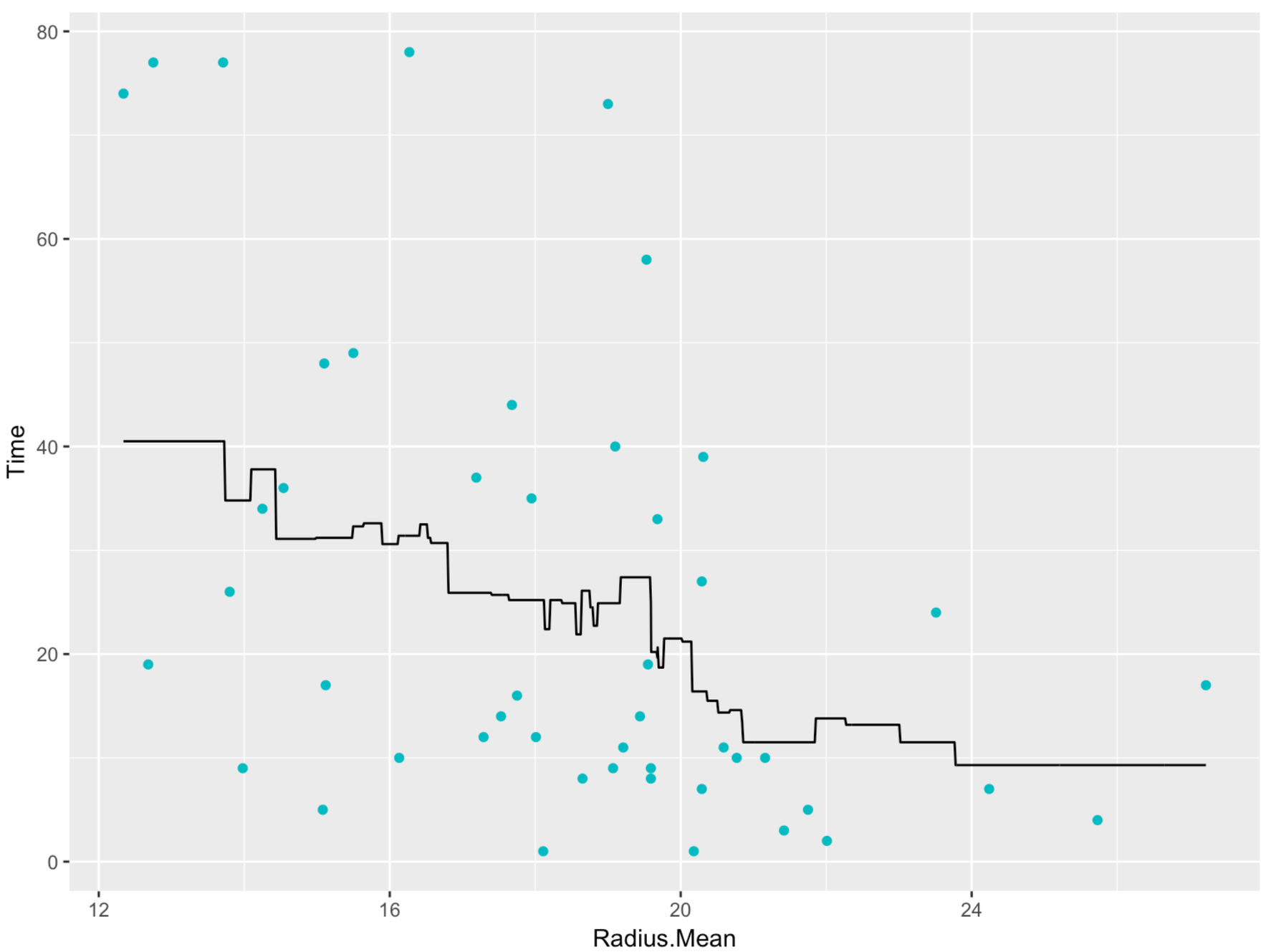
k-NN regression, Mean, k=3



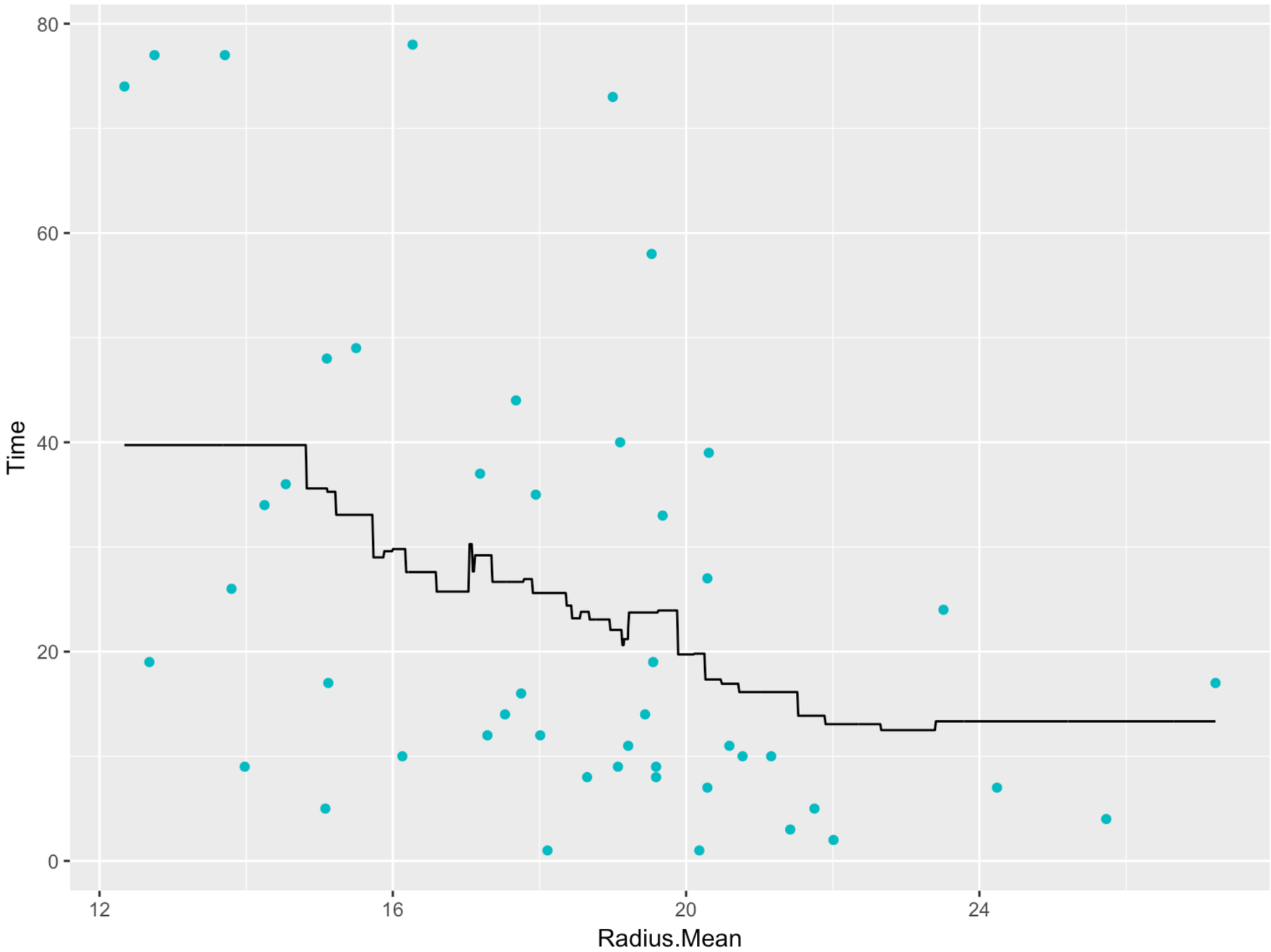
k-NN regression, Mean, k=5



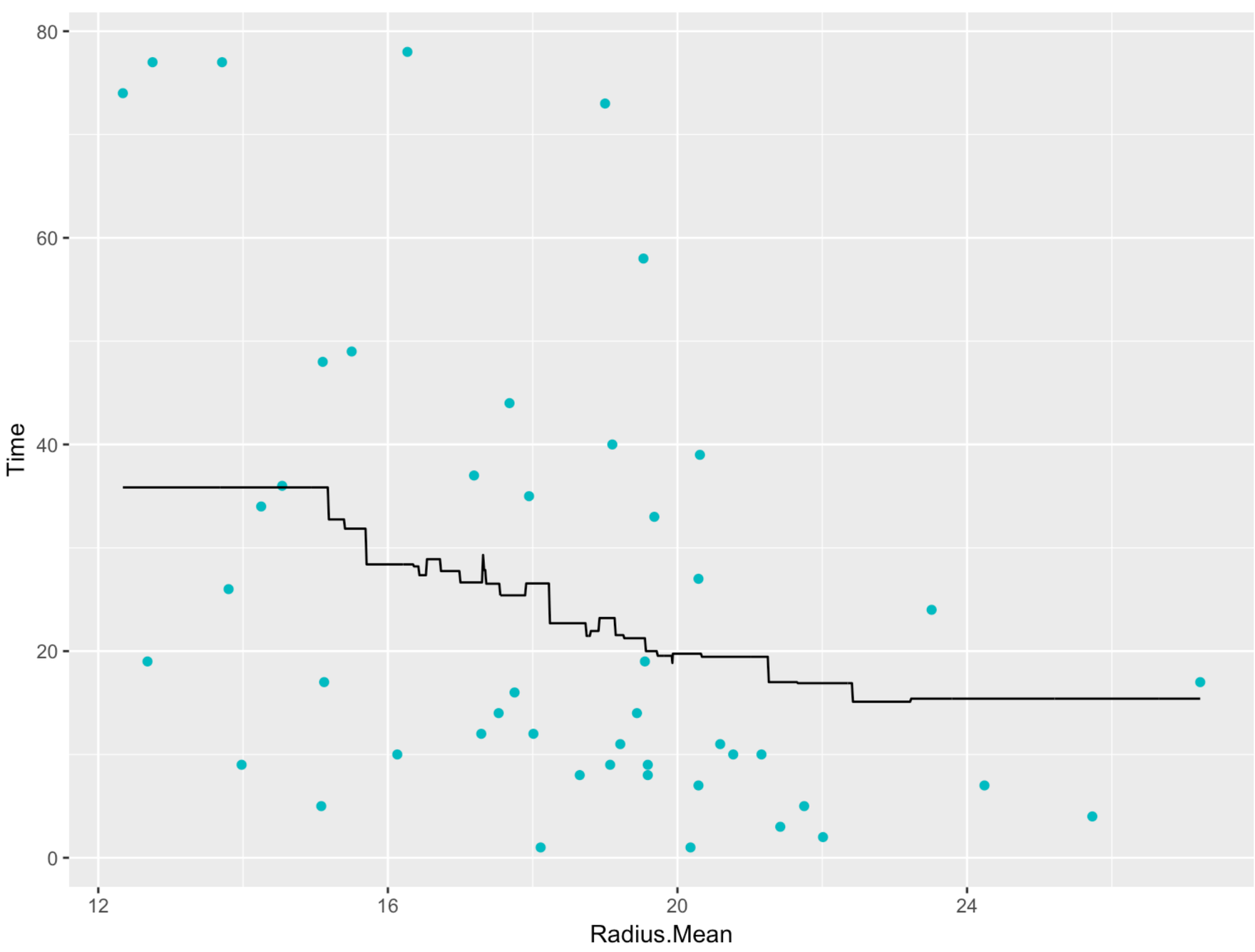
k-NN regression, Mean, k=10



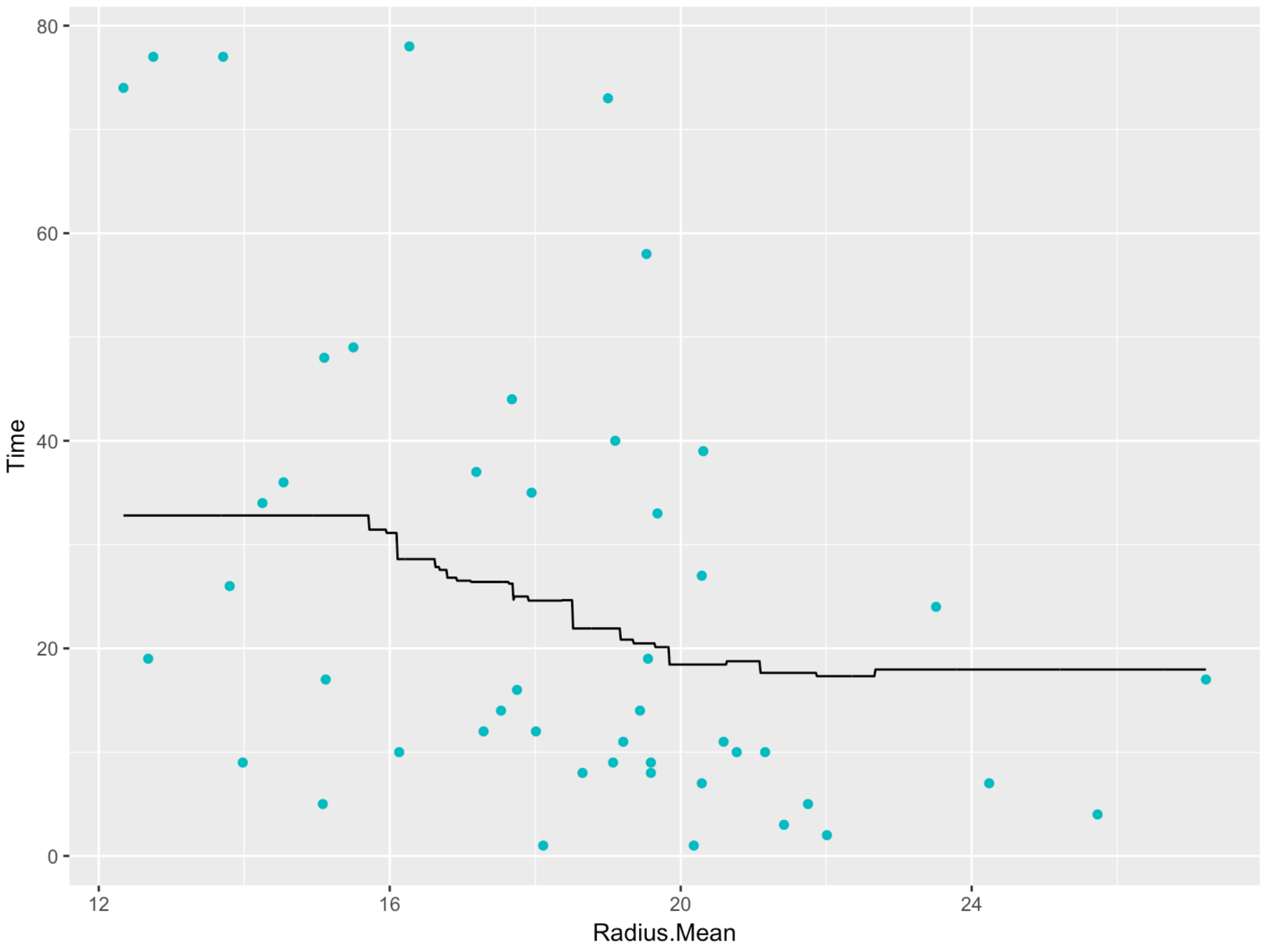
k-NN regression, Mean, k=15



k-NN regression, Mean, k=20



k-NN regression, Mean, k=25



Bias-variance trade-off

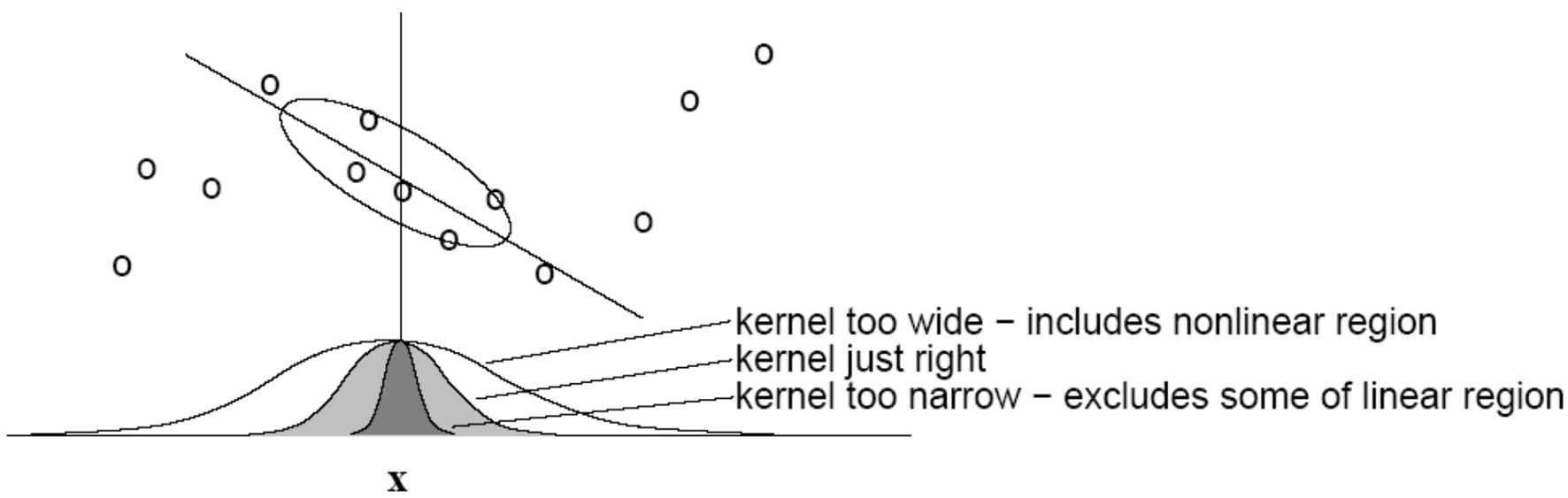
- If k is low, very non-linear functions can be approximated, but we also capture the noise in the data
  Bias is low, variance is high
- If k is high, the output is much smoother, less sensitive to data variation
  High bias, low variance
- A validation set can be used to pick the best k

Locally-weighted regression

- Weighted regression: different weights in the error function for different points

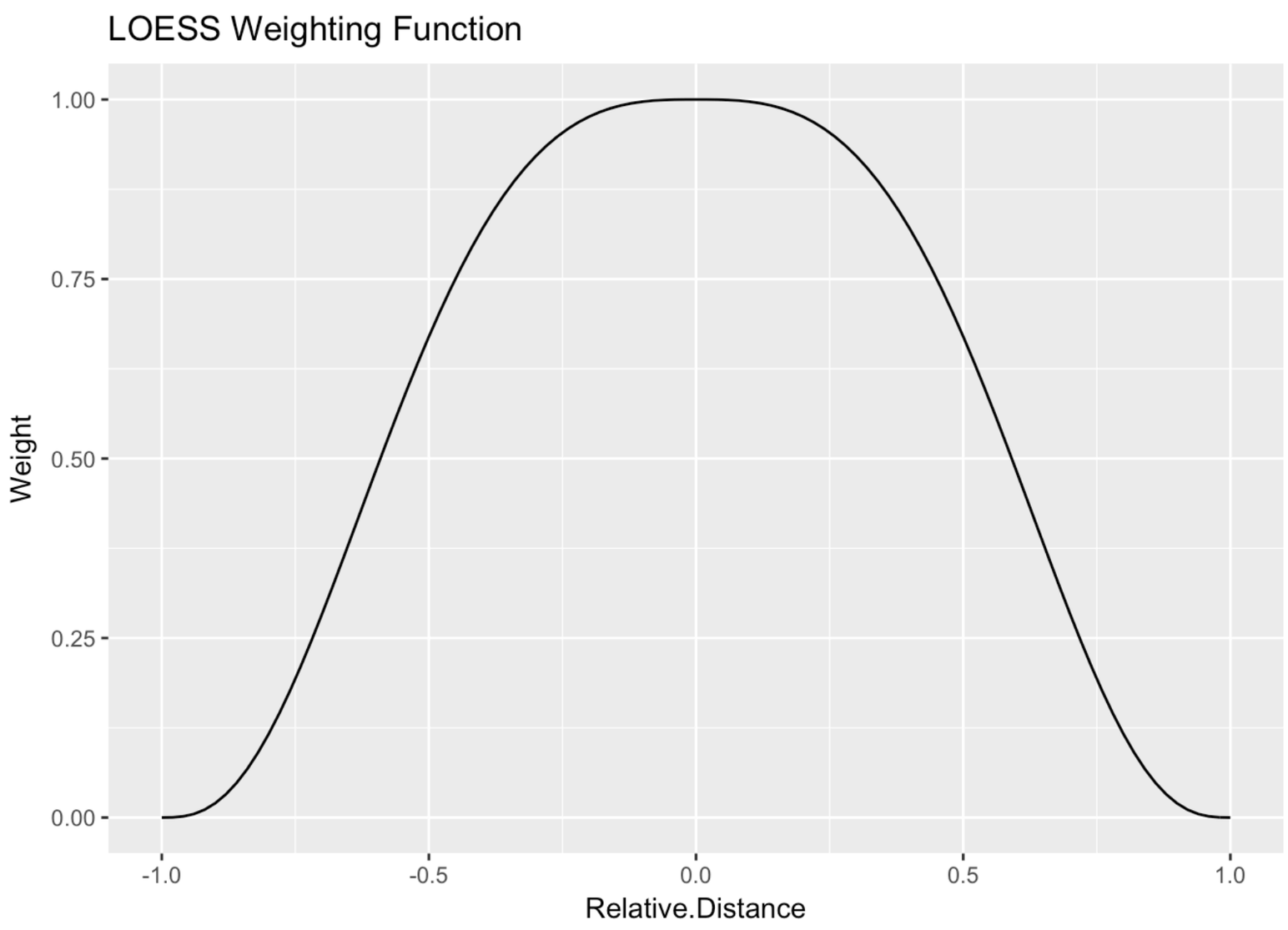
$$J(\mathbf{w}) = \sum_i w_i \cdot (h_{\mathbf{w}}(\mathbf{x}_i) - y_i)^2$$

- Locally weighted regression: weights *depend on the distance to the query point*

