Trying to learn a function f

Reality **x** → **Nature** → **y**

f(x)

Trying to learn a function f

Reality	**x** →	**Nature**	→ **y**	
		f(x)		
Natural processes culture	**x** →	**Mechanistic model**	→ **y**	**Natural process algorithms**
Generative modeling culture	**x** →	**Generic model**	→ **y**	**Phenomenological algorithms**
Machine learning				
Algorithmic modeling culture	**x** →	**Generic algorithm**	→ **y**	**Arbitrary algorithms**

f can mean different things in different cultures

f(x) for prediction

Reality $\boldsymbol{Z_1, Z_2, \ldots, Z_\Omega}$ $\boldsymbol{Y = \mathbf{nature}(Z)}$

Some set of causally-connected variables

Data $\boldsymbol{X_1, X_2, \ldots, X_p}$

A set of potential predictor variables

$$\boldsymbol{Y = f(X) + \epsilon}$$

Systematic component Error

Prediction $\boldsymbol{\hat{Y} = \hat{f}(X)}$ Hats indicate predicted Y and estimated f

Goal of prediction

Use data to find a function $\hat{f}$ that has good predictive performance given X

That is, $\hat{f}$ is accurate on new observations

Goal of machine learning

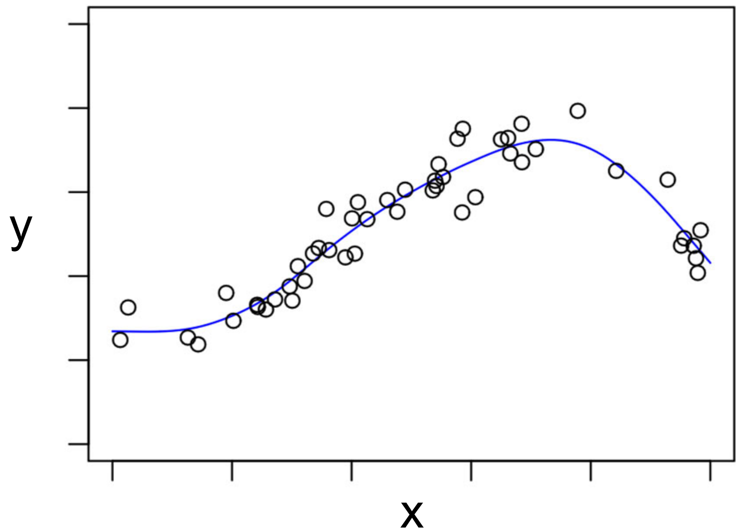
To predict accurately!

- Species distribution
  - map
  - predict accurately for places we won’t visit
- Climate change forecast
  - predict accurately for the future
- Antelopes in camera trap images
  - hand over the identification task to a machine so we don’t have to look at images!
  - predict accurately for images that we’ll never look at

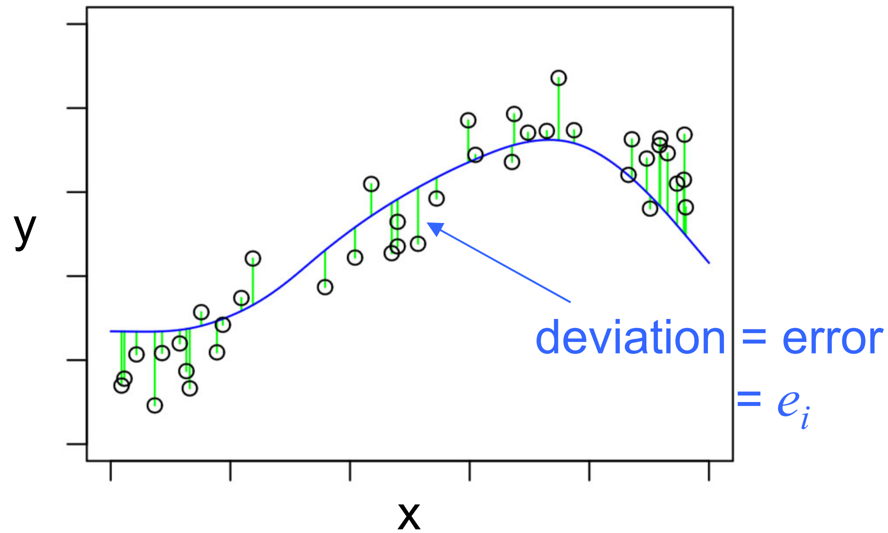
Predictive skill

Basic idea: out-of-sample accuracy

$\hat{f}$ trained on a sample of data



$\hat{f}$ predicting new data



e.g. mean square error (MSE) $\frac{1}{n}\sum_{i}^{n} e_i^2$

Machine learning workflow

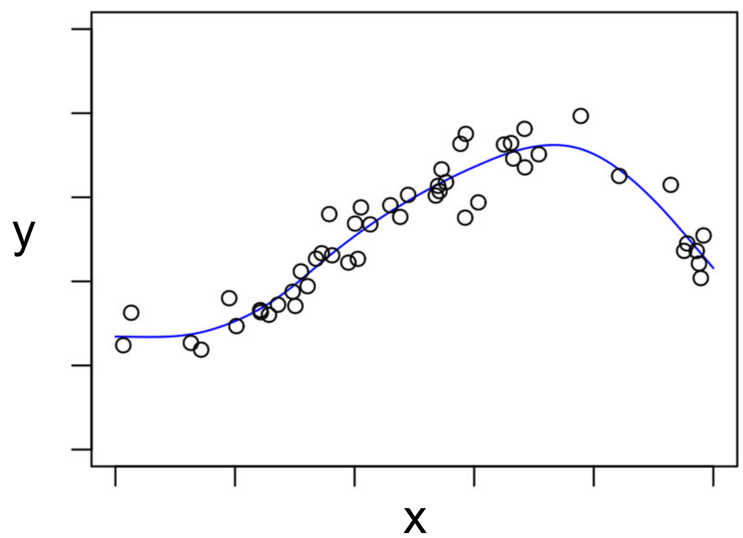
Overall algorithm:

1. Create model algorithm(s) for $\hat{f}(x)$
2. Use a training algorithm to find parameter values of $\hat{f}(x)$
3. Use an inference algorithm to compare predictive skill among models (model families, tuning parameters, x sets, etc).

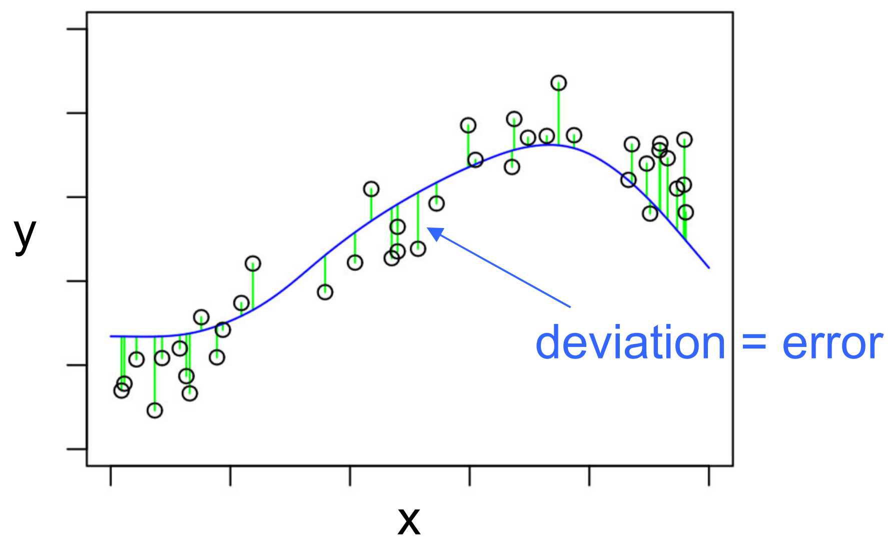
Inference algorithm

Basic idea: out-of-sample validation

Fit model to training dataset



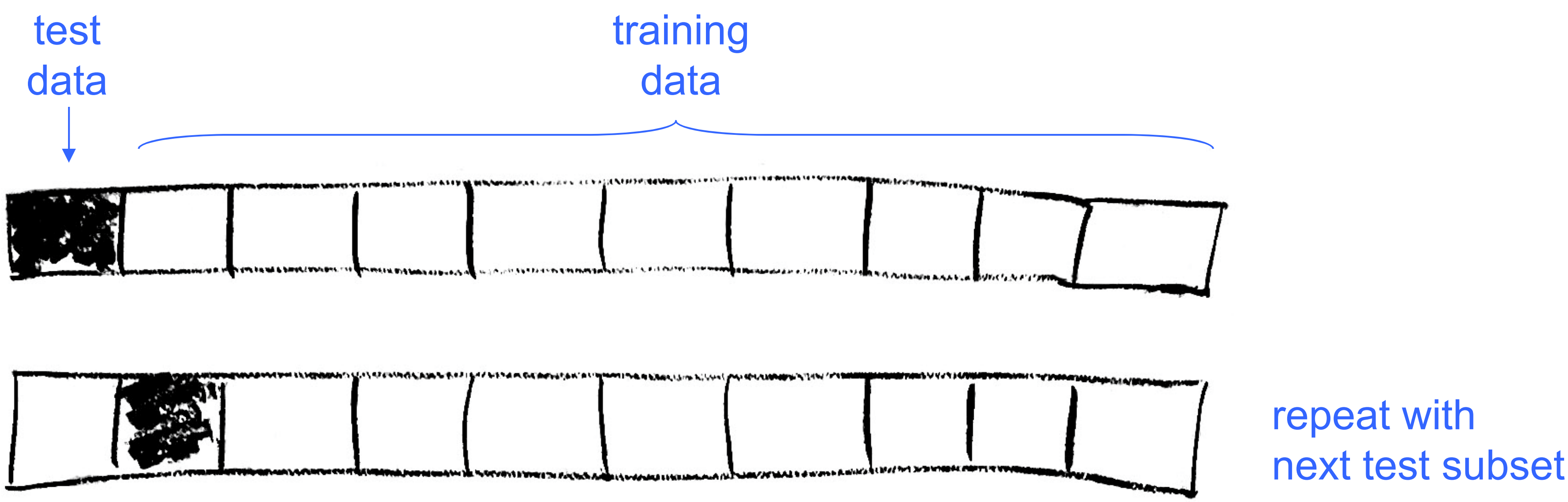
Test model on validation dataset



e.g. mean square error (MSE)

k-fold cross validation (CV)

Divide dataset into k parts (preferably randomly)



... repeat with each test subset

k-fold CV inference algorithm

Algorithm

divide dataset into k parts i = 1...k

for each i

    test dataset = part i

    training dataset = remaining data

    find f using training dataset

    use f to predict for test dataset

    e_i = prediction error

CV_error = mean(e)

