Regression and practical advice

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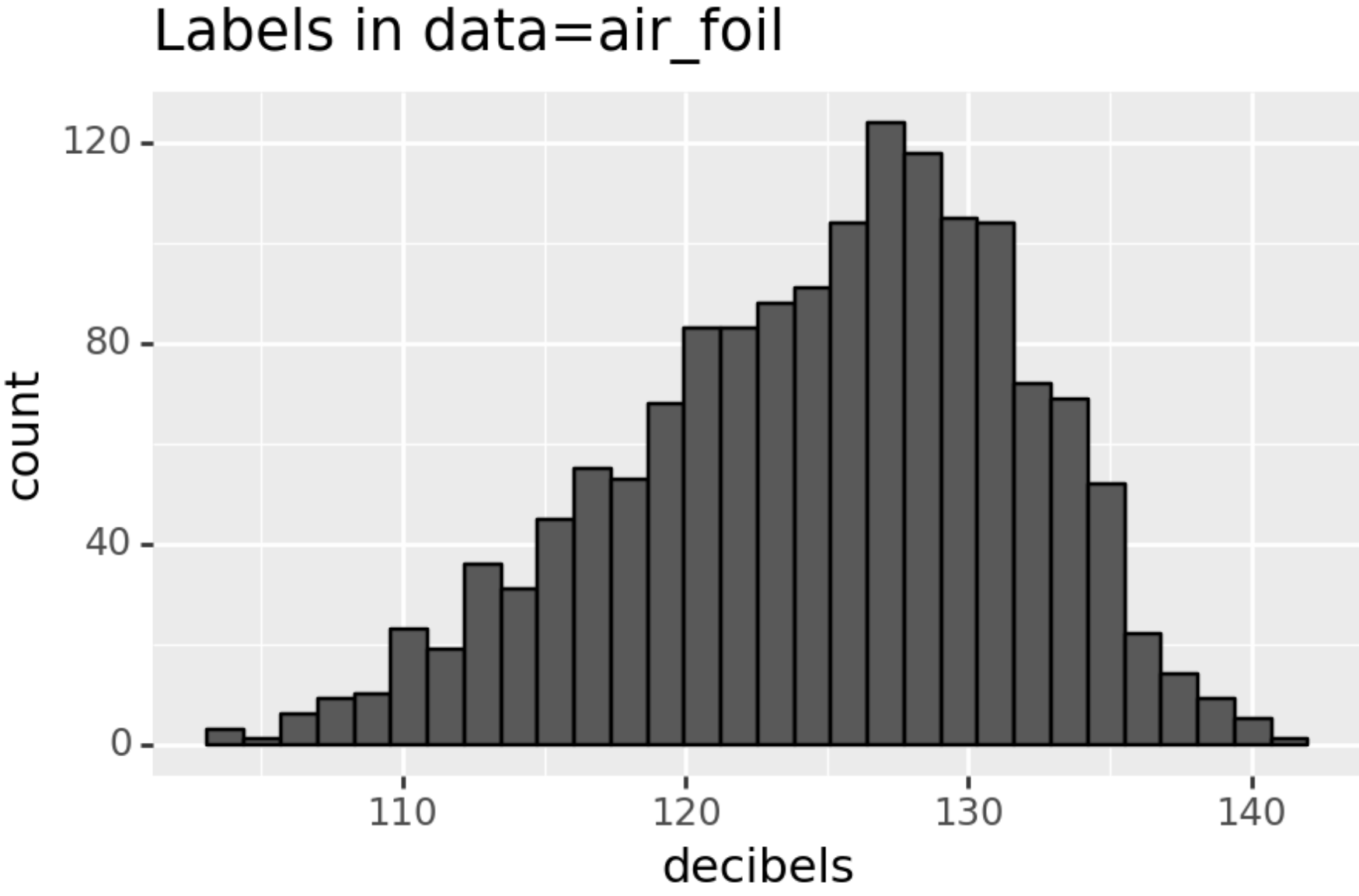
Supervised machine learning