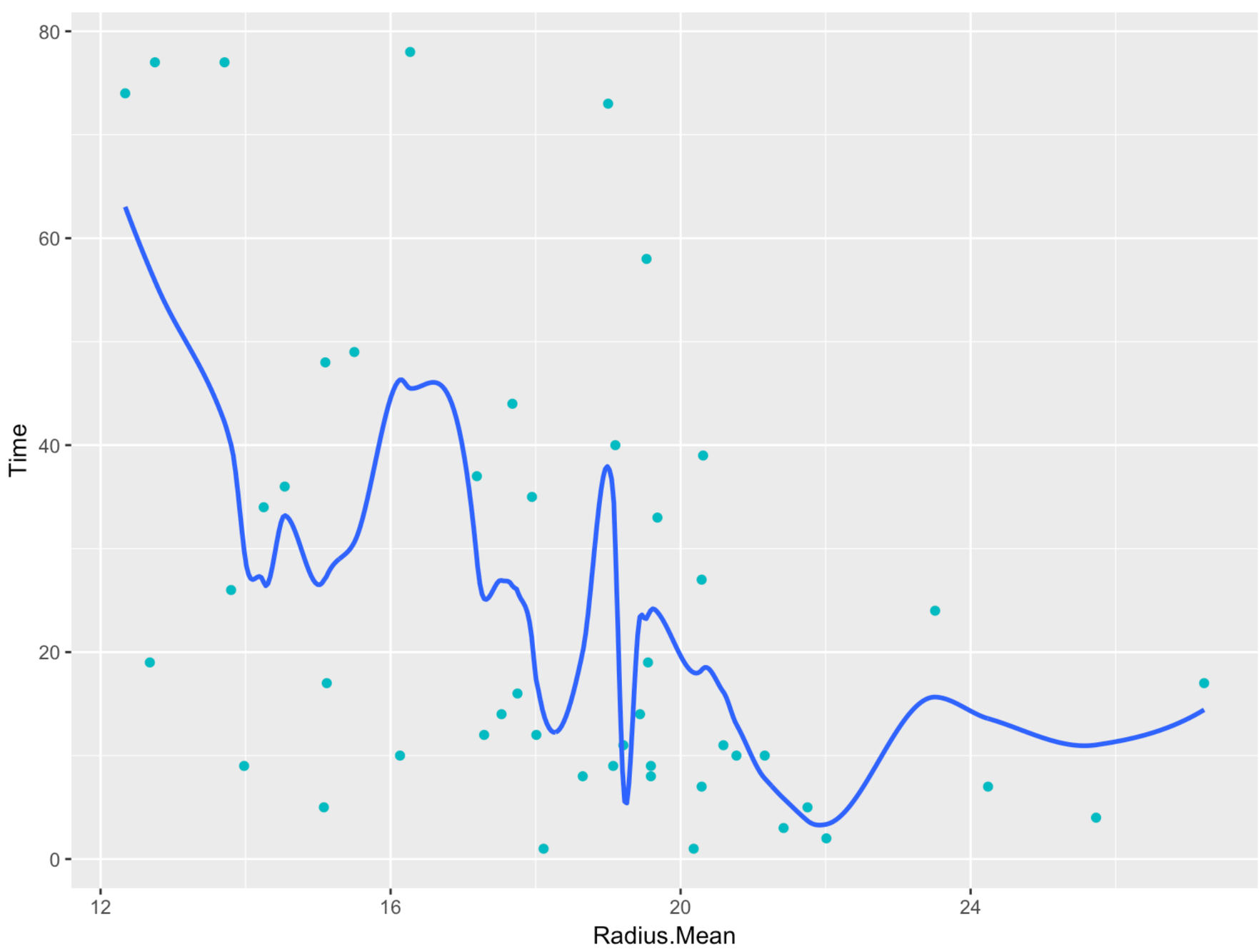


LOESS Smoothing

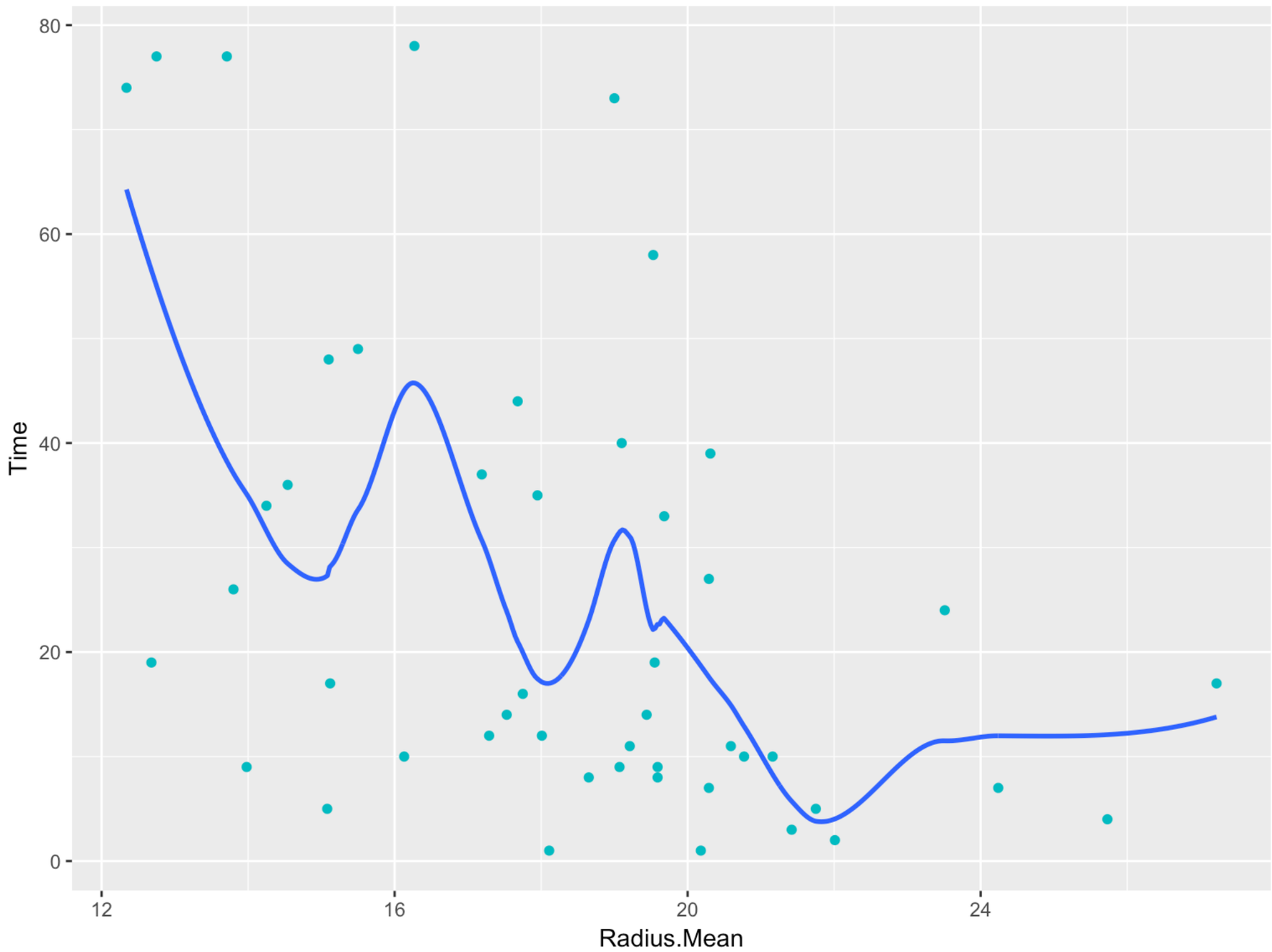
- Quadratic Regression
- Uses the closest α percent of the training set to make each prediction, called “span”