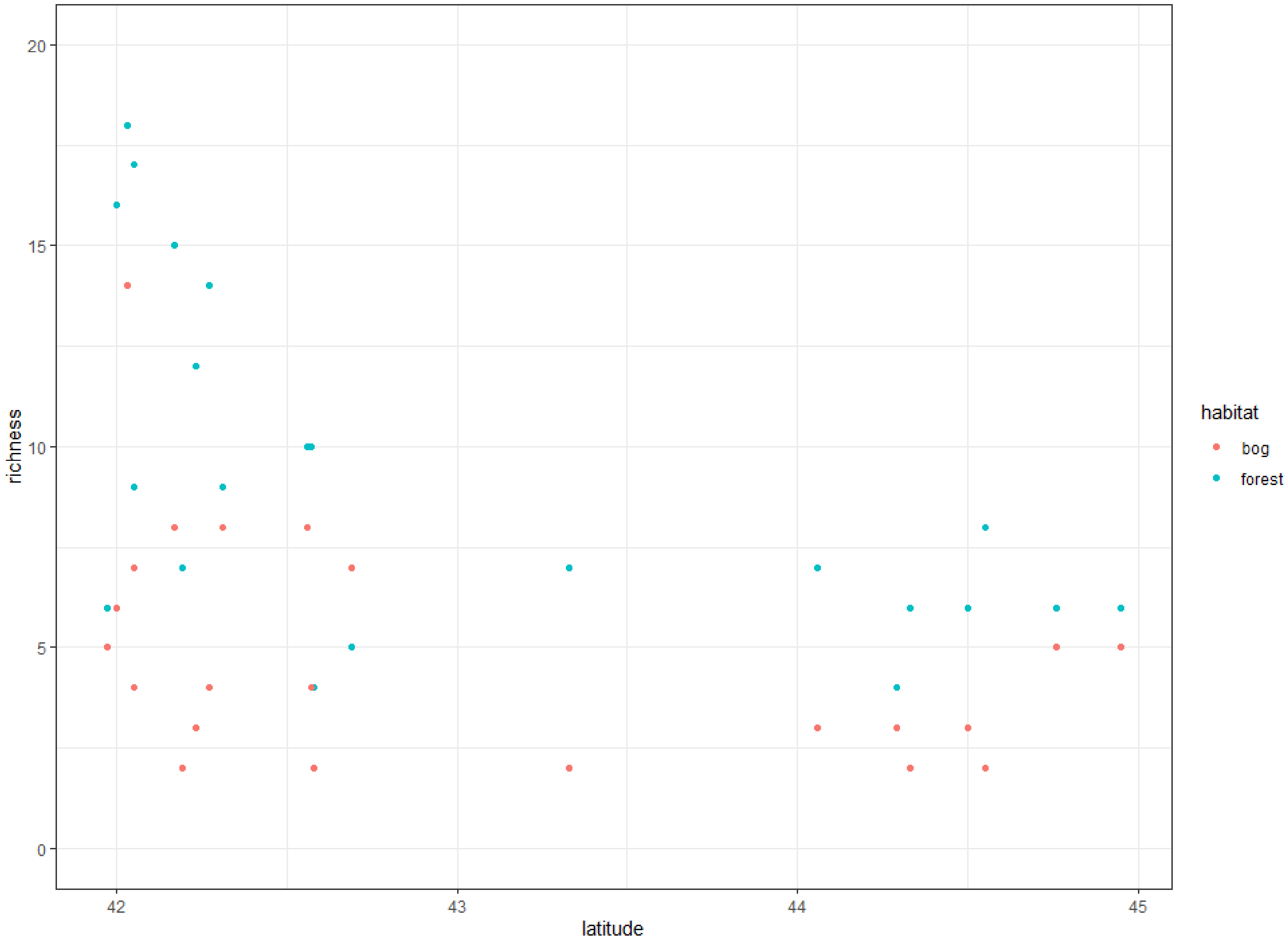
Typical values for k: 5, 10, k

Regression & classification

- Regression:
  - numerical response variable
  - predict a numerical value given x
  - e.g. number of species given latitude
- Classification:
  - categorical response variable
  - predict the category given x
  - e.g. is it a bird, deer, tree, or mountain lion?
  - e.g. is it dead or alive?; present or absent?

Ants data

```
> head(ants)
  site habitat latitude elevation richness
1  TPB  forest    41.97       389        6
2  HBC  forest    42.00         8       16
3  CKB  forest    42.03       152       18
4  SKP  forest    42.05         1       17
5   CB  forest    42.05       210        9
6   RP  forest    42.17        78       15
```


richness
20
15
10
5
0
42
43
44
45
latitude
habitat
bog
forest

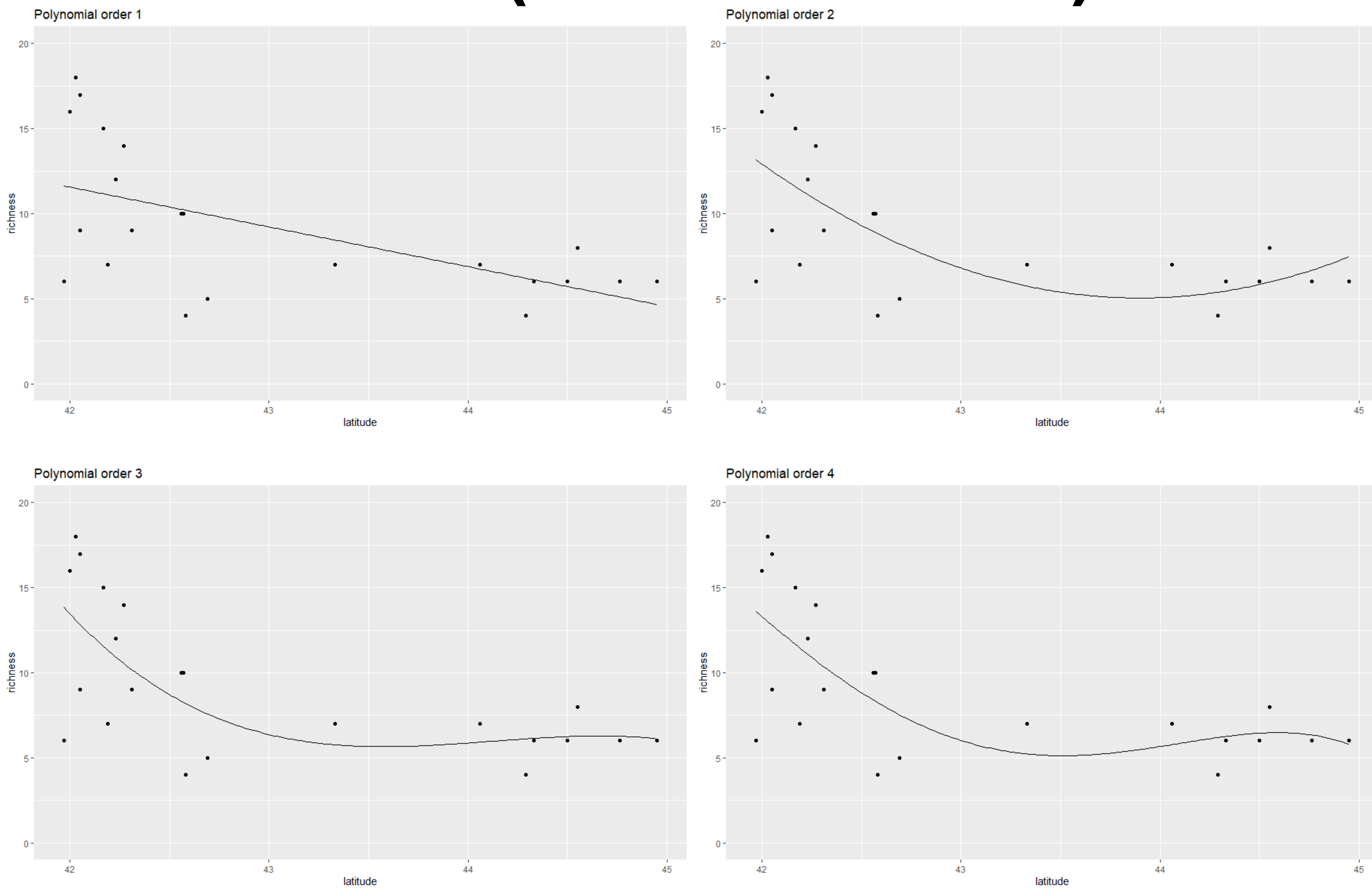
Basic full ML setup

- Polynomial example, 3 algorithms:
  - model: flexible function $\hat{f}(x)$; polynomial linear model

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ \dots + \beta_m x^m$$

m=order

Ants (forest habitat)



Basic full ML setup

- Polynomial example, 3 algorithms:
  - model: flexible function $\hat{f}(x)$; polynomial linear model

    $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ldots + \beta_m x^m$ m=order
  - training: optimize least squares objective function
  - minimize $SSQ = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ for training data

```
lm(richness ~ poly(latitude, order), data=forest_ants)
```

Basic full ML setup

- Polynomial example, 3 algorithms:
  - model: flexible function $\hat{f}(x)$; polynomial linear model

    $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ldots + \beta_m x^m$ m=order
  - training: optimize least squares objective function
  - minimize $SSQ = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ for training data
  - inference: tuning parameter (order of poly); k-fold cross validation

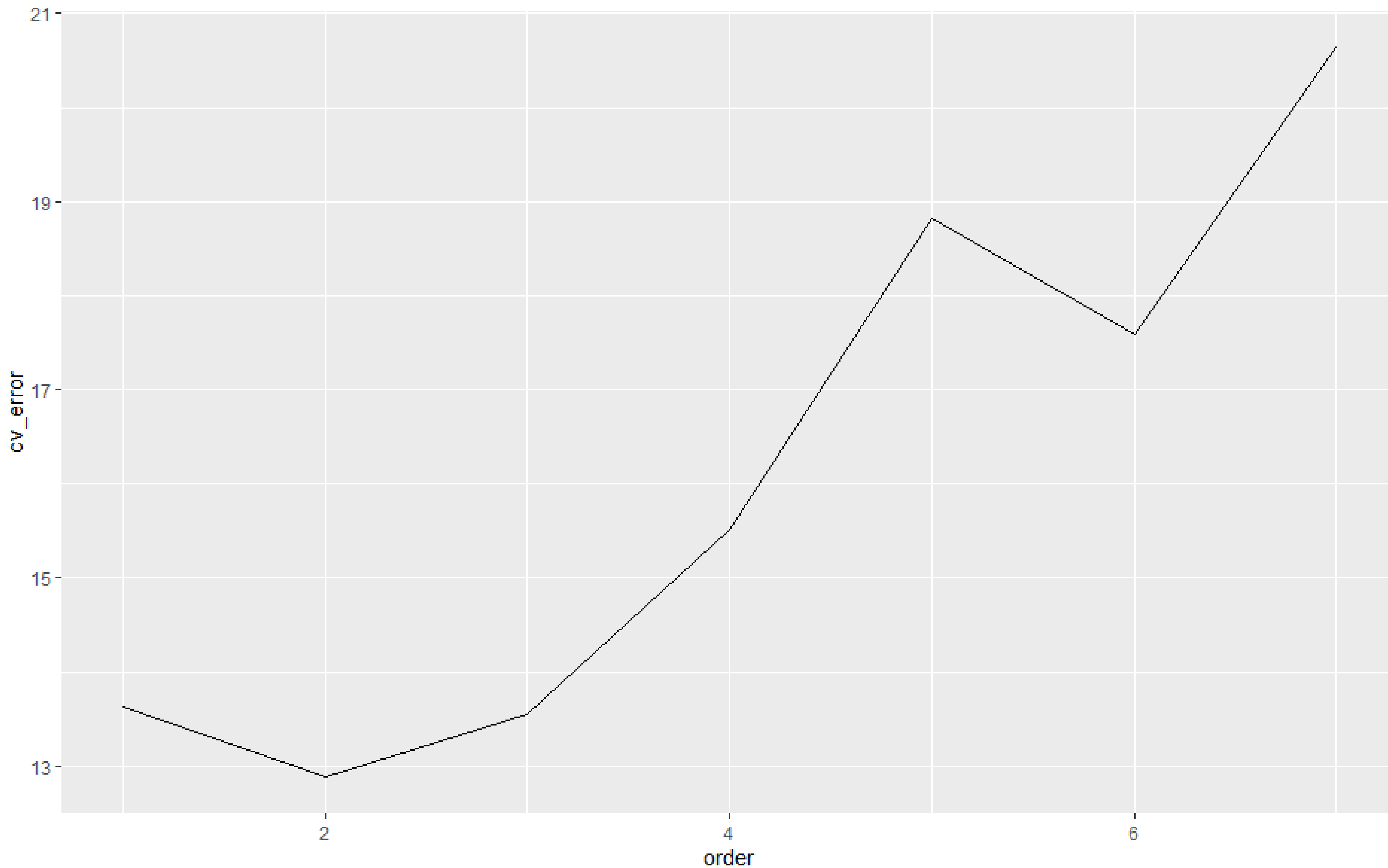
Leave-one-out cross validation

- LOOCV
- special case of k-fold CV: $k = n$

Algorithm
for each data point
    fit model without point
    predict for that point
    measure prediction error (compare to observed)
CV_error = mean error across points

(AIC and Bayesian WAIC are equivalent as $n \to \infty$)