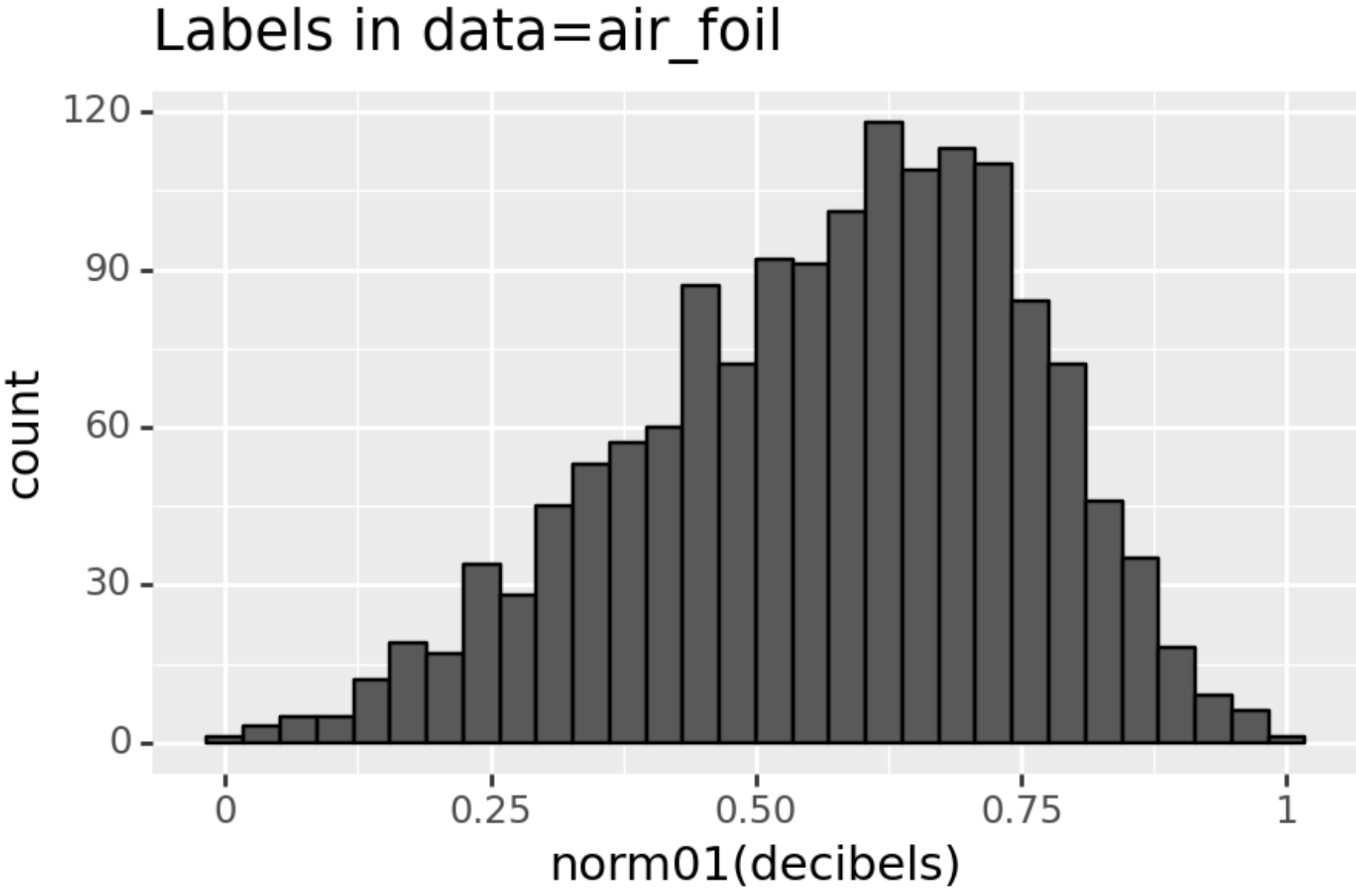
- Goal is to learn a function $f(\mathbf{x}) = y$ where $\mathbf{x} \in \mathbb{R}^p$ is an input/feature vector and y is an output/label.
- This week we will study linear models and neural networks for regression, meaning labels represented by $y \in \mathbb{R}$ is a real number.
- air foil self-noise data: $\mathbf{x}$ = Frequency (Hertz), Angle of attack (degrees), Chord length (meters), Free-stream velocity (meters per second), $y \in \mathbb{R}$ Scaled sound pressure level, in decibels.
- forest fires data: $\mathbf{x}$ =meteorological and other data, $y \in \mathbb{R}_+$ burned area.
- some practical advice for getting gradient descent learning to work better (scaling, log transform, feature transform)