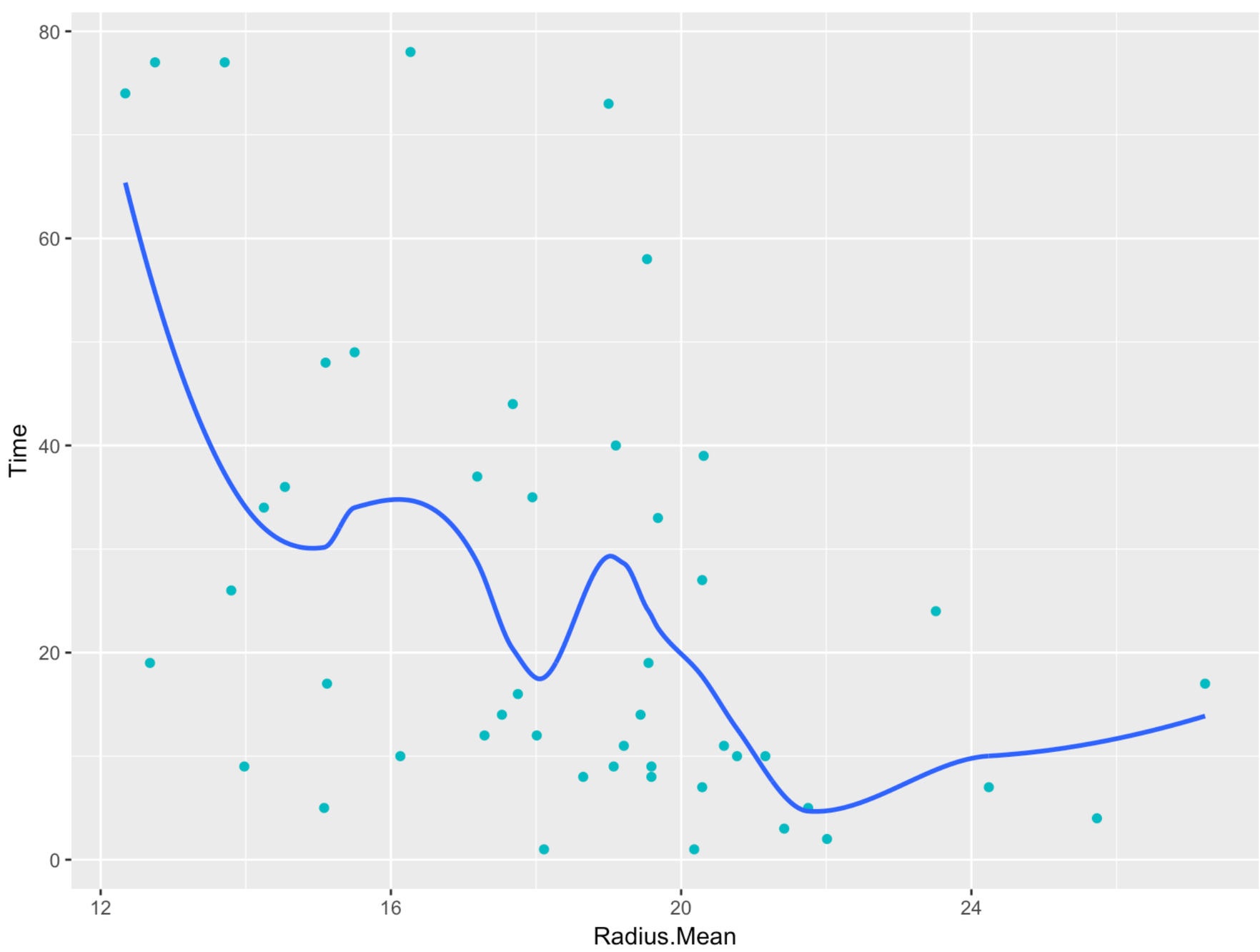
LOESS Smoothing, alpha=0.200



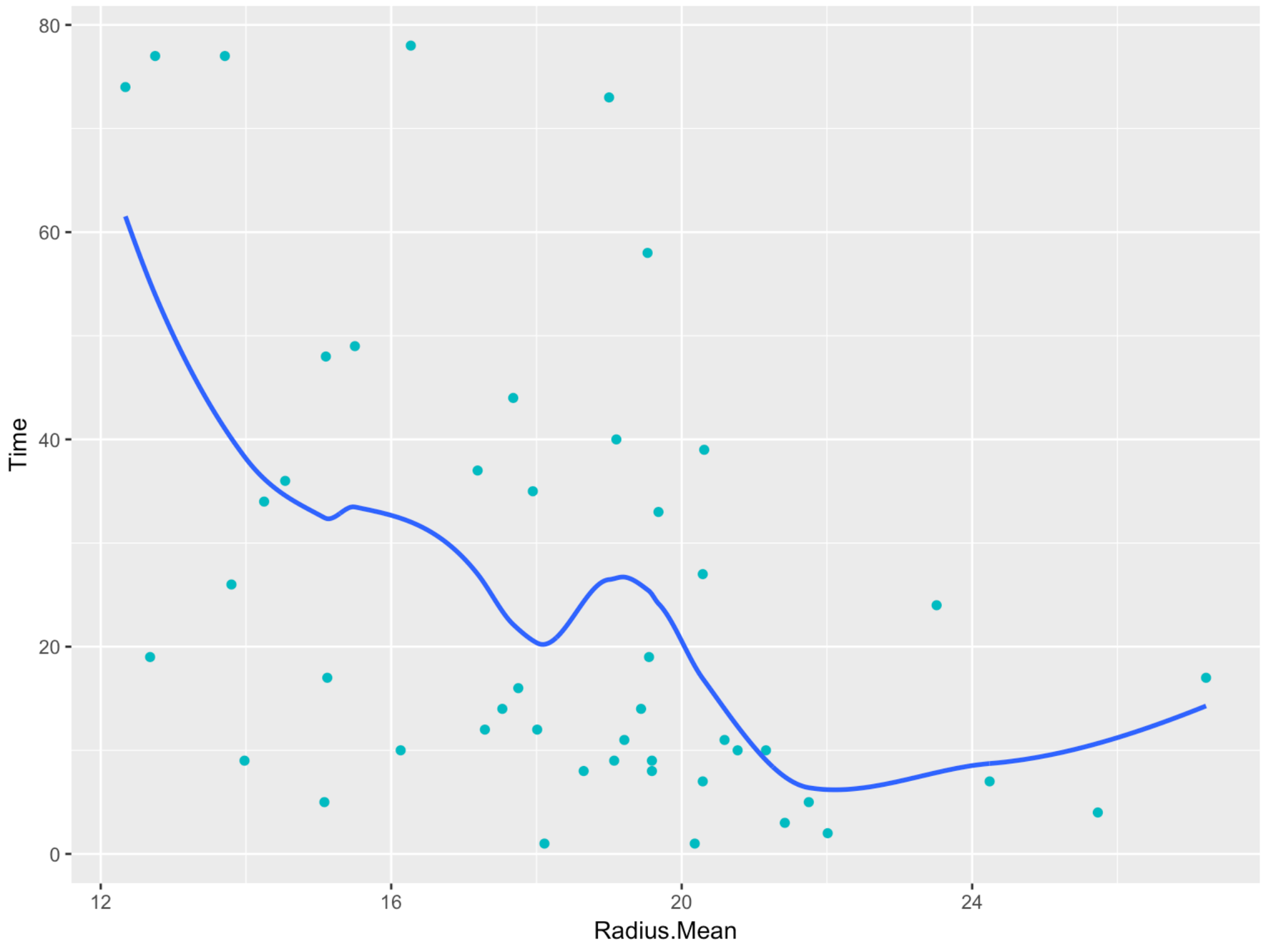
LOESS Smoothing, alpha=0.300



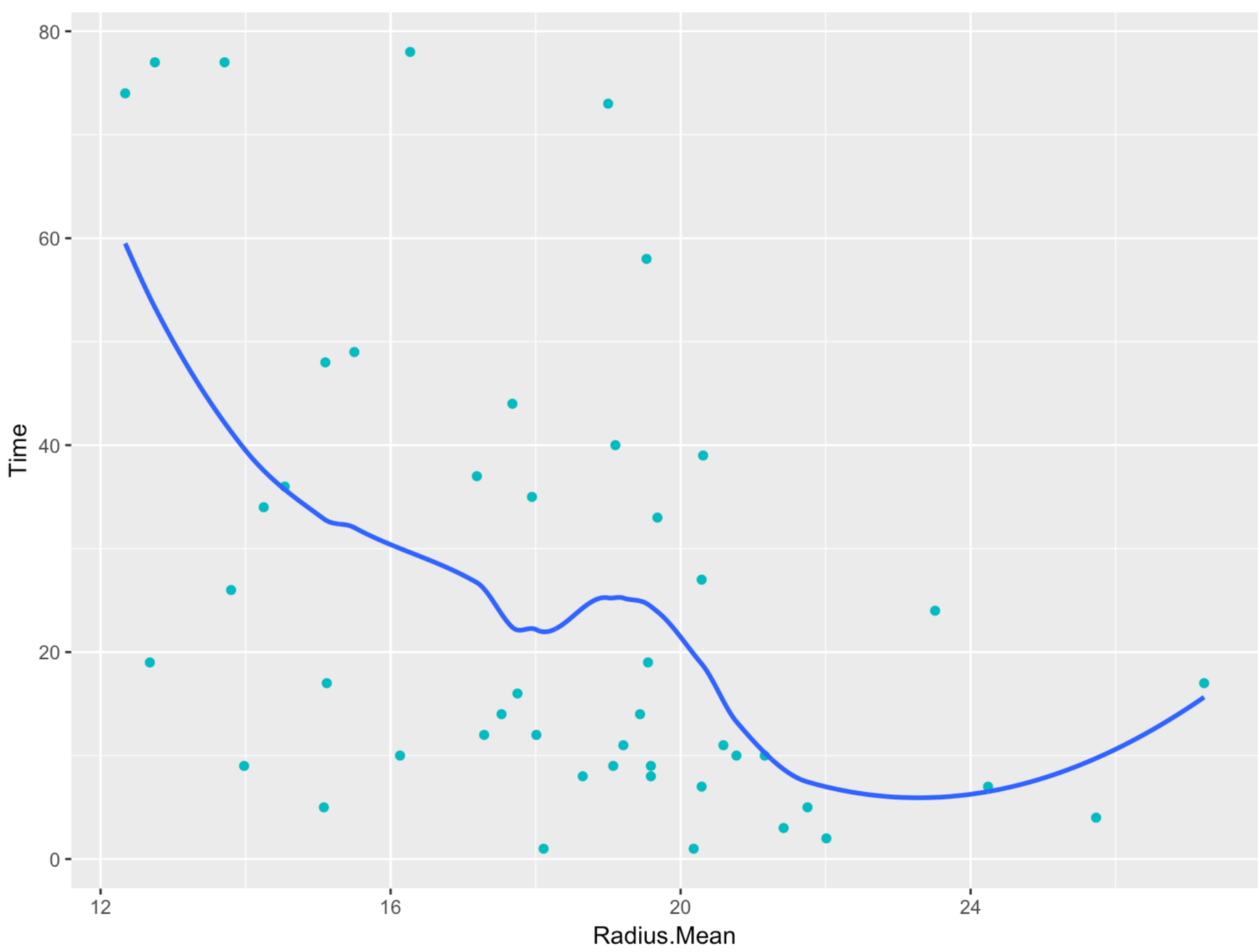
LOESS Smoothing, alpha=0.400



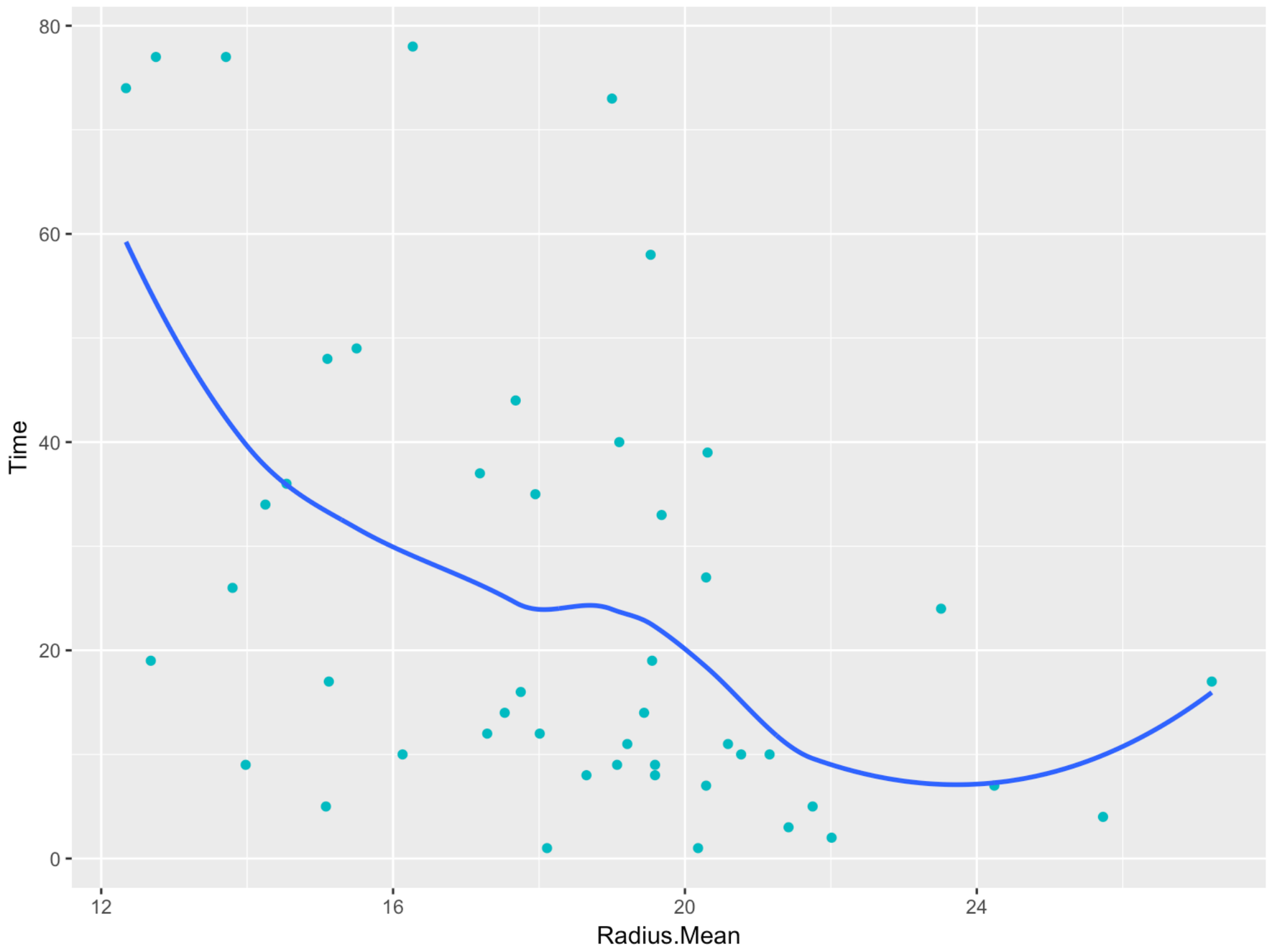
LOESS Smoothing, alpha=0.500



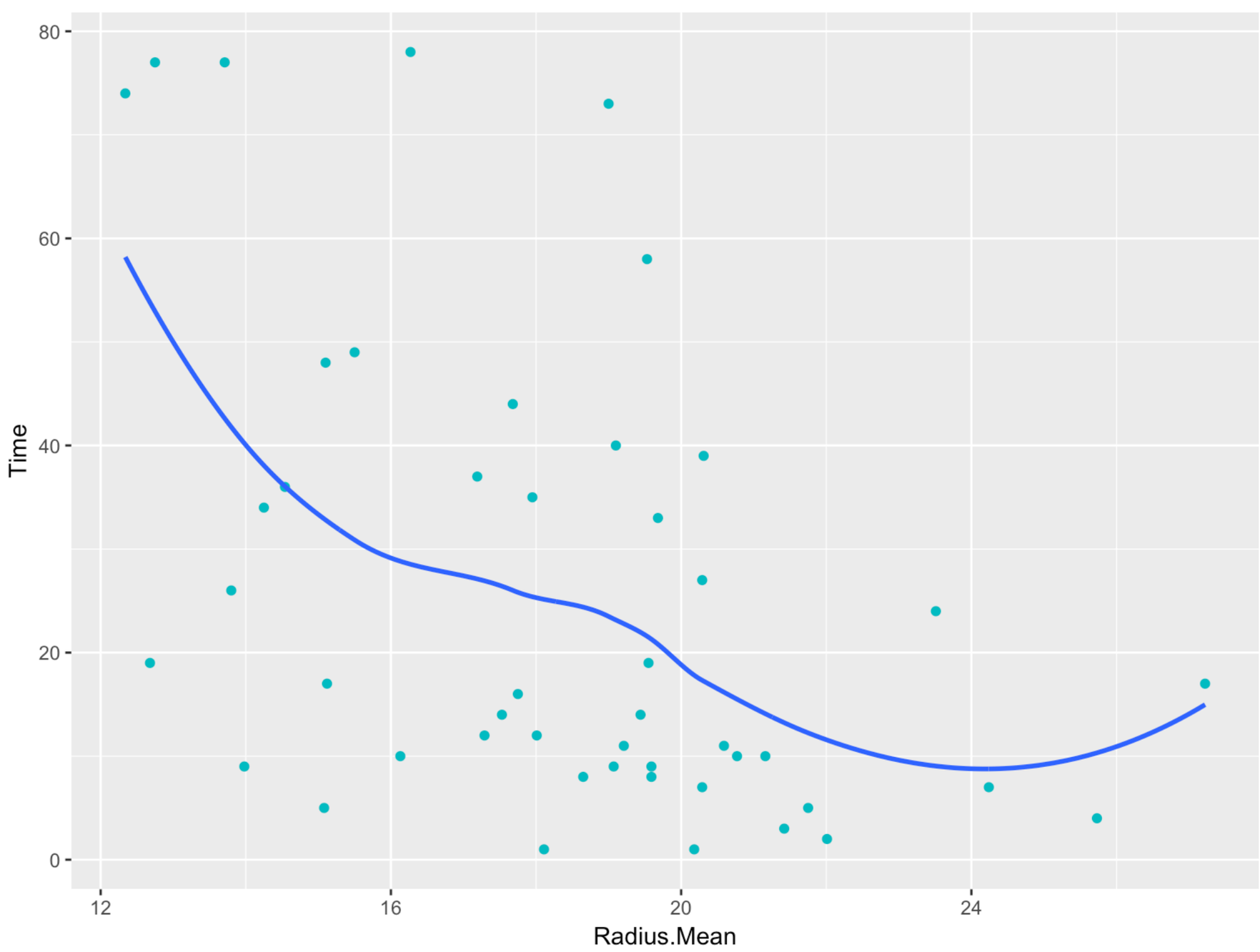
LOESS Smoothing, alpha=0.600



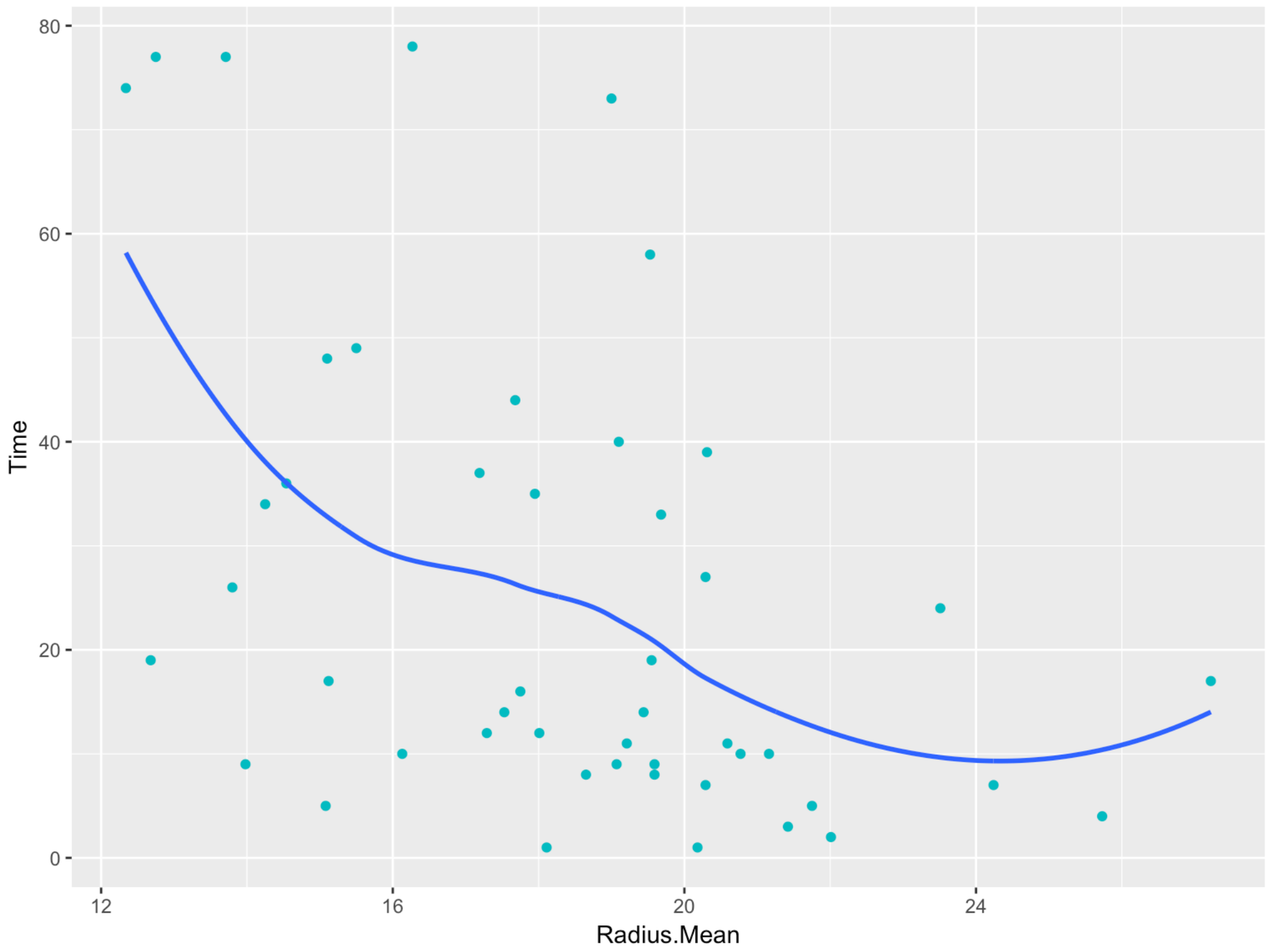
LOESS Smoothing, alpha=0.700



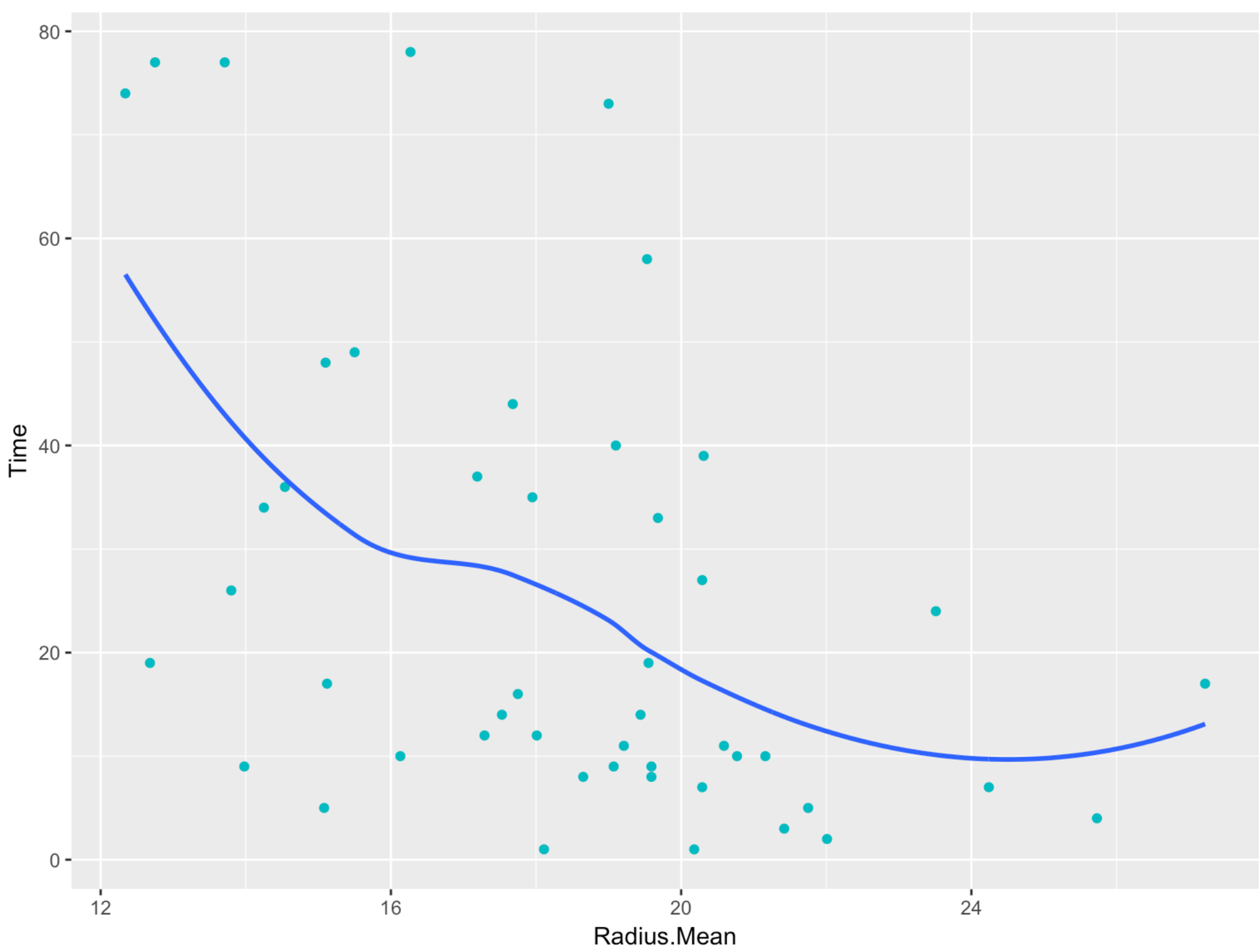
LOESS Smoothing, alpha=0.750



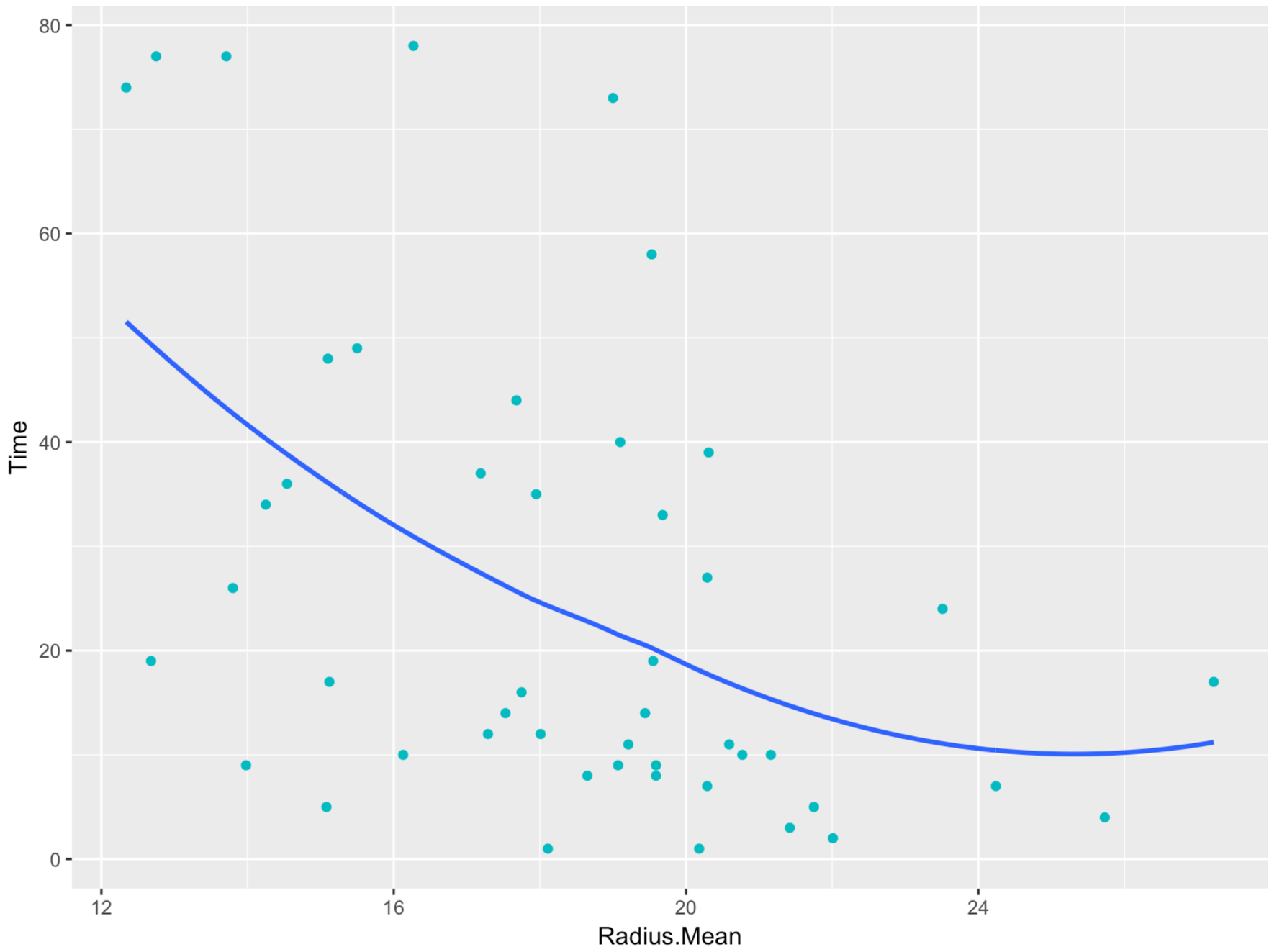
LOESS Smoothing, alpha=0.800



LOESS Smoothing, alpha=0.900



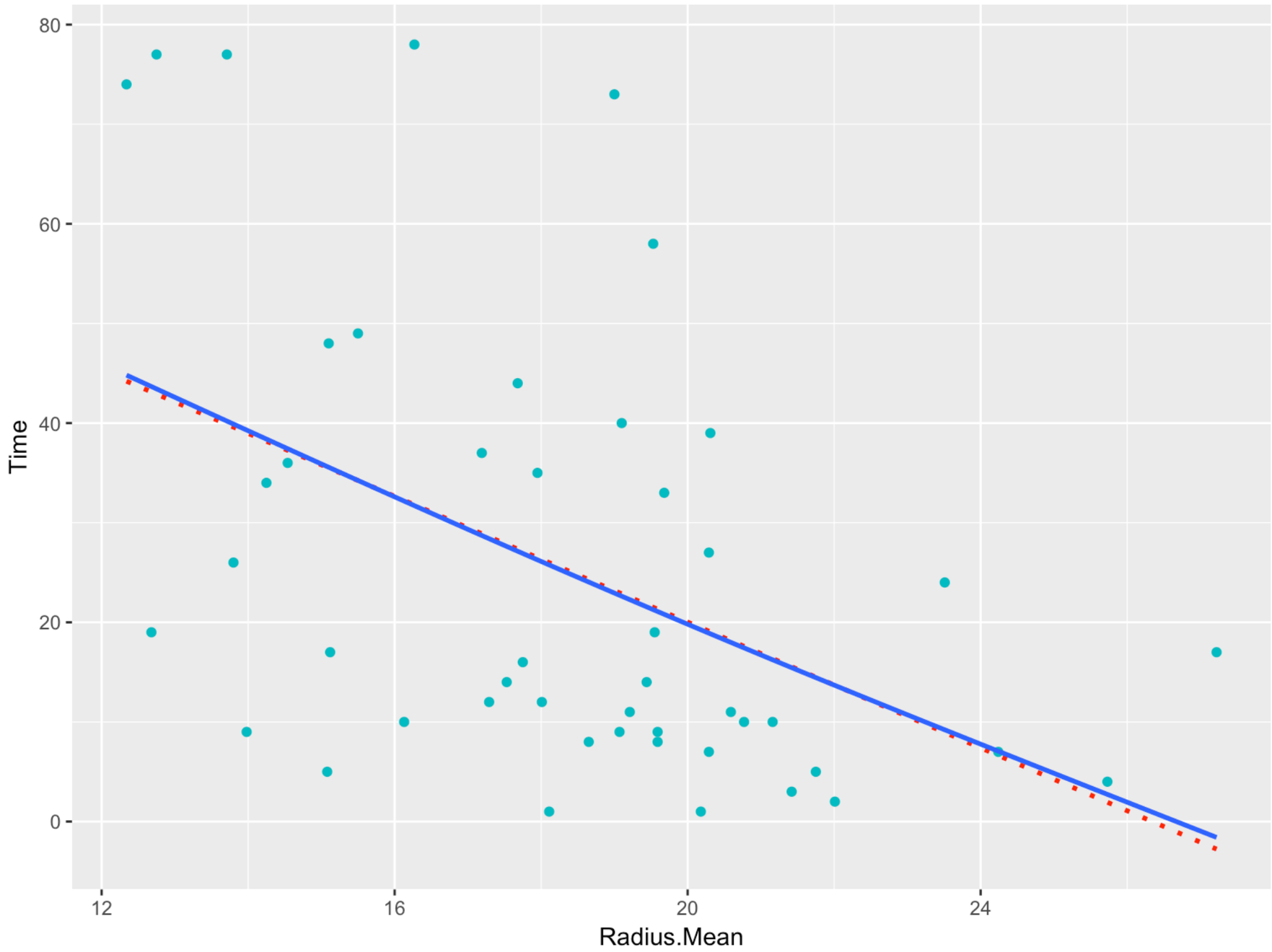
LOESS Smoothing, alpha=1.000



Generalized Additive Models

- Also smooth functions of the input variables; appearance similar to LOESS but with deeper theory.
- Based on regression splines

GAM Smoothed Example



Lazy and eager learning

- *Lazy*: wait for query before generalizing

  E.g. Nearest Neighbor

- *Eager*: generalize before seeing query