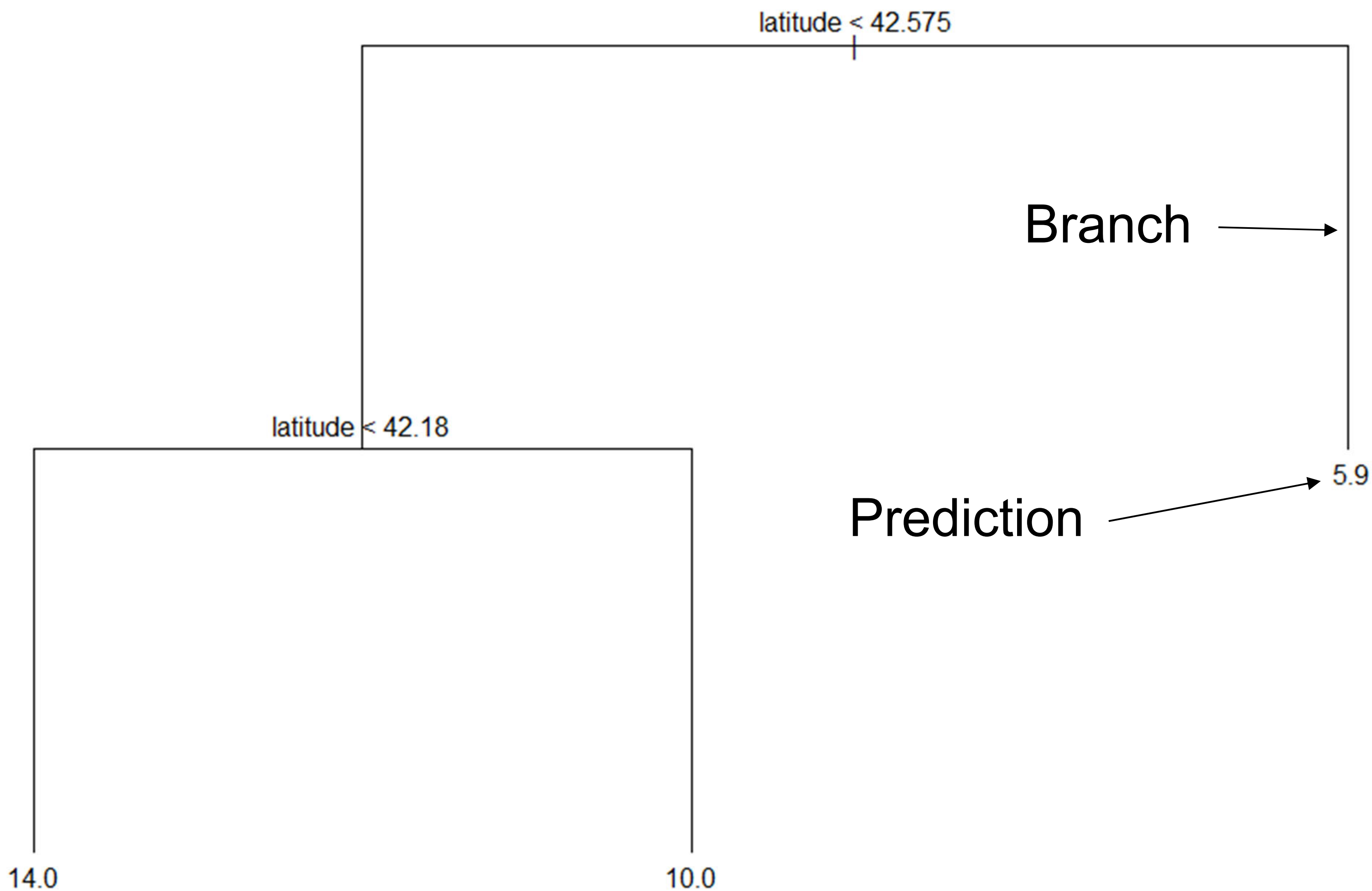
Leave one out CV (k-fold CV, k=n)