  E.g. SVM, Linear regression

Does it matter?

Pros and cons of lazy and eager learning

- Eager learners must create global approximation
- Lazy learners can create many local approximations
- An eager learner does the work off-line, summarizes lots of data with few parameters
- A lazy learner has to do lots of work sifting through the data at query time
- Typically lazy learners take longer time to answer queries and require more space

When to consider nonparametric methods

- When you have: instances that map to points in $\mathbb{R}^p$, not too many attributes per instance (< 20), lots of data
- Advantages:
  - Training is very fast
  - Easy to learn complex functions over few variables
  - Can give back confidence intervals in addition to the prediction
  - *Often wins* if you have enough data
- Disadvantages:
  - Slow at query time
  - Query answering complexity depends on the number of instances
  - *Easily fooled by irrelevant attributes* (for most distance metrics)
  - “Inference” is not possible

Decision Trees

- What are decision trees?
- Methods for constructing decision trees
- Overfitting avoidance

Non-metric learning

- The result of learning is not a set of parameters, but there is **no distance metric** to assess similarity of different instances
- Typical examples:
  - Decision trees
  - Rule-based systems

Example: Decision tree for Wisconsin data

- Internal nodes are tests on the values of different attributes
- Tests can be binary or multi-valued
- Each training example $\langle \mathbf{x}_i, y_i \rangle$ falls in precisely one leaf.

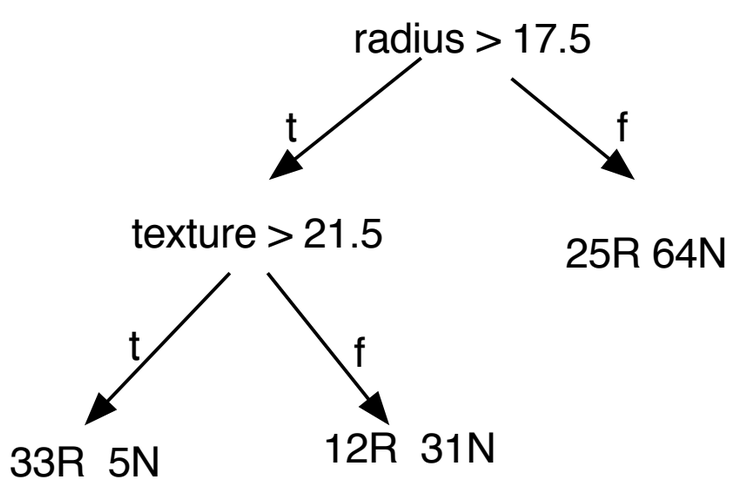
Using decision trees for classification

How do we classify a new a new instance, e.g.: *radius=18, texture=12, …*

- At every node, test the corresponding attribute
- Follow the appropriate branch of the tree
- At a leaf, one can predict the class of the majority of the examples for the corresponding leaf, or the probabilities of the two classes.

Decision trees as logical representations

A decision tree can be converted an equivalent set of if-then rules.

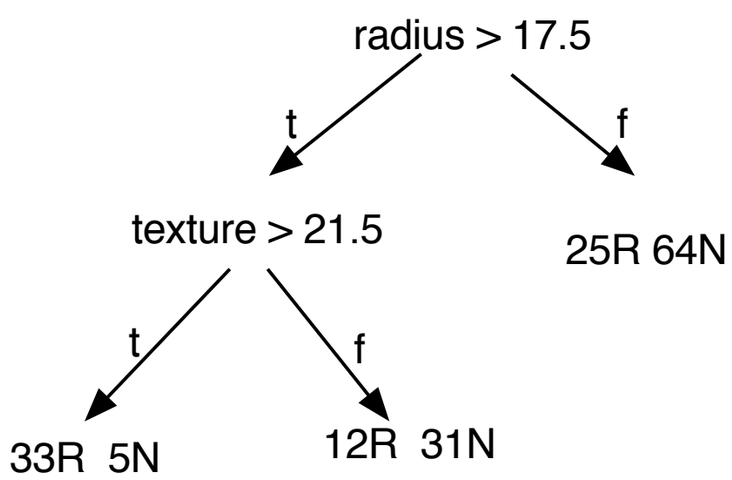


IF	THEN most likely class is

radius $>$ 17.5 AND texture $>$ 21.5	R
radius $>$ 17.5 AND texture $\leq$ 21.5	N
radius $\leq$ 17.5	N

Decision trees as logical representations

A decision tree can be converted an equivalent set of if-then rules.



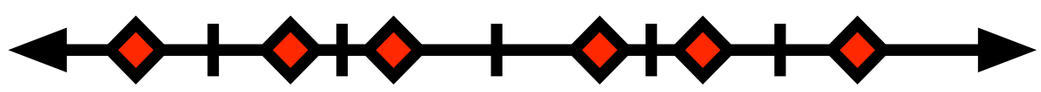
IF	THEN P(R) is
radius$>$ 17.5 AND texture$>$ 21.5	$33/(33+5)$
radius$>$ 17.5 AND texture$\leq$ 21.5	$12/(12+31)$
radius$\leq$ 17.5	$25/(25+64)$

Decision trees, more formally

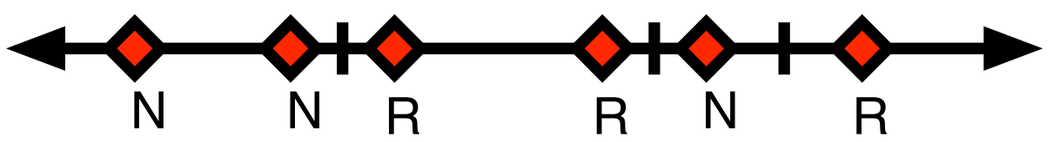
- Each internal node contains a *test*, on the value of one (typically) or more feature values
- A test produces discrete outcomes, e.g.,
  - radius > 17.5
  - radius $\in [12, 18]$
  - grade is $\in \{A, B, C\}$
  - color is RED
- For discrete features, typically branch on some, or all, possible values
- For real features, typically branch based on a threshold value
- *A finite set of possible tests* is usually decided before learning the tree; learning comprises choosing the shape of the tree and the tests at every node.

More on tests for real-valued features

- Suppose feature j is real-valued,
- How do we choose a finite set of possible thresholds, for tests of the form $x_j > \tau$?
  - Regression: choose midpoints of the observed data values, $x_{1,j}, x_{2,j}, \ldots, x_{m,j}$



  - Classification: choose midpoints of data values with different y values



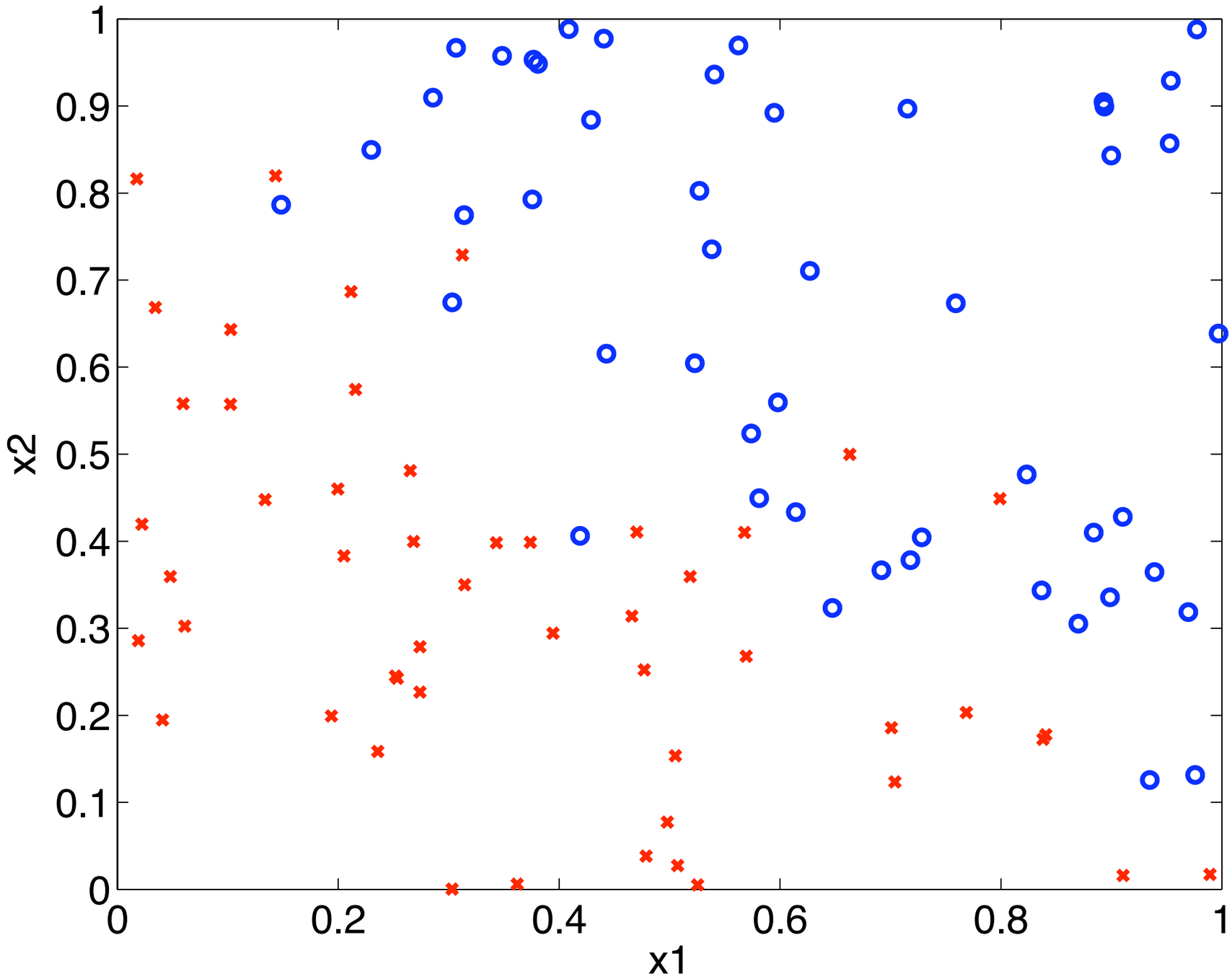
Representational power and efficiency of decision trees

- Suppose the input $\mathbf{x}$ consists of n binary features
- How can a decision tree represent:
  - $y = x_1$ AND x_2 AND … AND x_n
  - $y = x_1$ OR x_2 OR … OR x_n
  - $y = x_1$ XOR x_2 XOR … XOR x_n

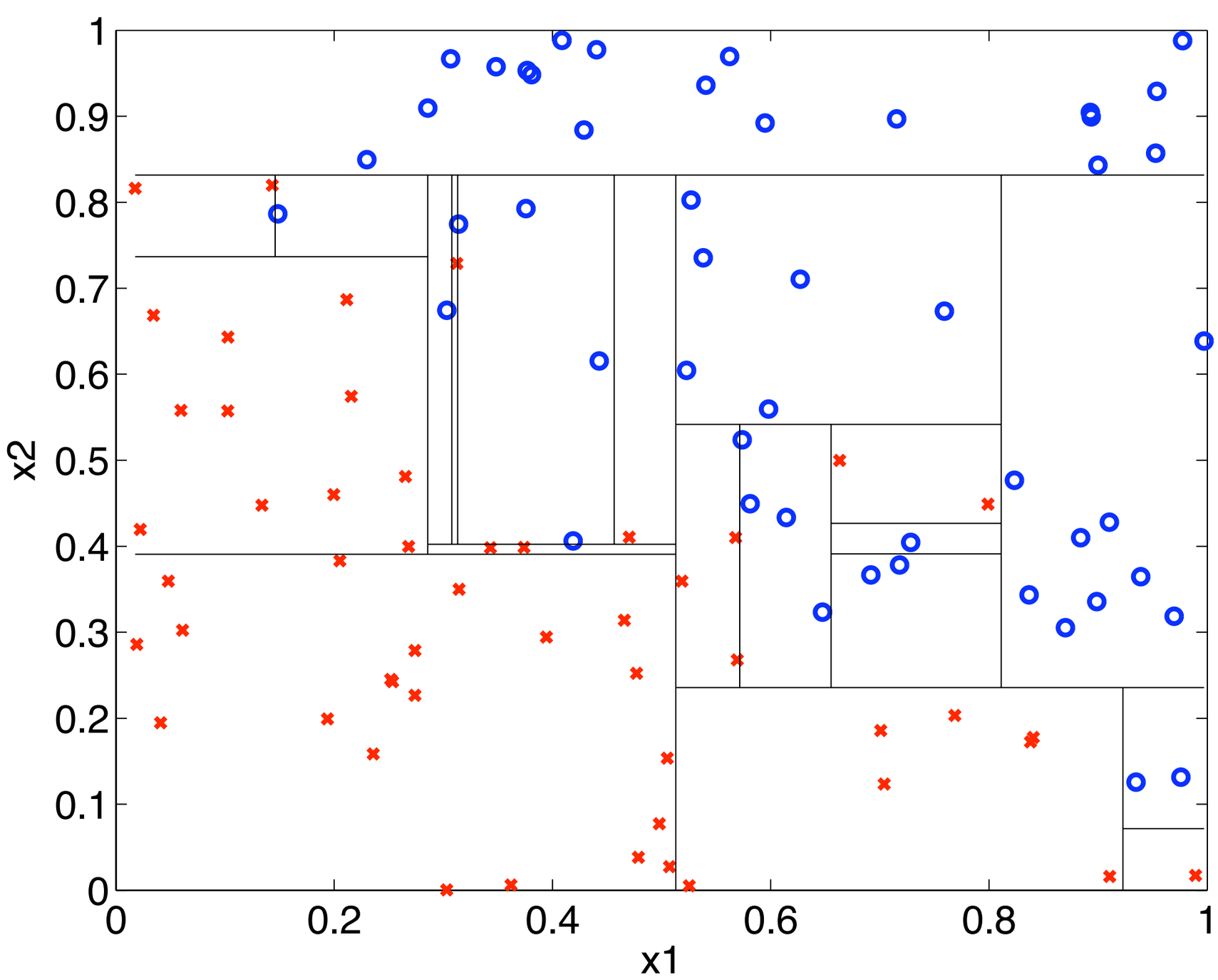
Representational power and efficiency of decision trees

- With typical univariate tests, AND and OR are easy, taking $O(n)$ tests
- Parity/XOR type problems are hard, taking $O(2^n)$ tests
- With real-valued features, decision trees are good at problems in which the class label is **constant in large, connected, axis-orthogonal regions of the input space.**

An artificial example



Example: Decision tree decision surface



How do we learn decision trees?