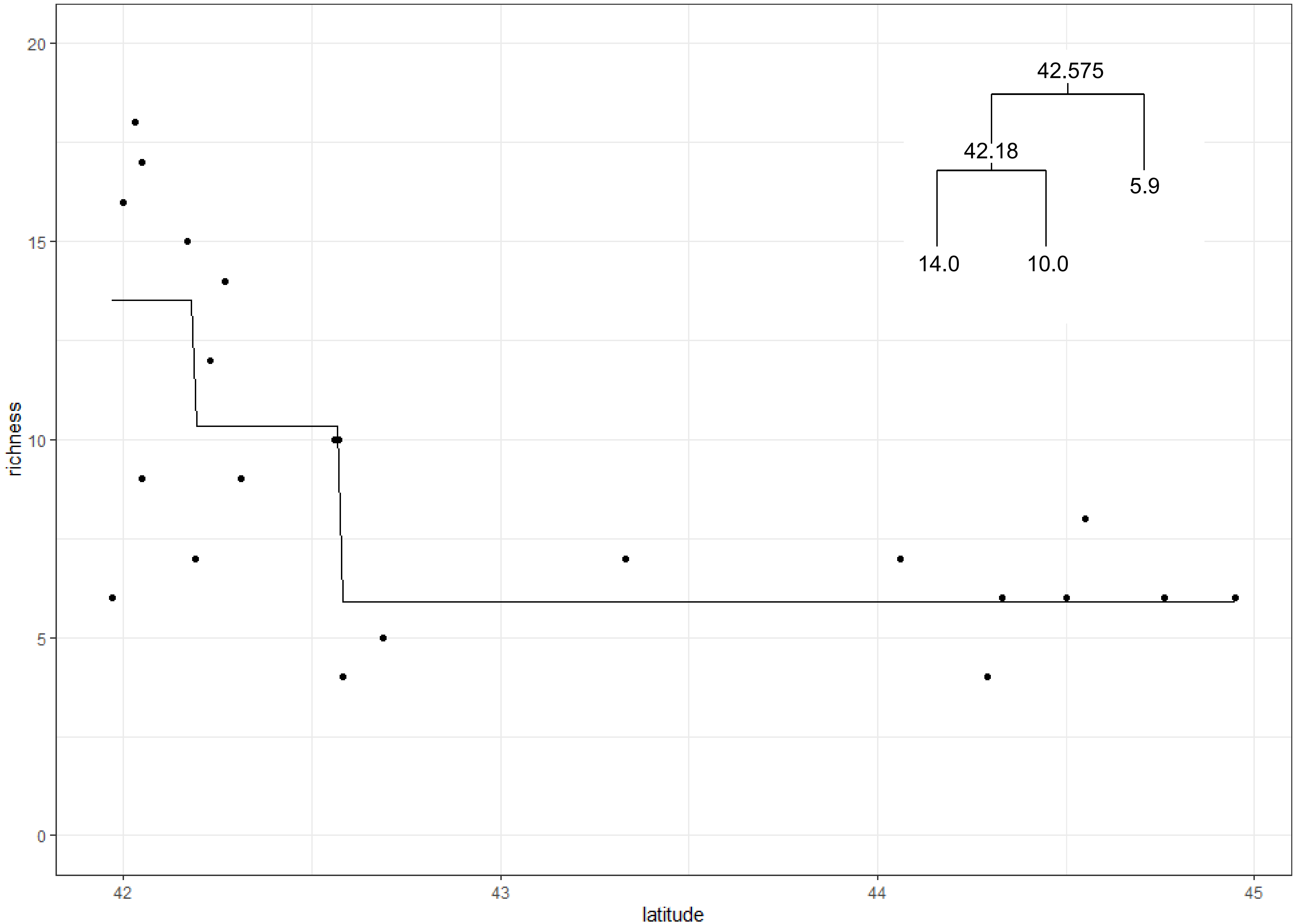


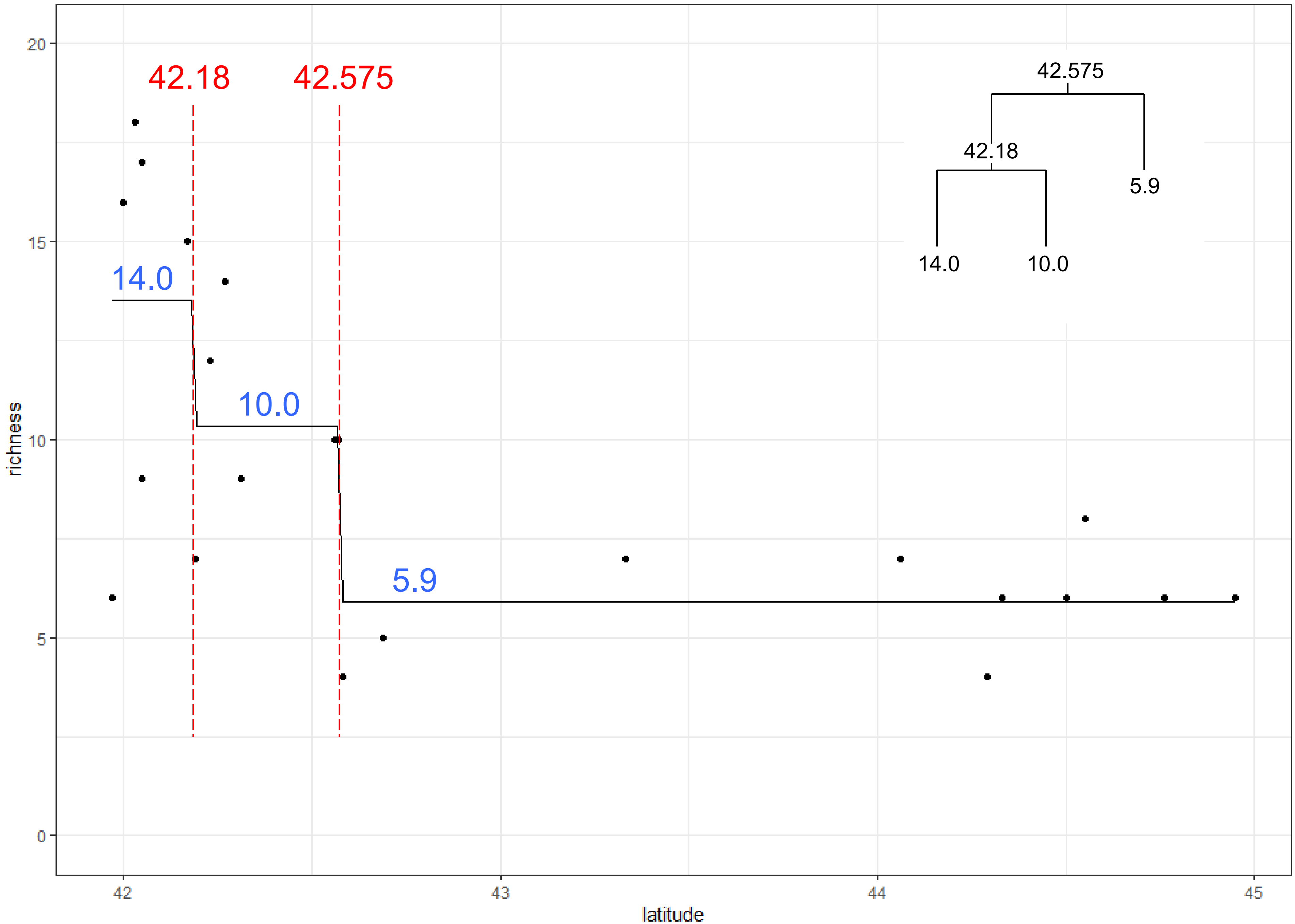
Basic model algorithms

- Ensemble methods
  - Bagging
  - Random forest
  - Boosting
- Neural networks

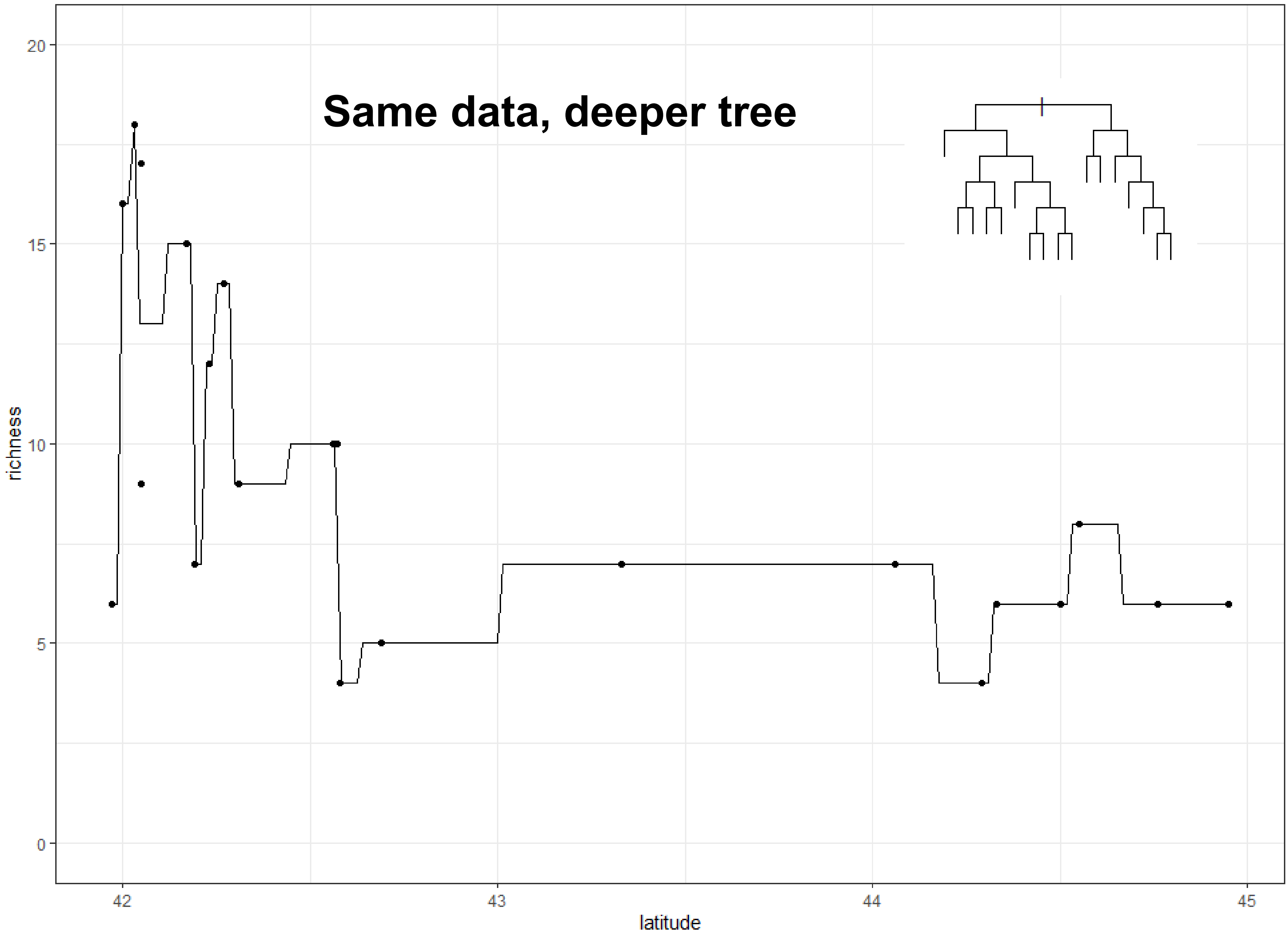
Regression tree base model



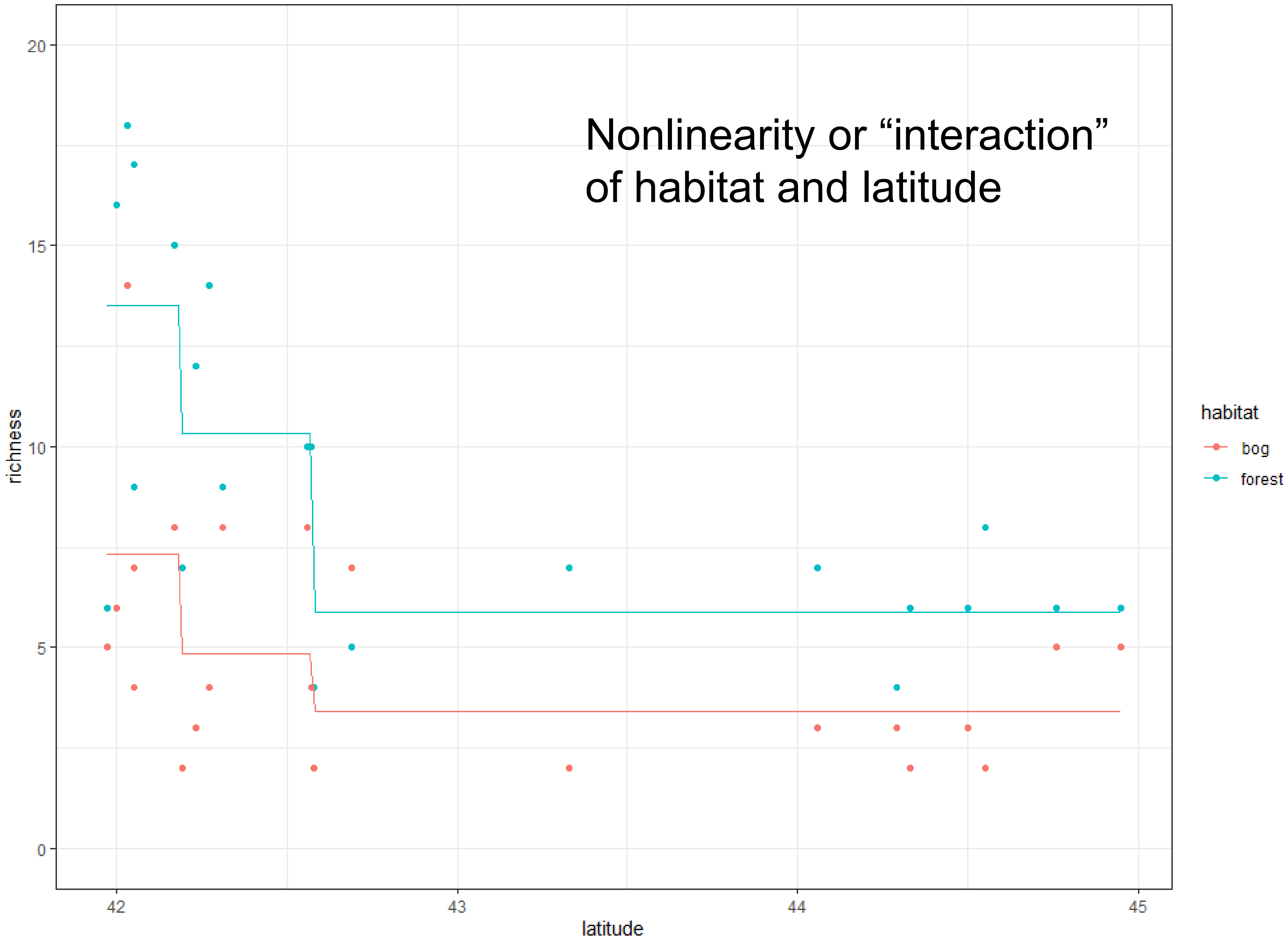

42.575
42.18
5.9
14.0
10.0
20
15
10
5
0
richness
42
43
44
45
latitude

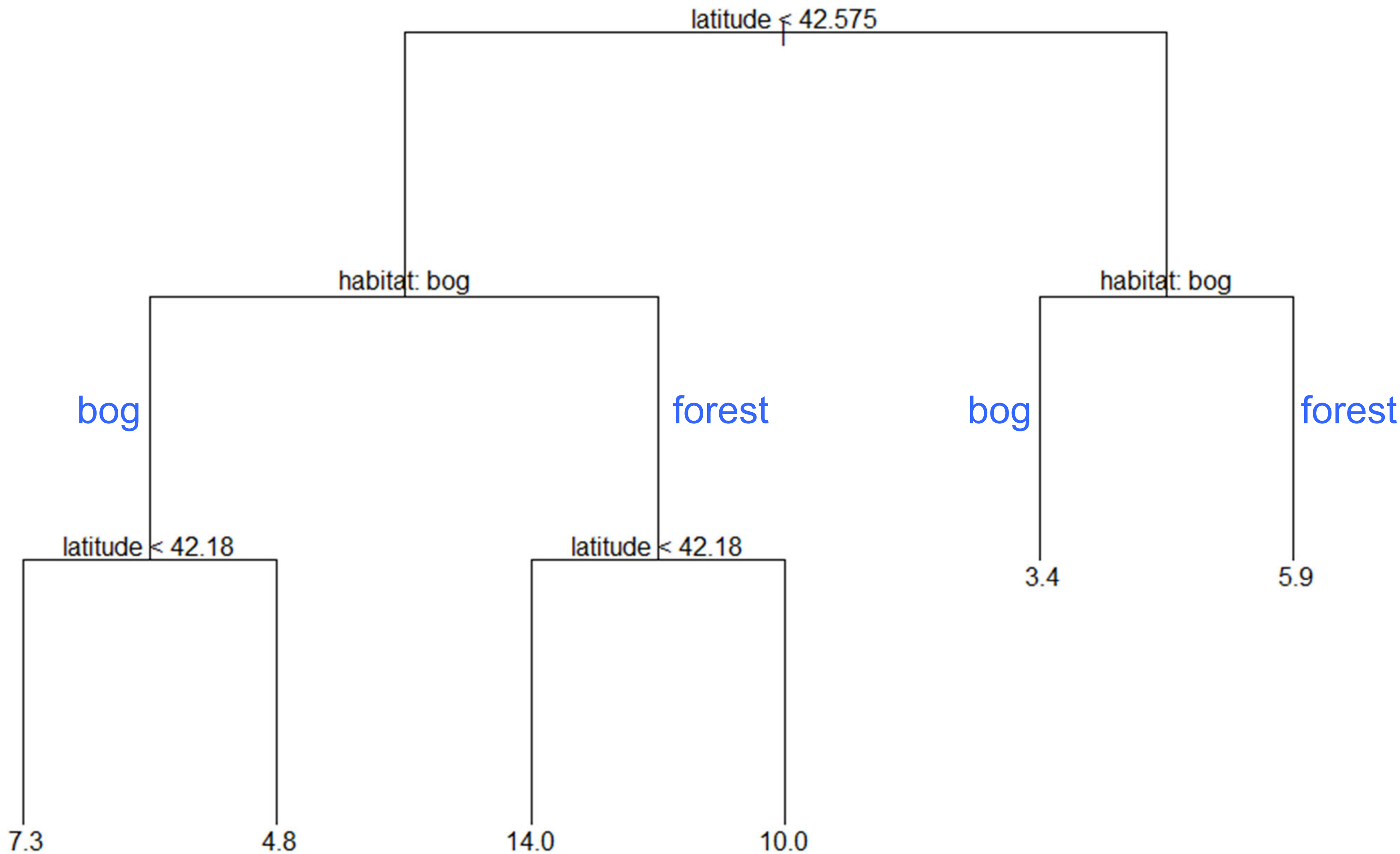


42.18
42.575
14.0
10.0
5.9
42.575
42.18
5.9
14.0
10.0
richness
latitude
20
15
10
5
0
42
43
44
45



Same data, deeper tree
richness
latitude
20
15
10
5
0
42
43
44
45


Nonlinearity or “interaction”
of habitat and latitude
richness
latitude
habitat
bog
forest
0
5
10
15
20
42
43
44
45


latitude < 42.575
habitat: bog
habitat: bog
bog
forest
bog
forest
latitude < 42.18
latitude < 42.18
3.4
5.9
7.3
4.8
14.0
10.0

Ensemble methods

- Train many models
- Average the models to predict
- Averaging reduces variance

e.g. $$\mathrm{Var}(\bar{y}) = \frac{\sigma_y^2}{n}$$

Bagging

- Bootstrap
  - form new datasets by resampling from the data
- Aggregate
  - average over bootstrapped model fits

Bagging algorithm

for many repetitions

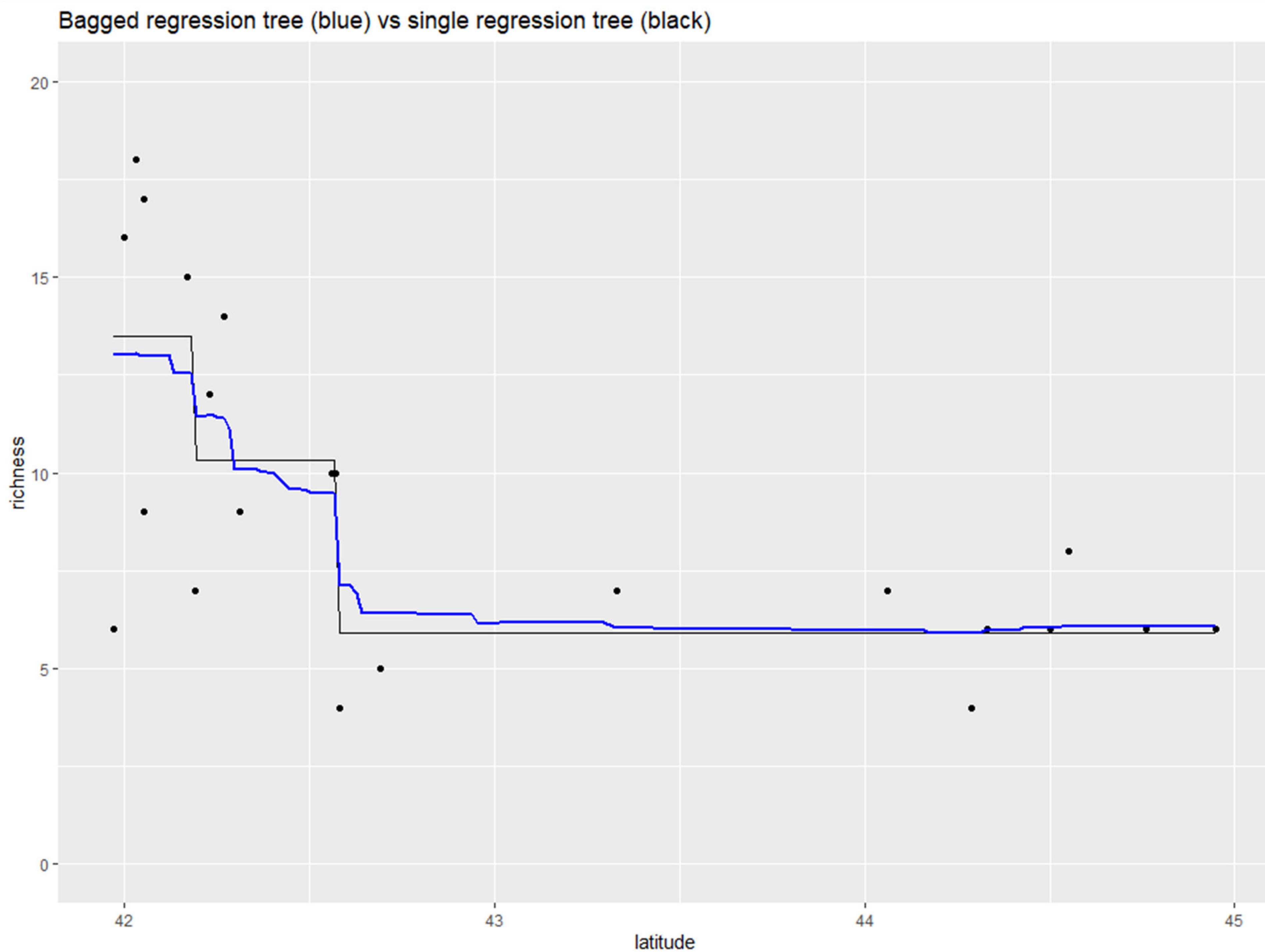
    resample the data with replacement

    train the base model

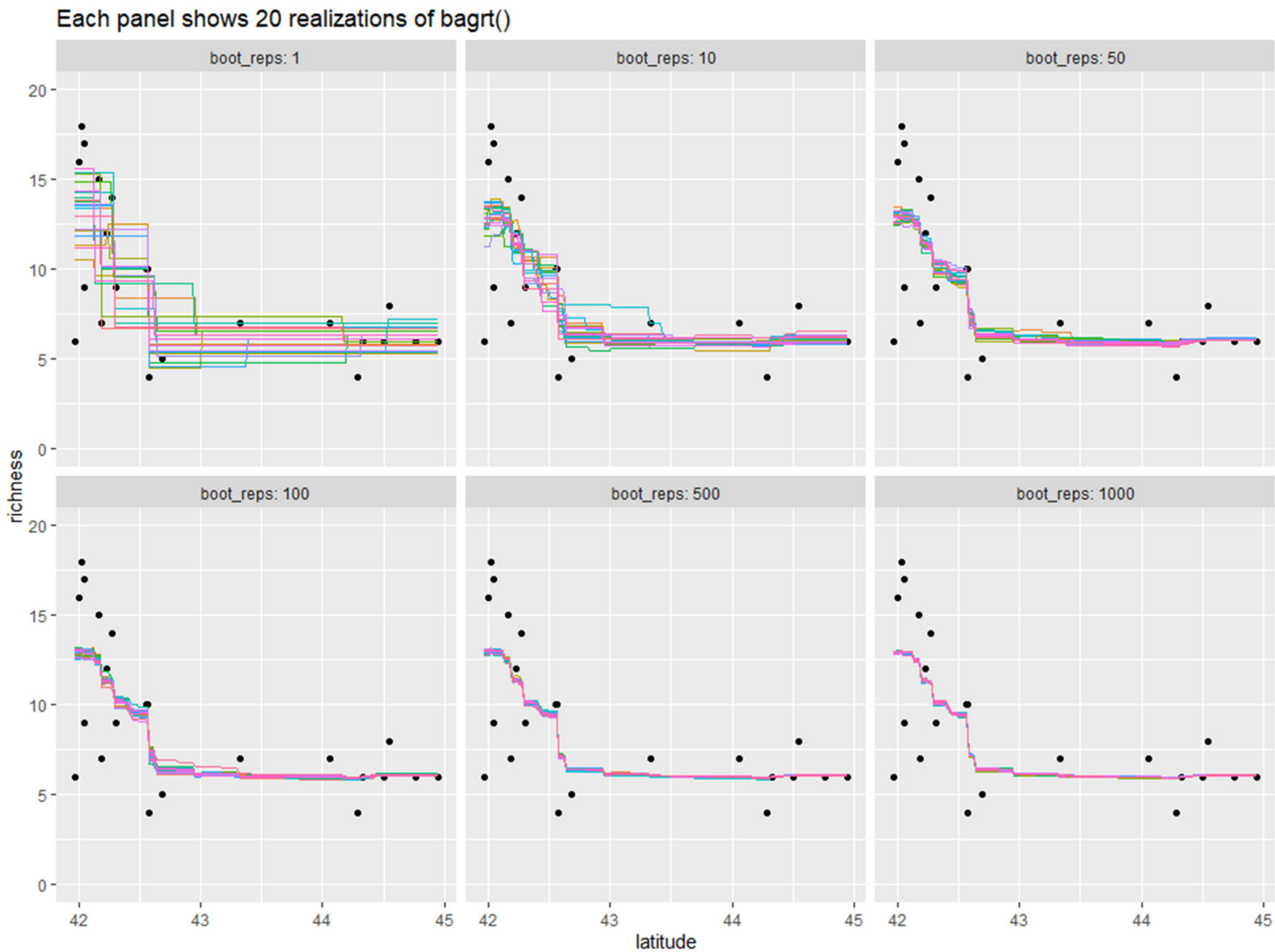
    record prediction

final prediction = mean of predictions

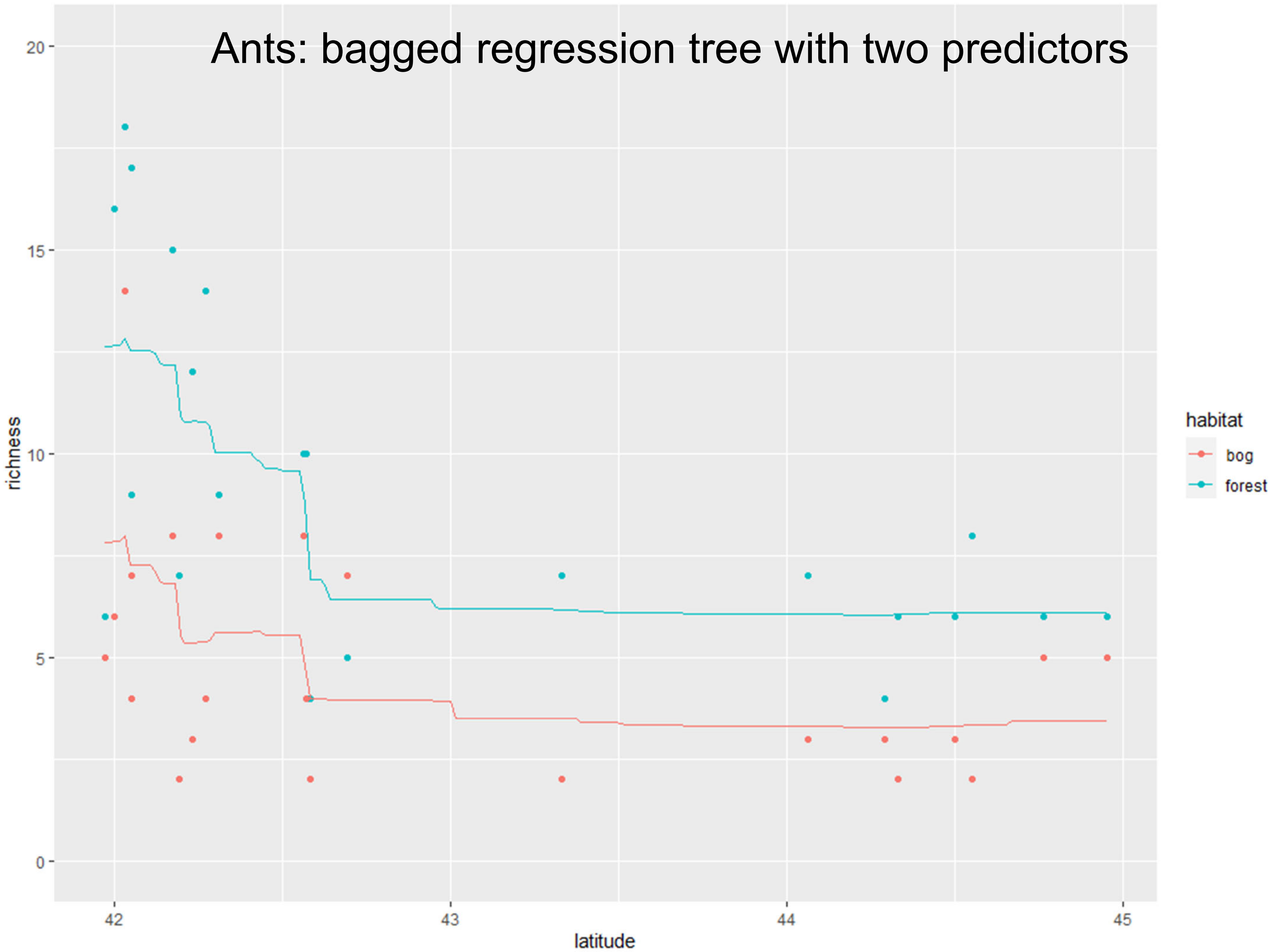
Base model: can be any type of model


Bagged regression tree (blue) vs single regression tree (black)
richness
latitude
0
5
10
15
20
42
43
44
45

Bagging reduces prediction variance



Ants: bagged regression tree with two predictors



Random forest

Algorithm

for many repetitions

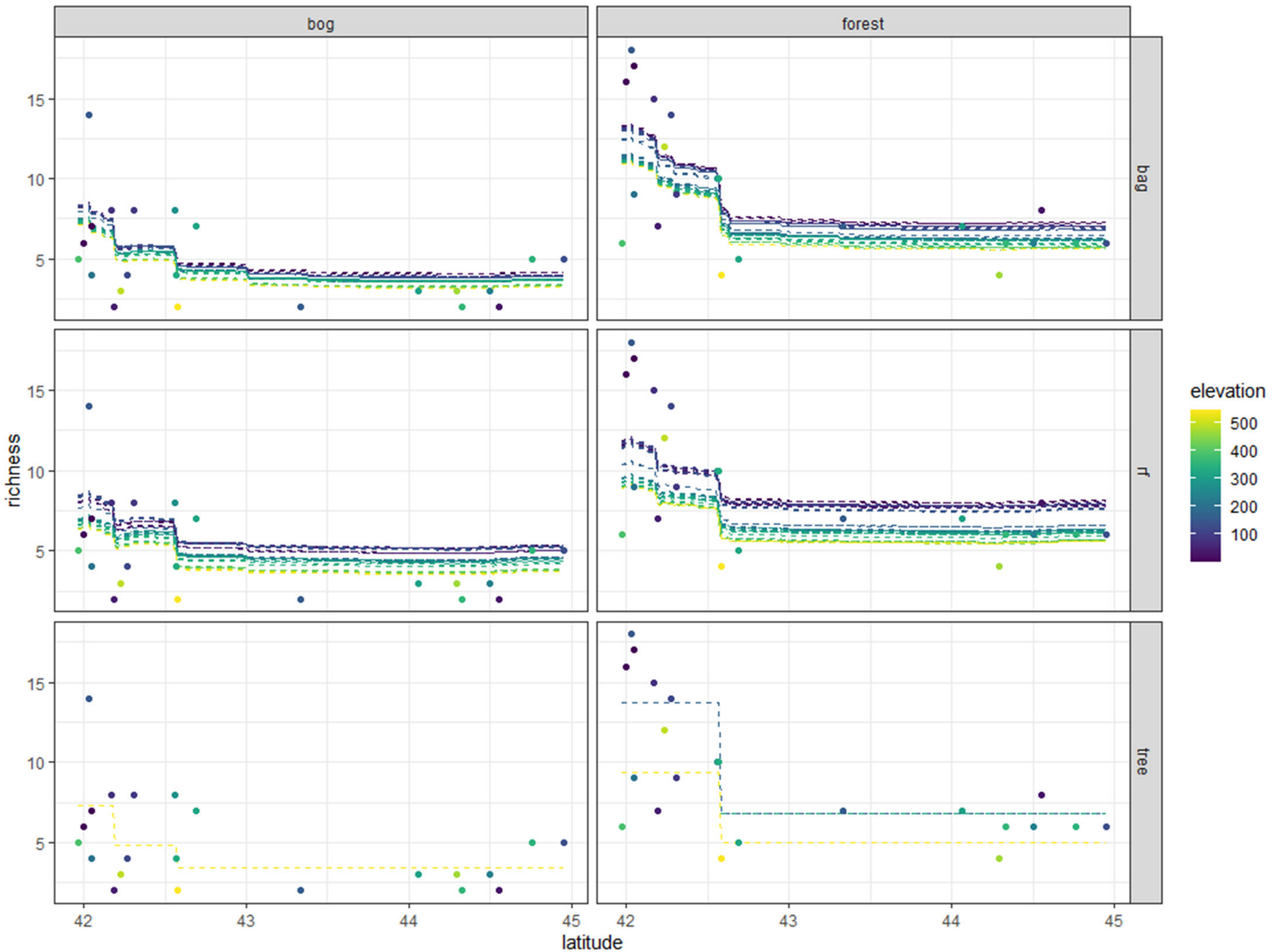
    randomly select m predictor variables