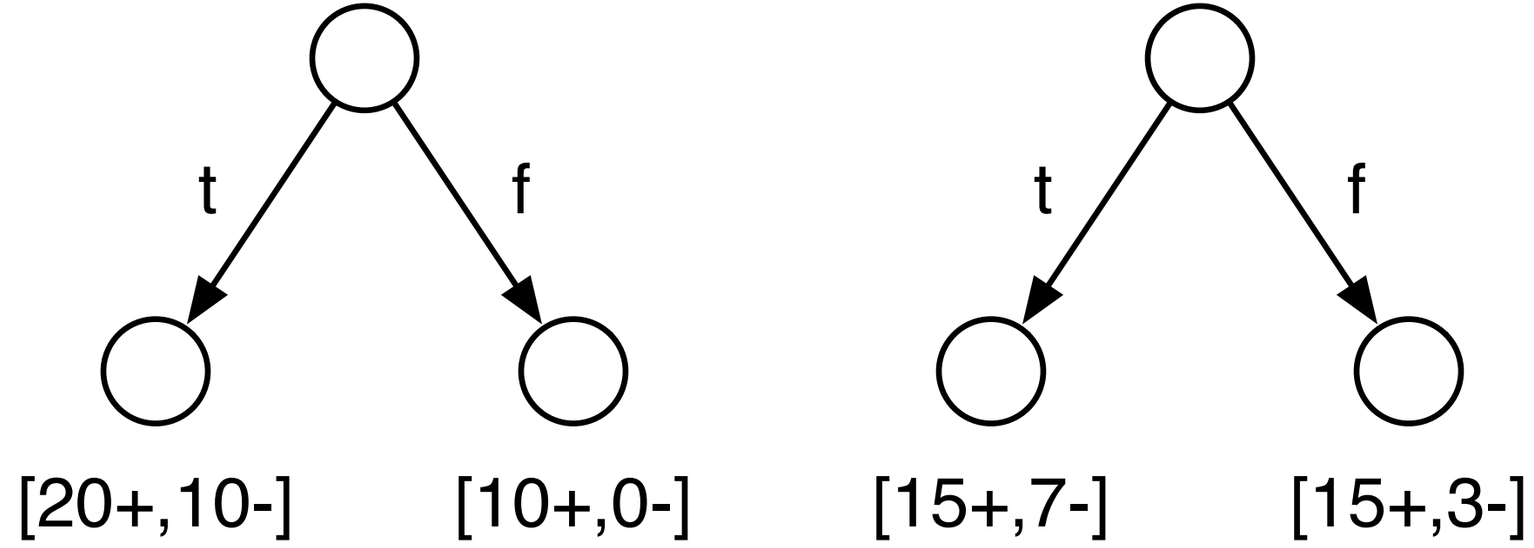
- We could enumerate all possible trees (assuming number of possible tests is finite),
  - Each tree could be evaluated using the training set or, better yet, a validation set
  - But there are many possible trees! Combinatorial problem…
  - We'd probably overfit the data anyway
- Usually, decision trees are constructed in two phases:
  1. An recursive, top-down procedure "grows" a tree (possibly until the training data is completely fit)
  2. The tree is "pruned" back to avoid overfitting
- Both typically use *greedy heuristics*

Top-down induction of decision trees

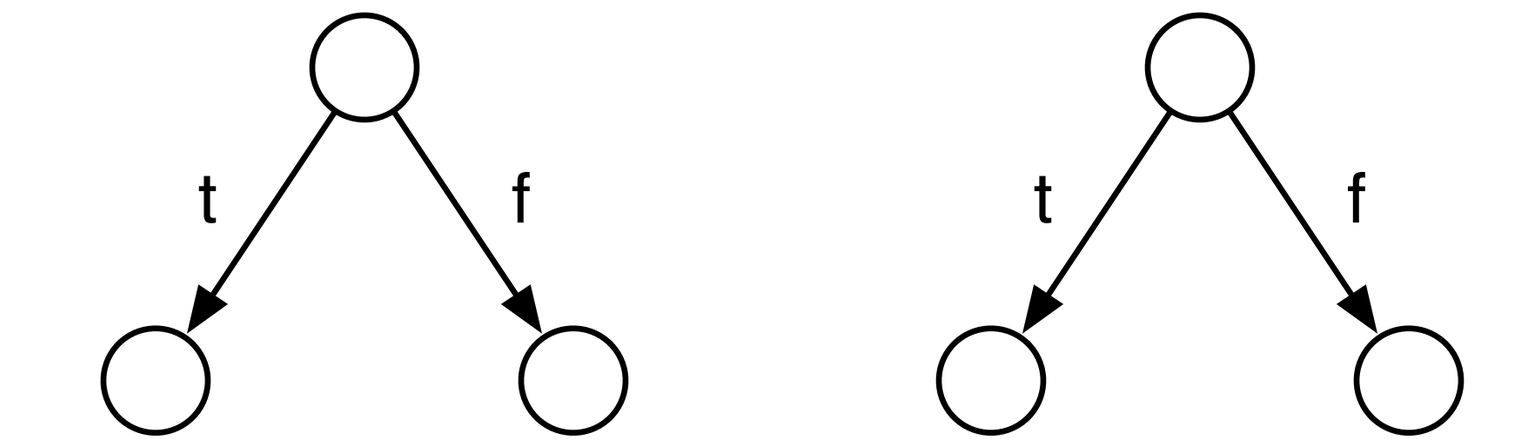
- For a classification problem:
  1. If all the training instances have the same class, create a leaf with that class label and exit.
  2. Pick the *best test* to split the data on
  3. Split the training set according to the value of the outcome of the test
  4. Recurse on each subset of the training data
- For a regression problem - same as above, except:
  - The decision on when to stop splitting has to be made earlier
  - At a leaf, either predict the mean value, or do a linear fit

Which test is best?

- The test should provide *information* about the class label.
- Suppose we have 30 positive examples, 10 negative ones, and we are considering two tests that would give the following splits of instances:



Which test is best?

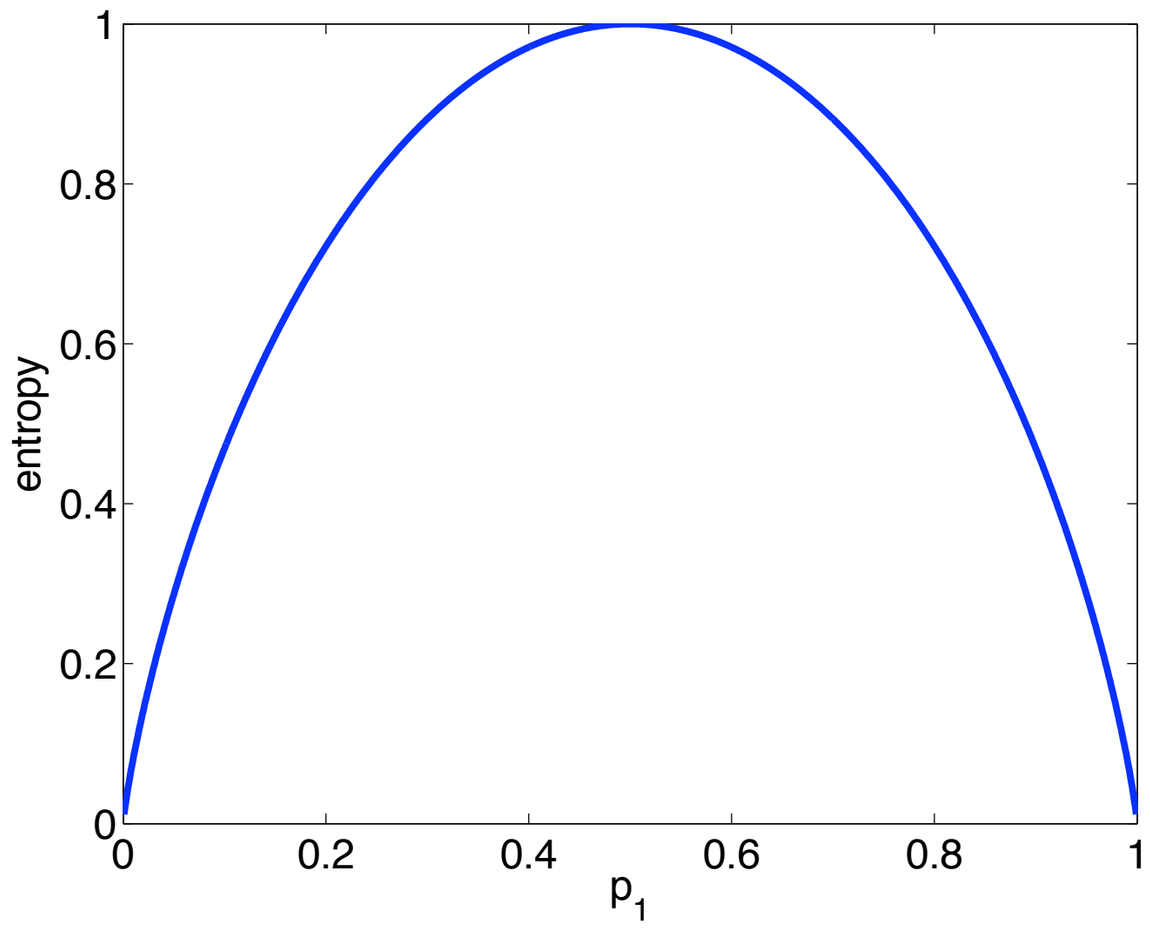


- Intuitively, we would like an attribute that *separates* the training instances as well as possible
- If each leaf was pure, the attribute would provide maximal information about the label at the leaf
- We need a mathematical measure for the purity of a set of instances

Entropy

$$H(P) = \sum_{i=1}^{k} p_i \log_2 \frac{1}{p_i}$$

- The further P is from uniform, the lower the entropy



Entropy applied to binary classfication

- Consider data set D and let
  - $p_{\oplus}$ = the proportion of positive examples in D
  - $p_{\ominus}$ = the proportion of negative examples in D
- Entropy measures the impurity of D, based on empirical probabilities of the two classes:

$$H(D) \equiv p_{\oplus} \log_2 \frac{1}{p_{\oplus}} + p_{\ominus} \log_2 \frac{1}{p_{\ominus}}$$

Marginal Entropy

$x =$**HasKids**	$y =$**OwnsDoraVideo**
Yes	Yes
Yes	Yes
Yes	Yes
Yes	Yes
No	No
No	No
Yes	No
Yes	No

- From the table, we can estimate $P(Y = \text{Yes}) = 0.5 = P(Y = \text{No})$.
- Thus, we estimate $H(Y) = 0.5 \log \frac{1}{0.5} + 0.5 \log \frac{1}{0.5} = 1$.

Specific Conditional entropy

$x =$**HasKids**	$y =$**OwnsDoraVideo**
Yes	Yes
Yes	Yes
Yes	Yes
Yes	Yes
No	No
No	No
Yes	No
Yes	No

Specific conditional entropy is the uncertainty in Y given a particular x value. E.g.,

- $P(Y = \text{Yes}|X = \text{Yes}) = \frac{2}{3}, P(Y = \text{No}|X = \text{Yes}) = \frac{1}{3}$
- $H(Y|X = \text{Yes}) = \frac{2}{3}\log \frac{1}{(\frac{2}{3})} + \frac{1}{3}\log \frac{1}{(\frac{1}{3})} \approx 0.9183.$

(Average) Conditional entropy

$x =$**HasKids**	$y =$**OwnsDoraVideo**
Yes	Yes
Yes	Yes
Yes	Yes
Yes	Yes
No	No
No	No
Yes	No
Yes	No

- *The conditional entropy,* $H(Y|X)$, is the average specific conditional entropy of y given the values for x:

$$H(Y|X) = \sum_x P(X = x)H(Y|X = x)$$

- $H(Y|X = \text{Yes}) = \frac{2}{3}\log \frac{1}{(\frac{2}{3})} + \frac{1}{3}\log \frac{1}{(\frac{1}{3})} \approx 0.9183$
- $H(Y|X = \text{No}) = 0 \log \frac{1}{0} + 1 \log \frac{1}{1} = 0.$
- $H(Y|X) = H(Y|X = \text{Yes})P(X = \text{Yes}) + H(Y|X = \text{No})P(X = \text{No})$
  $= 0.9183 \cdot \frac{3}{4} + 0 \cdot \frac{1}{4} \approx 0.6887$
- Interpretation: the expected number of bits needed to transmit y if both the emitter and the receiver know the possible values of x (but before they are told x's specific value).

Information gain

- Suppose one has to transmit y. How many bits on the average would it save if both the transmitter and the receiver knew x?

$$IG(Y|X) = E[H(Y) - H(Y|X)]$$

  This is called *information gain*

- Alternative interpretation: what reduction in entropy would be obtained by knowing X
- Intuitively, this has the meaning we seek for decision tree construction

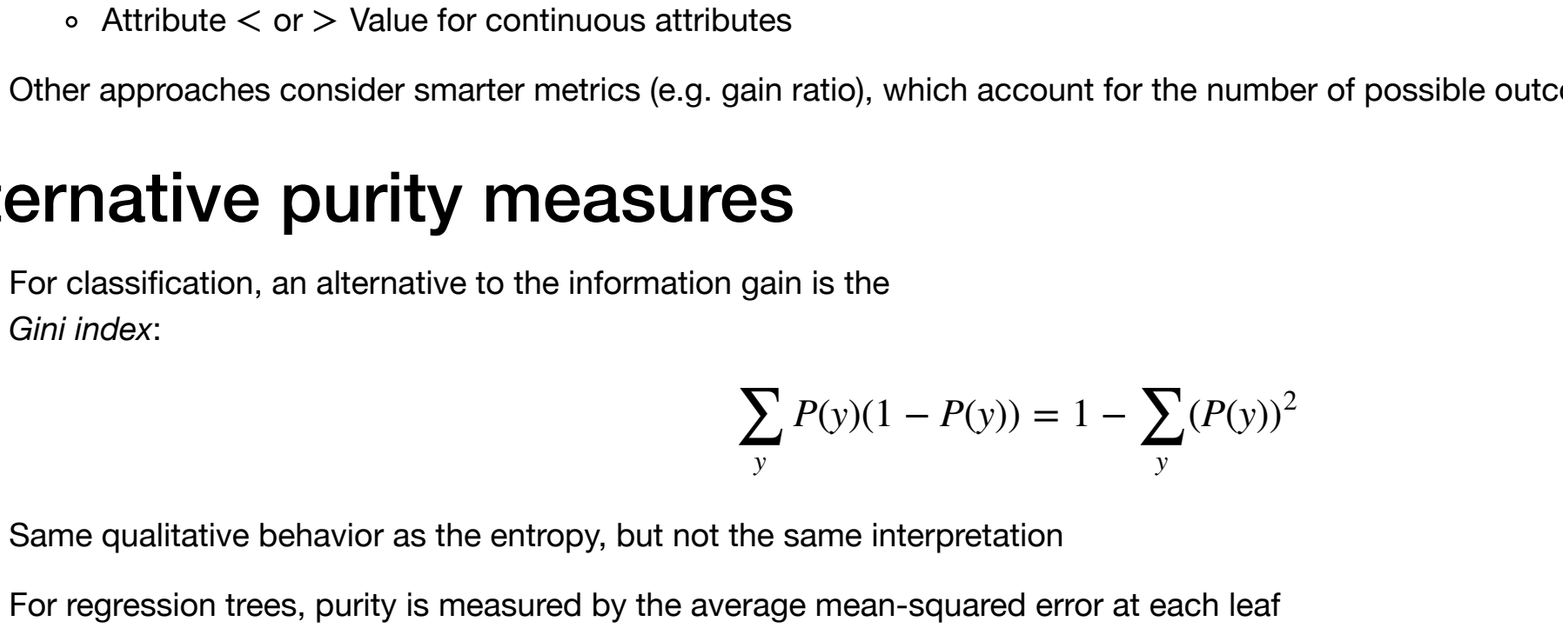
Information gain to determine best test

- We choose, recursively at each interior node, the test that has highest empirical information gain (on the training set.)