    resample the data (rows) with replacement

    train the tree model

    record prediction

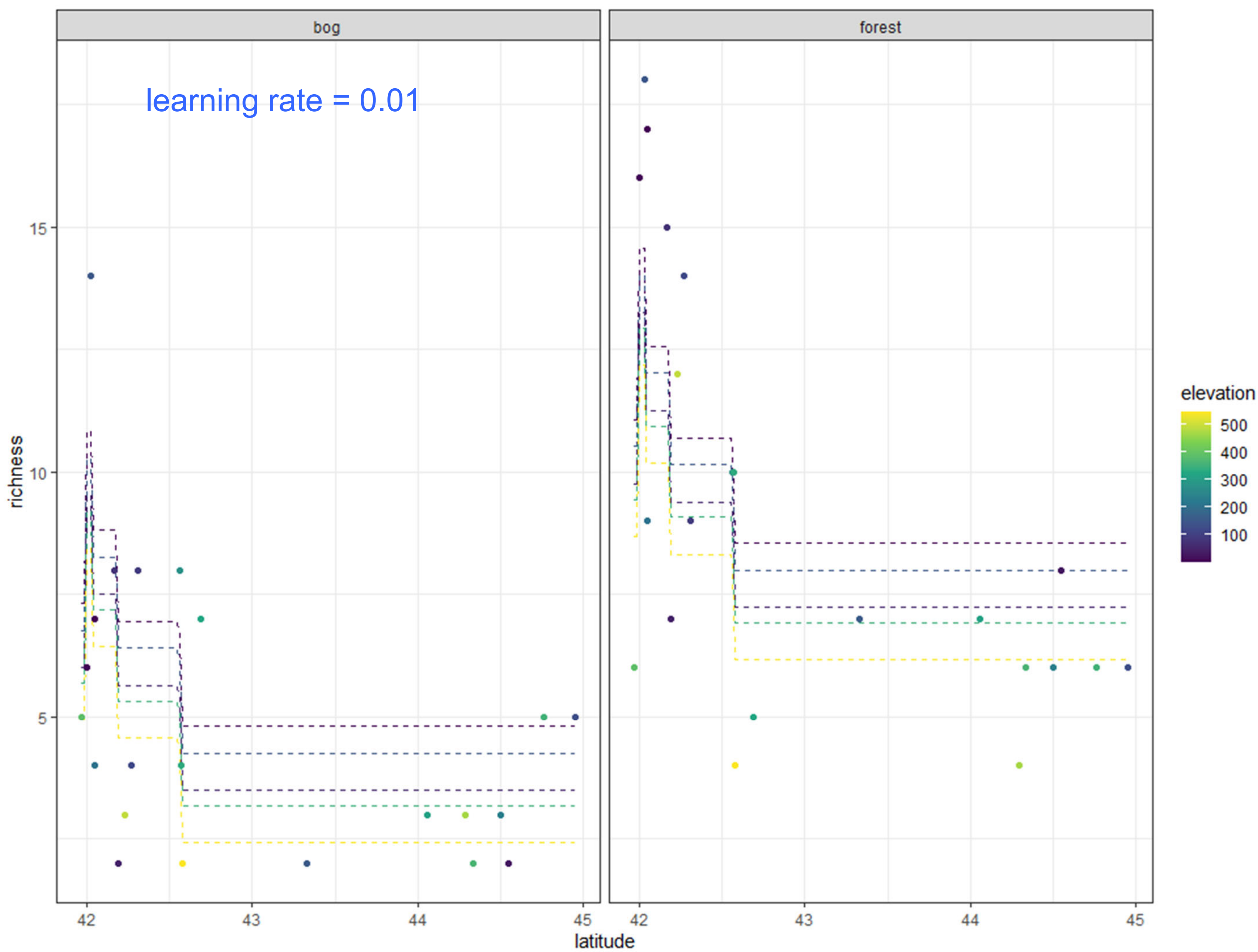
final prediction = mean of predictions



bog
forest
bag
rf
tree
richness
latitude
elevation
500
400
300
200
100
15
10
5
42
43
44
45

Boosting algorithm

- Too complex for this quick overview
- Basic idea: learn slowly by building up an ensemble iteratively from many models, each with small weight
- Key tuning parameter: learning rate
- Can include aspects of bagging and RF
- Training algorithm: gradient descent

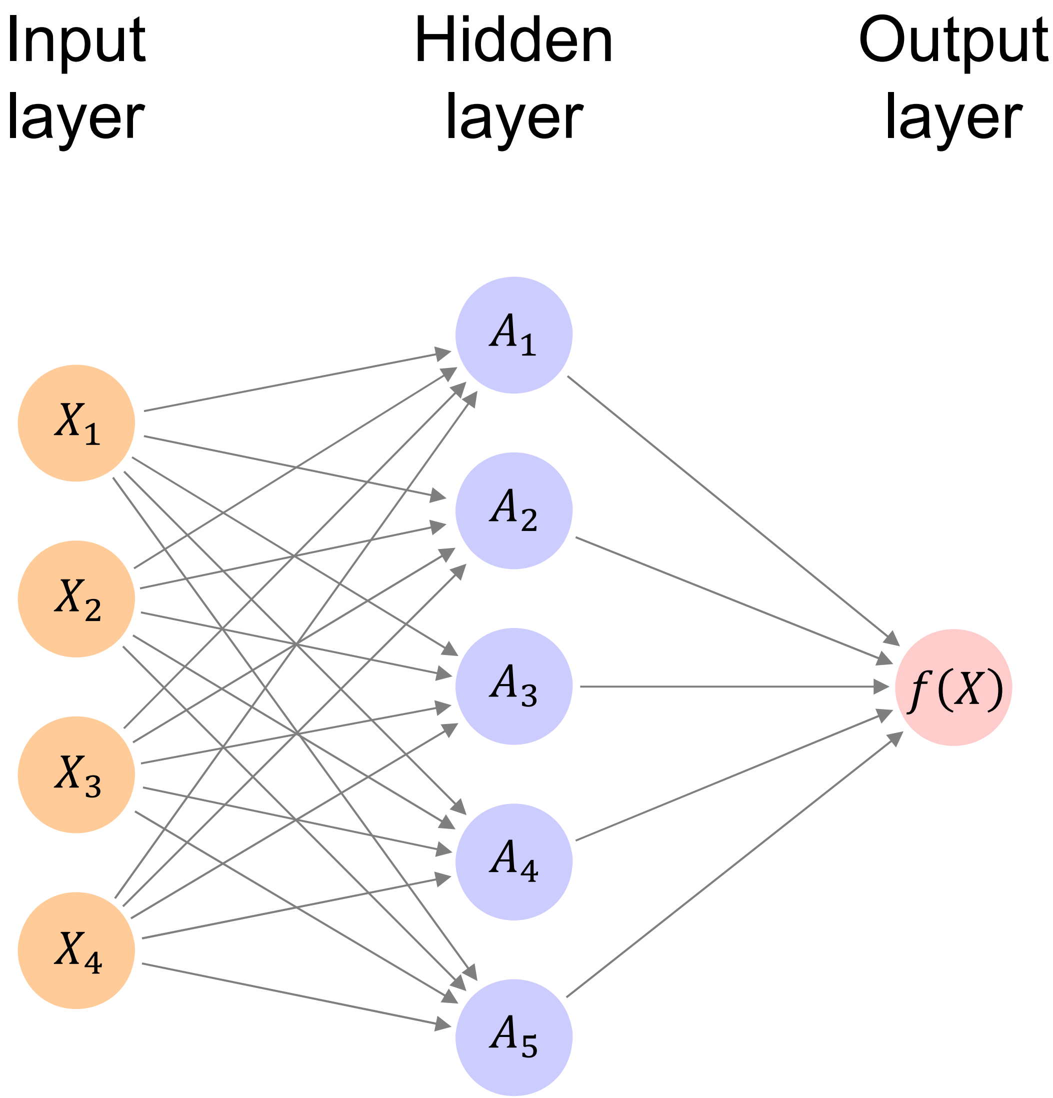


bog
forest
learning rate = 0.01
richness
15
10
5
42
43
44
45
latitude
elevation
500
400
300
200
100

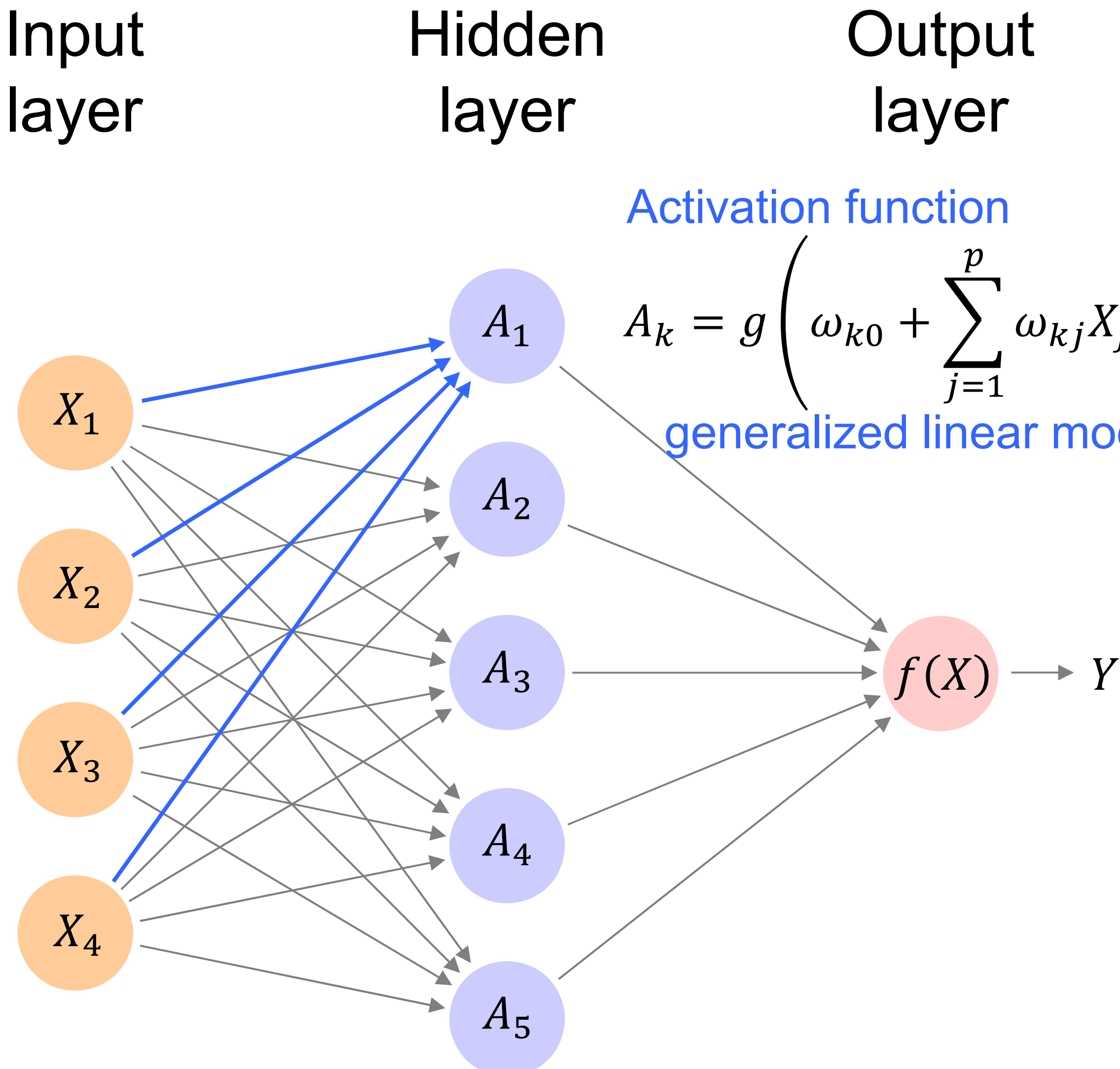
Neural Networks in R

- Interfaces to:
  - keras - google
  - torch - facebook

Single layer NN



Single layer NN



Activation function

$$A_k = g\left(\omega_{k0} + \sum_{j=1}^{p} \omega_{kj} X_j\right)$$

generalized linear model

Transform from X to A

Single layer NN

Input layer

Hidden layer

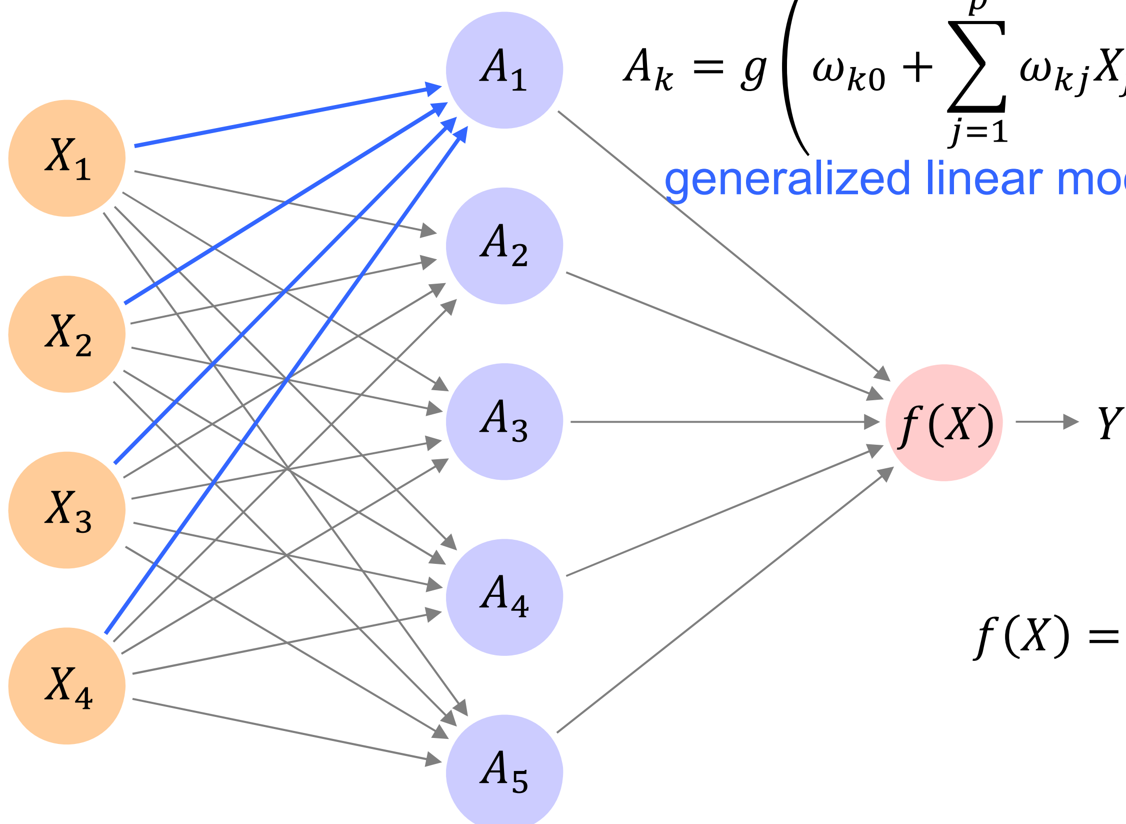
Output layer

Activation function

$$A_k = g\left(\omega_{k0} + \sum_{j=1}^{p} \omega_{kj} X_j\right)$$

generalized linear model

Transform from X to A



$$f(X) = \beta_0 + \sum_{k=1}^{K} \beta_k A_k$$

multiple linear regression

Training algorithm

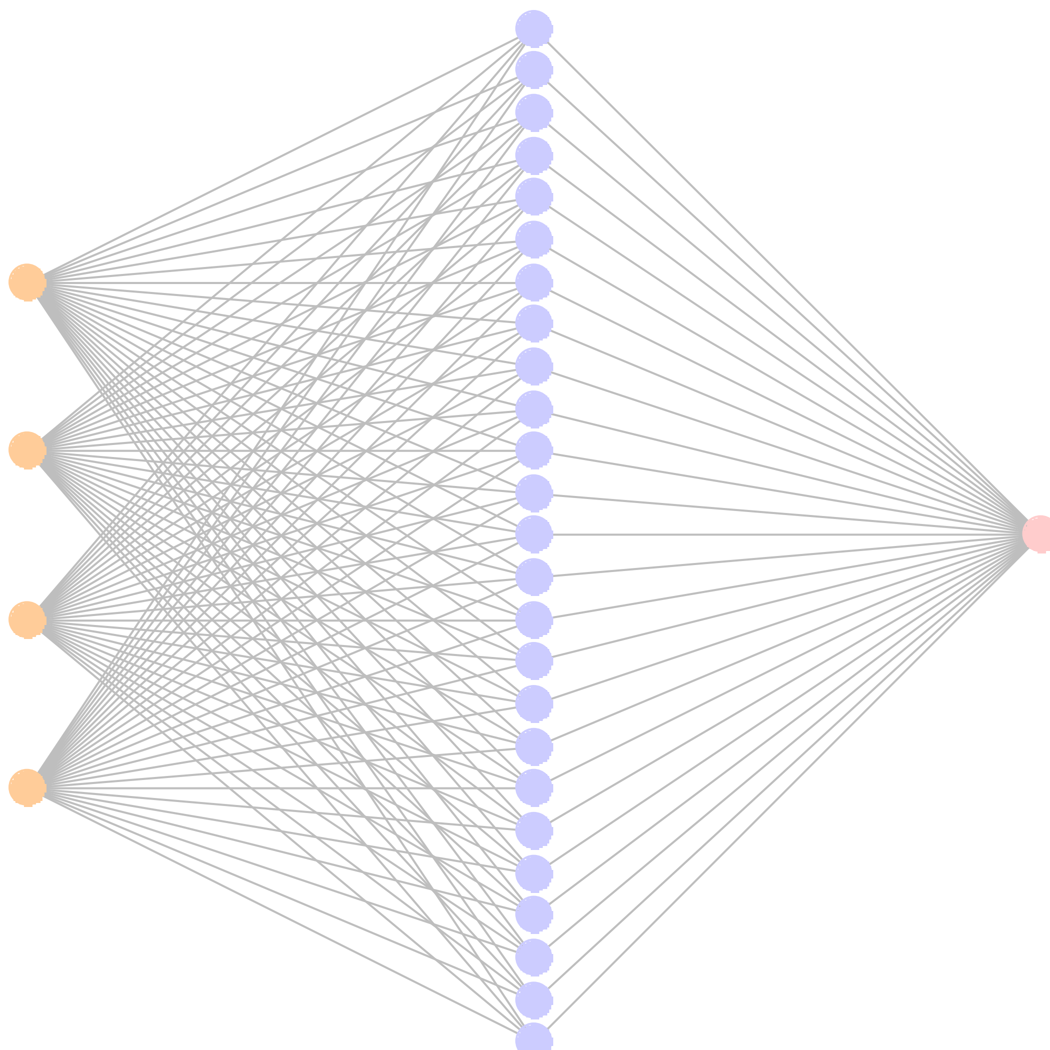
- Stochastic gradient descent
  - with back propagation

- Model and training algorithms incorporate many previous strategies

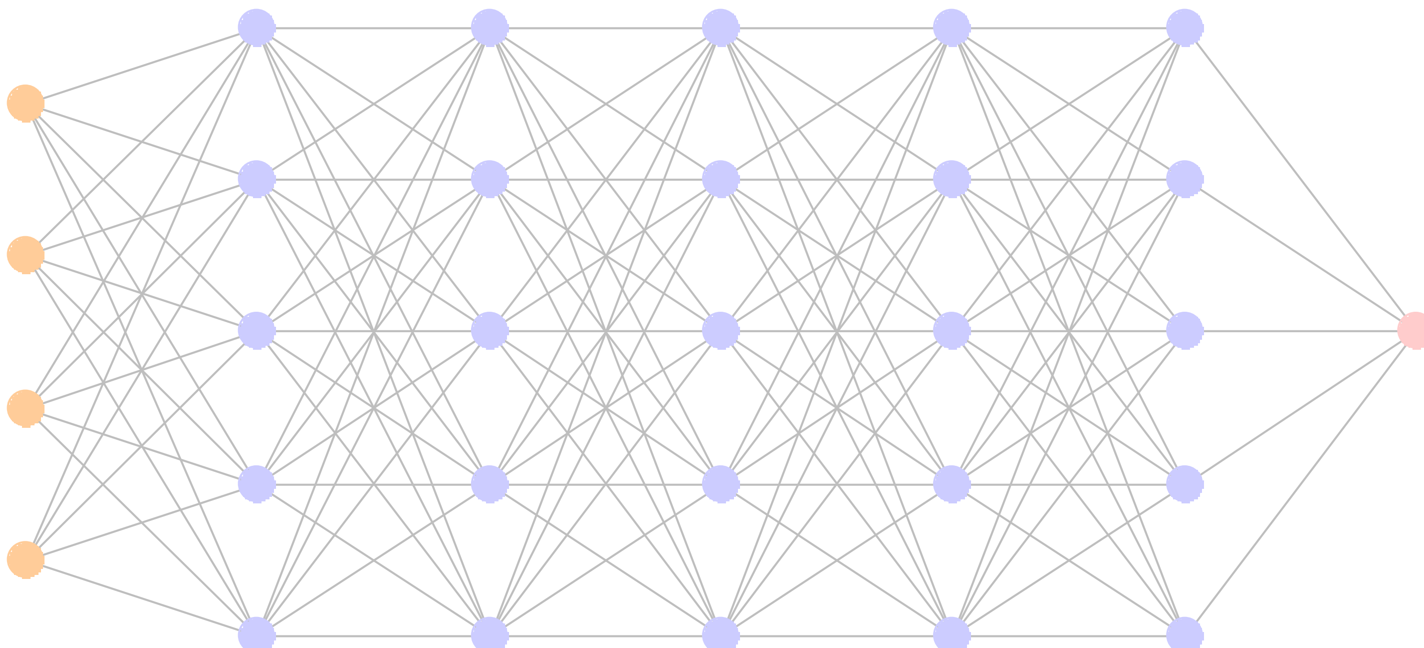
Deep learning

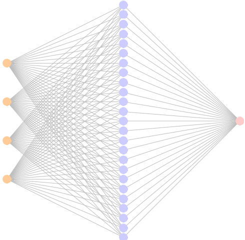
- Multilayer neural networks
- Model algorithm
  - expressiveness
    - ability to approximate complex nonlinearity
  - architecture: width versus depth