  Equivalently, test that results in lowest conditional entropy.

- If tests are binary:

$$\begin{aligned} IG(D, \text{Test}) &= H(D) - H(D|\text{Test}) \\ &= H(D) - \frac{|D_{\text{Test}}|}{|D|} H(D_{\text{Test}}) - \frac{|D_{\neg\text{Test}}|}{|D|} H(D_{\neg\text{Test}}) \end{aligned}$$



Check that in this case, the test on the left has higher IG.

Caveats on tests with multiple values

- If the outcome of a test is *multi-valued*, the number of possible values influences the information gain
- The more possible values, the higher the gain! (the more likely it is to form small, but pure partitions)
- C4.5 (one famous decision tree construction algorithm) uses only binary tests:
  - Attribute $=$ Value for discrete attributes
  - Attribute $<$ or $>$ Value for continuous attributes
- Other approaches consider smarter metrics (e.g. gain ratio), which account for the number of possible outcomes

Alternative purity measures

- For classification, an alternative to the information gain is the *Gini index*:

$$\sum_y P(y)(1 - P(y)) = 1 - \sum_y (P(y))^2$$

  Same qualitative behavior as the entropy, but not the same interpretation

- For regression trees, purity is measured by the average mean-squared error at each leaf

  E.g. CART (Breiman et al., 1984)

Dealing with noise in the training data

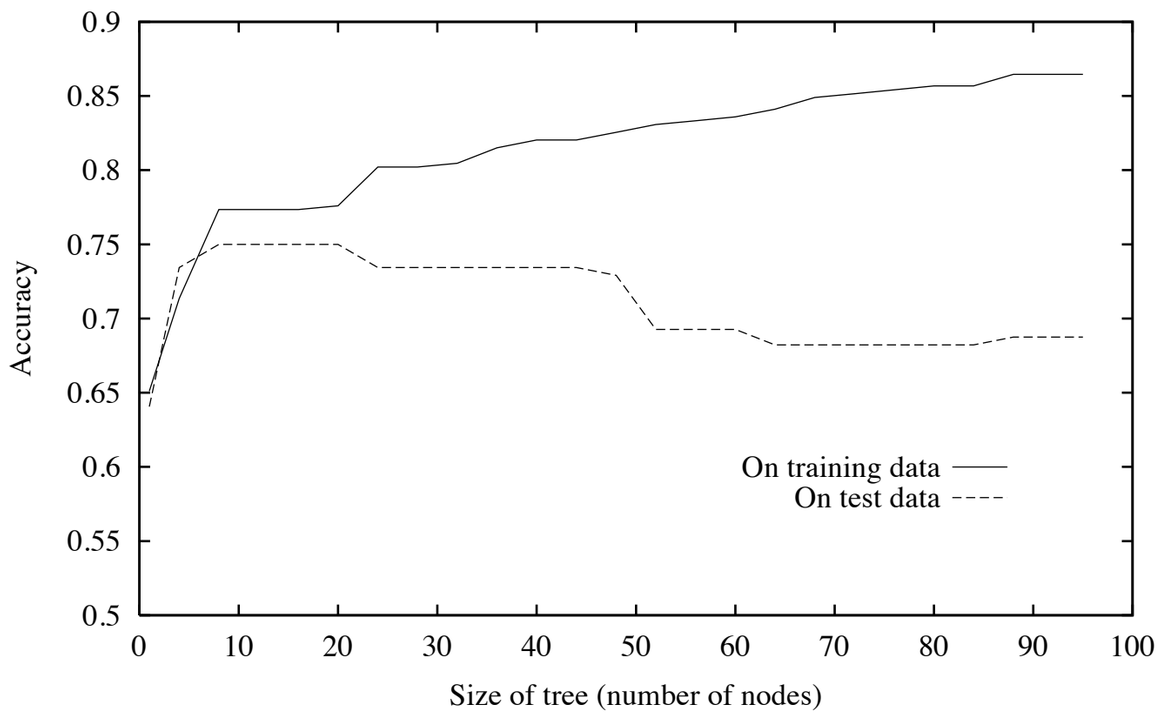
Noise is inevitable!

- Values of attributes can be misrecorded
- Values of attributes may be missing
- The class label can be misrecorded

What happens when adding a noisy example?

Overfitting in decision trees

- Remember, decision tree construction proceeds until all leaves are pure – all examples having the same y value.
- As the tree grows, the generalization performance starts to degrade, because the algorithm is finding *irrelevant attributes* / *tests*.



Example from (Mitchell, 1997)

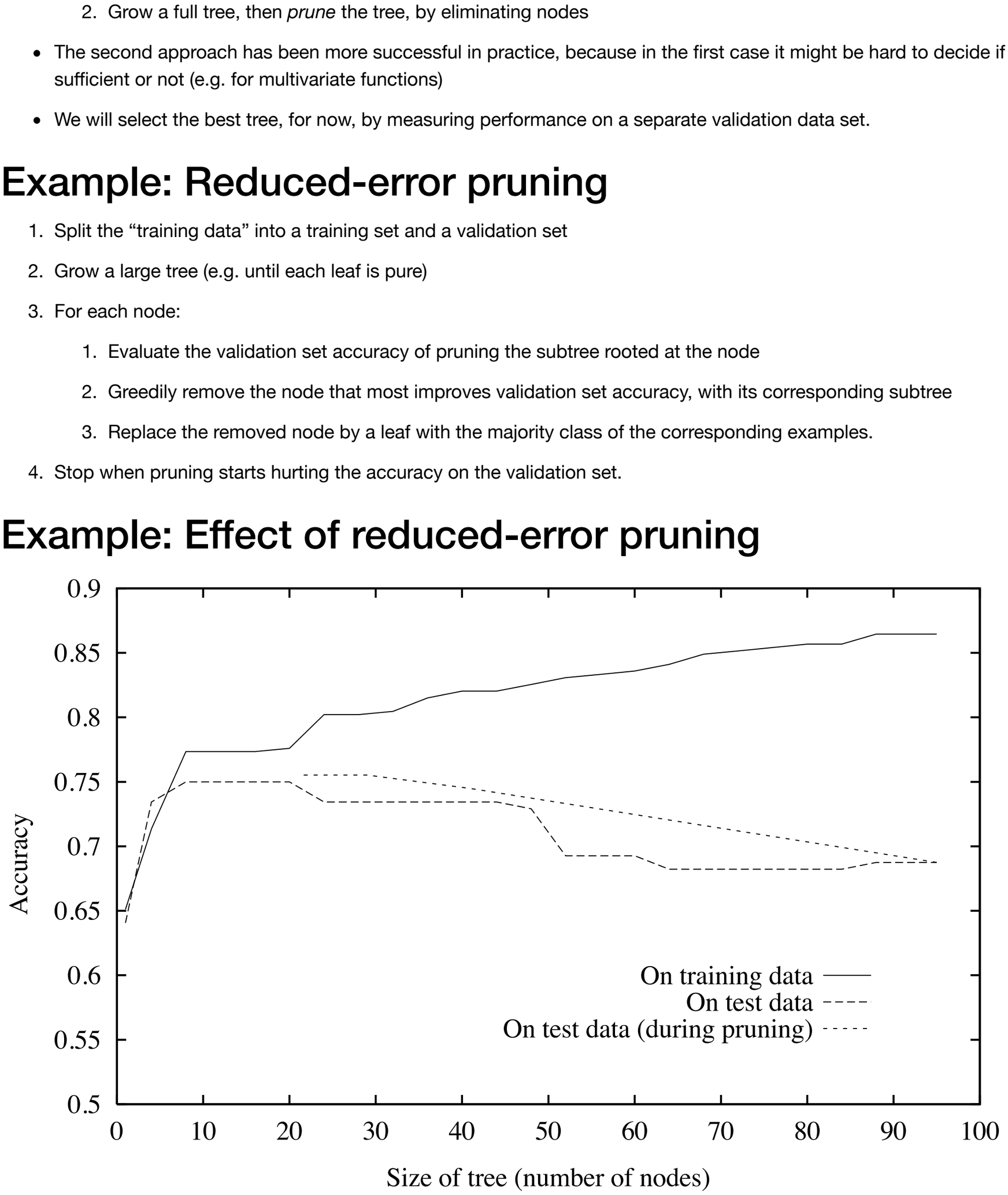
Avoiding overfitting

- Two approaches:
    1. Stop growing the tree when further splitting the data does not yield a statistically significant improvement
    2. Grow a full tree, then *prune* the tree, by eliminating nodes
- The second approach has been more successful in practice, because in the first case it might be hard to decide if the information gain is sufficient or not (e.g. for multivariate functions)
- We will select the best tree, for now, by measuring performance on a separate validation data set.

Example: Reduced-error pruning

1. Split the “training data” into a training set and a validation set
2. Grow a large tree (e.g. until each leaf is pure)
3. For each node:
    1. Evaluate the validation set accuracy of pruning the subtree rooted at the node
    2. Greedily remove the node that most improves validation set accuracy, with its corresponding subtree
    3. Replace the removed node by a leaf with the majority class of the corresponding examples.
4. Stop when pruning starts hurting the accuracy on the validation set.

Example: Effect of reduced-error pruning



Example: Rule post-pruning in C4.5

1. Convert the decision tree to rules
2. Prune each rule independently of the others, by removing preconditions such that the accuracy is improved
3. Sort final rules in order of estimated accuracy

Advantages:

- Can prune attributes higher up in the tree *differently on different paths*
- There is no need to reorganize the tree if pruning an attribute that is higher up
- Often people want rules anyway, for readability

Random Forests

- Draw B bootstrapped datasets, learn B decision trees.
- Average/vote the outputs.
- When choosing each split, only consider a random $\sqrt{p}$-sized subset of the features.
- Prevents overfitting
- Works extremely well

Missing values during classification

- Assign “most likely” value based on all the data that reaches the current node. This is a form of .
- Assign all possible values with some probability.
    - Count the occurrences of the different attribute values in the instances that have reached the same node.
    - Predict all the possible class labels with the appropriate probabilities
    - Introduce a value that means “unknown”

Decision Tree Summary (1)

- Very fast learning algorithms (e.g. C4.5, CART)
- Attributes may be discrete or continuous, no preprocessing needed
- Provide a general representation of classification rules
- Easy to understand! Though…
    - Exact tree output may be sensitive to small changes in data
    - With many features, tests may not be meaningful

Decision Tree Summary (2)

- In standard form, good for (nonlinear) piecewise axis-orthogonal decision boundaries – not good with smooth, curvilinear boundaries
- In regression, the function obtained is discontinuous, which may not be desirable
- Good accuracy in practice – many applications

Extra Slides

What is information?

- Imagine:
    1. You are about to observe the outcome of a dice roll
    2. You are about to observe the outcome of a coin flip
    3. You are about to observe the outcome of a biased coin flip
    4. Someone is about to tell you your own name
- Intuitively, in each situation you have a different amount of uncertainty as to what outcome / message you will observe.

Information = Reduction in uncertainty

Let E be an event that occurs with probability $P(E)$. If we are told that E has occurred with certainty, then we received

$$I(E) = \log_2 \frac{1}{P(E)}$$

bits of *information*.

- You can also think of information as the amount of “surprise” in the outcome (e.g., consider $P(E) = 1$, $P(E) \approx 0$)
- E.g., result of a fair coin flip provides $\log_2 2 = 1$ bit of information
- E.g., result of a fair dice roll provides $\log_2 6 \approx 2.58$ bits of information.
- E.g., result of being told your own name (or any other deterministic event) produces 0 bits of information

Interpretations of entropy

$$H(P) = \sum_i p_i \log_2 \frac{1}{p_i}$$

- Average amount of information per symbol
- Average amount of surprise when observing the symbol
- Uncertainty the observer has before seeing the symbol
- Average number of bits needed to communicate the symbol