Wide: 25 hidden units

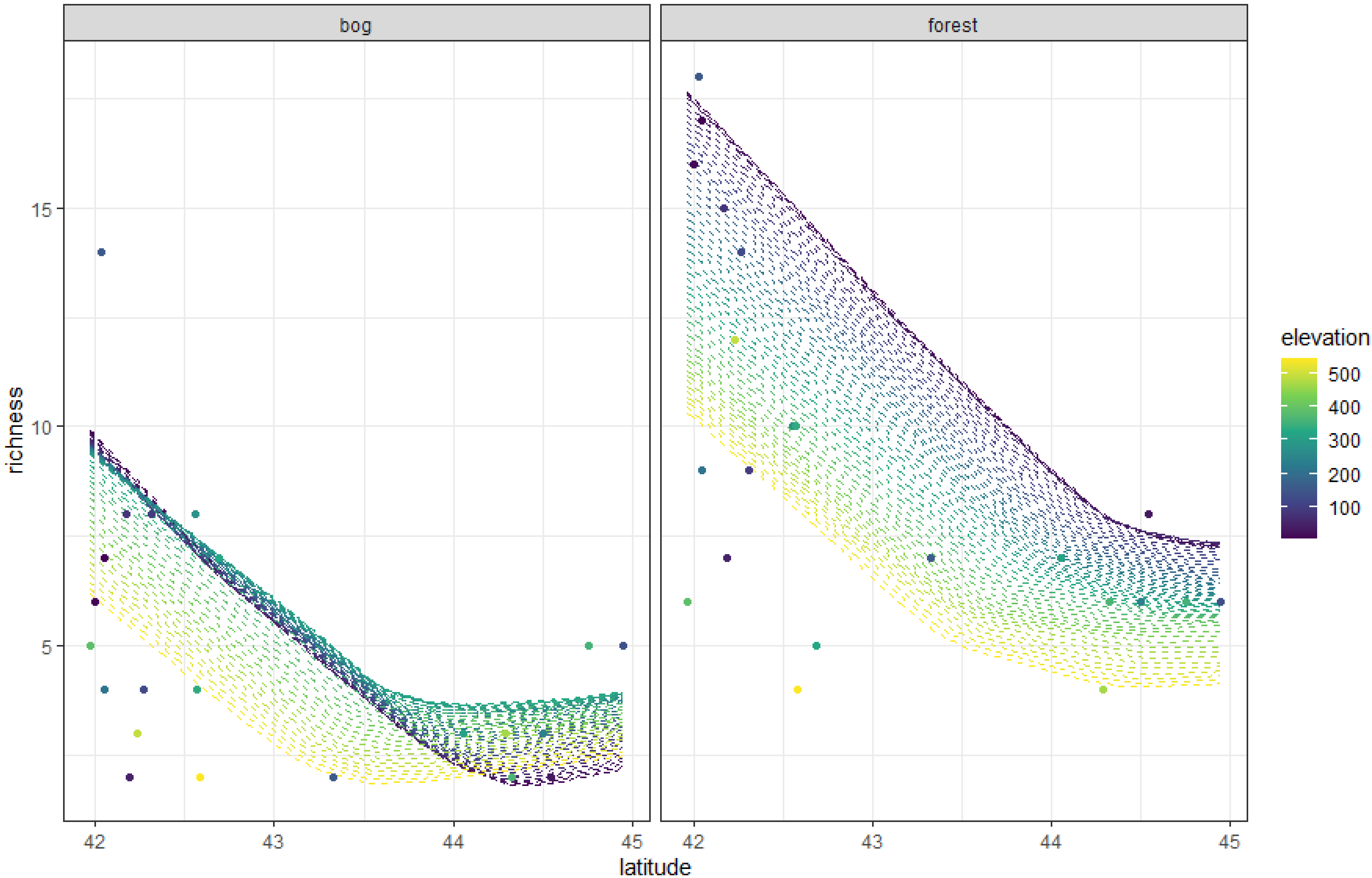


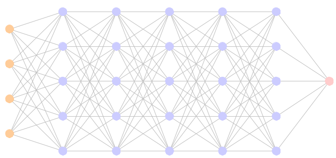
Deep: 25 hidden units



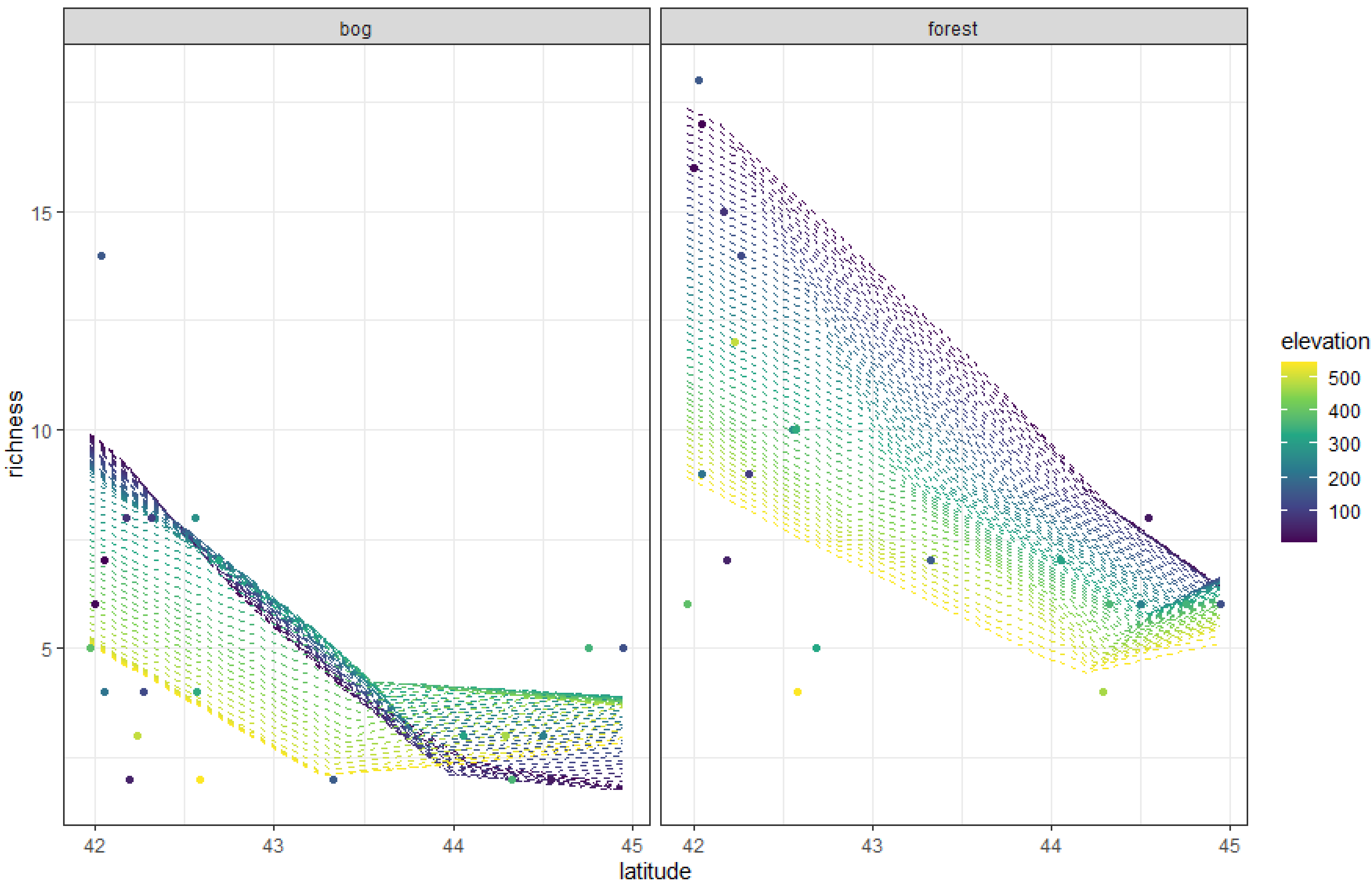


Ants data: wide





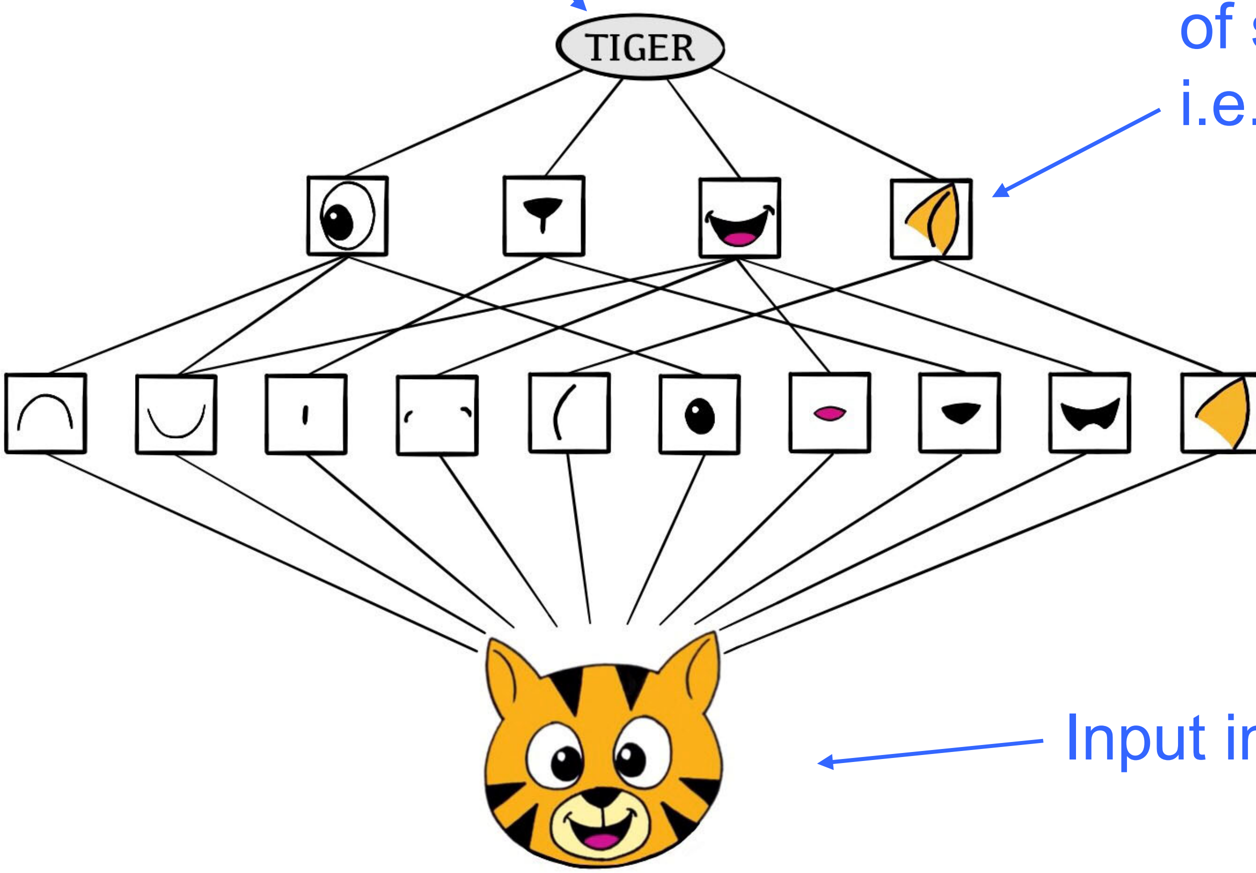
Ants data: deep



Convolutional NNs

Output is high-level concept

Conv layer 2
learns combinations
of small features
i.e. objects



Conv layer 1
learns small
features
e.g. edges

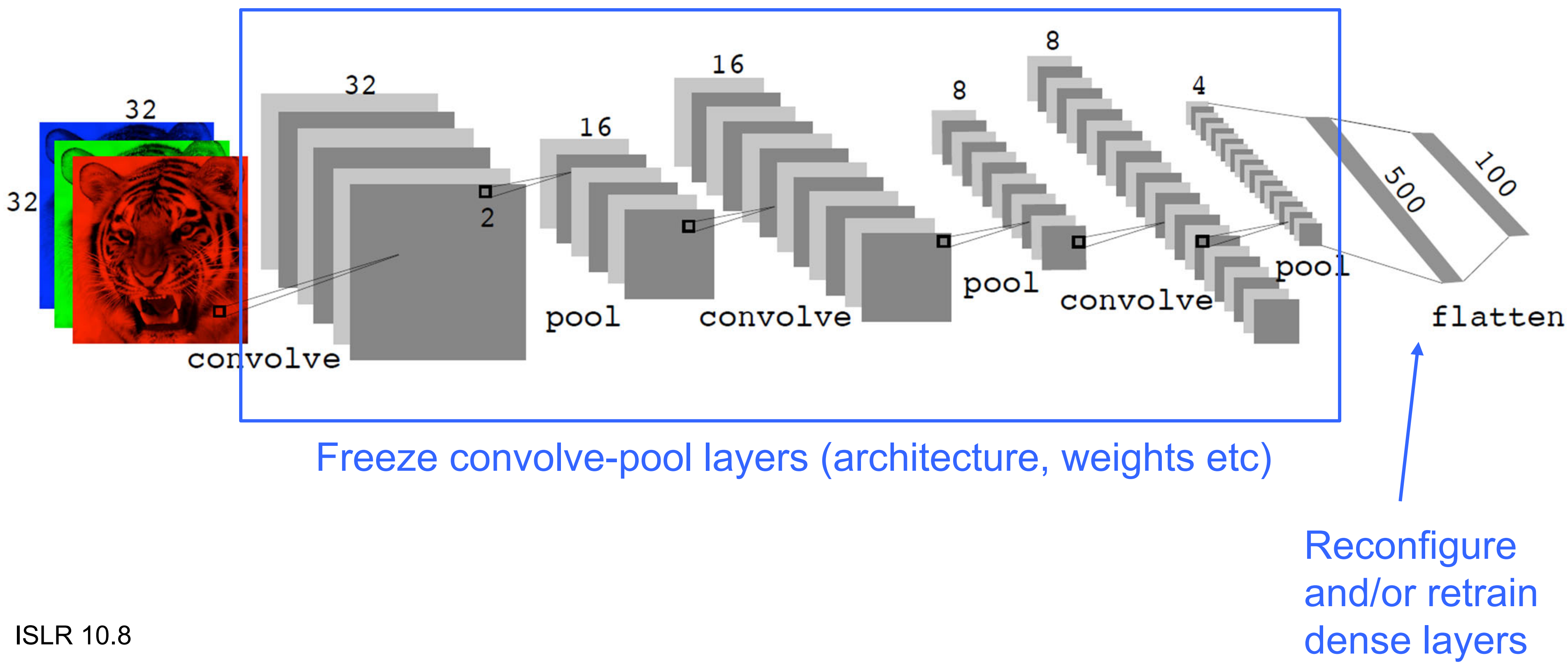
Input image

ISLR 10.6

Transfer learning

Pretrained model on related big data

Retrain last 1-2 layers on specialized little data



ISLR 10.8

Rapid innovation

- Architectures
- Algorithms
- Recent example: transformer

Outlook

Automated data collection

+

machine learning

=

revolutionary