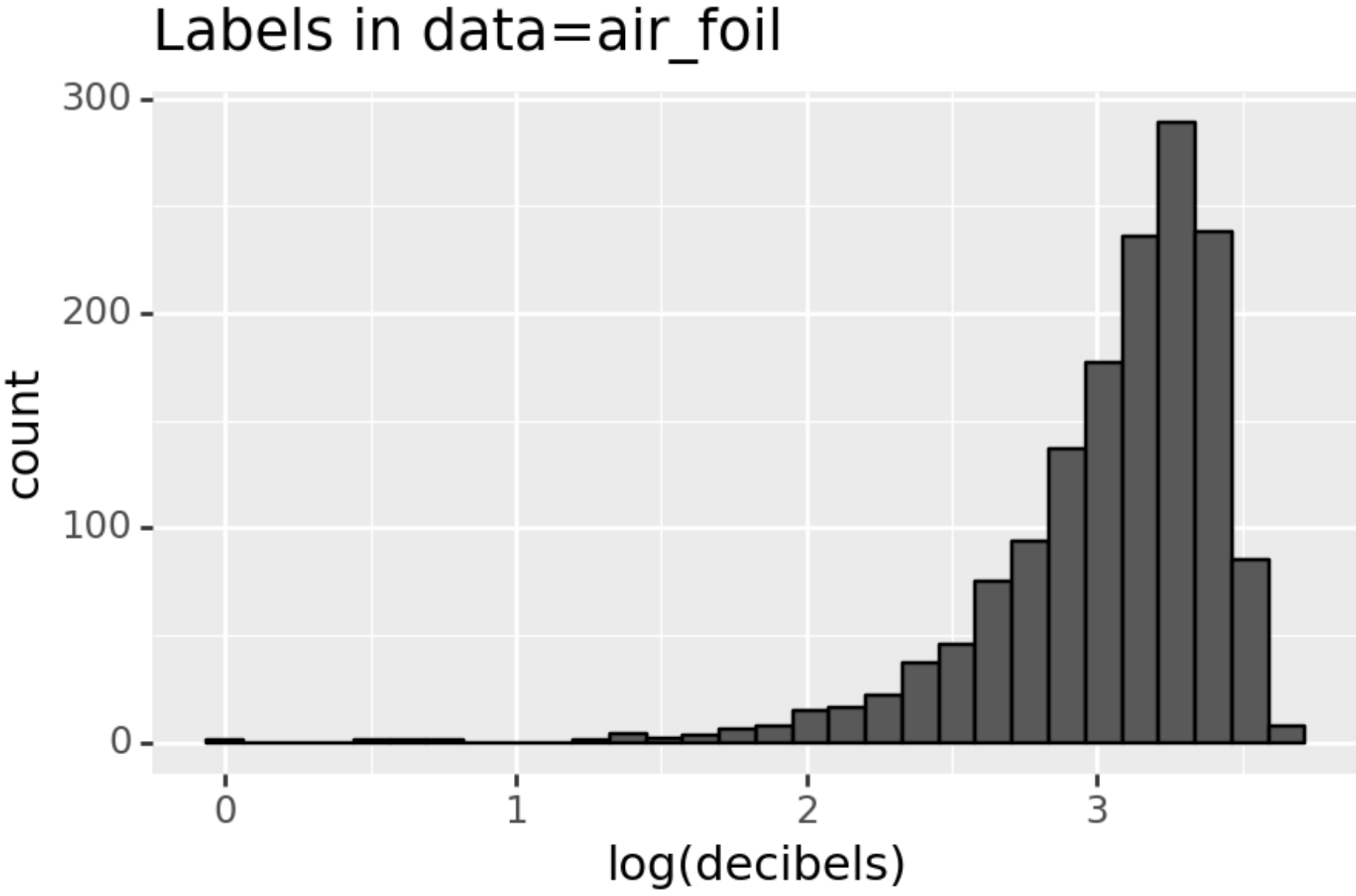
air foil self-noise data

```
##        Hertz  degrees   ...     meters  decibels
## 0        800      0.0   ...   0.002663   126.201
## 1       1000      0.0   ...   0.002663   125.201
## 2       1250      0.0   ...   0.002663   125.951
## 3       1600      0.0   ...   0.002663   127.591
## 4       2000      0.0   ...   0.002663   127.461
## ...      ...      ...   ...        ...       ...
## 1498    2500     15.6   ...   0.052849   110.264
## 1499    3150     15.6   ...   0.052849   109.254
## 1500    4000     15.6   ...   0.052849   106.604
## 1501    5000     15.6   ...   0.052849   106.224
## 1502    6300     15.6   ...   0.052849   104.204
##
## [1503 rows x 6 columns]
```

Need to scale label vector, to avoid numerical instability in gradient descent.


Labels in data=air_foil
120
80
40
0
count
110
120
130
140
decibels

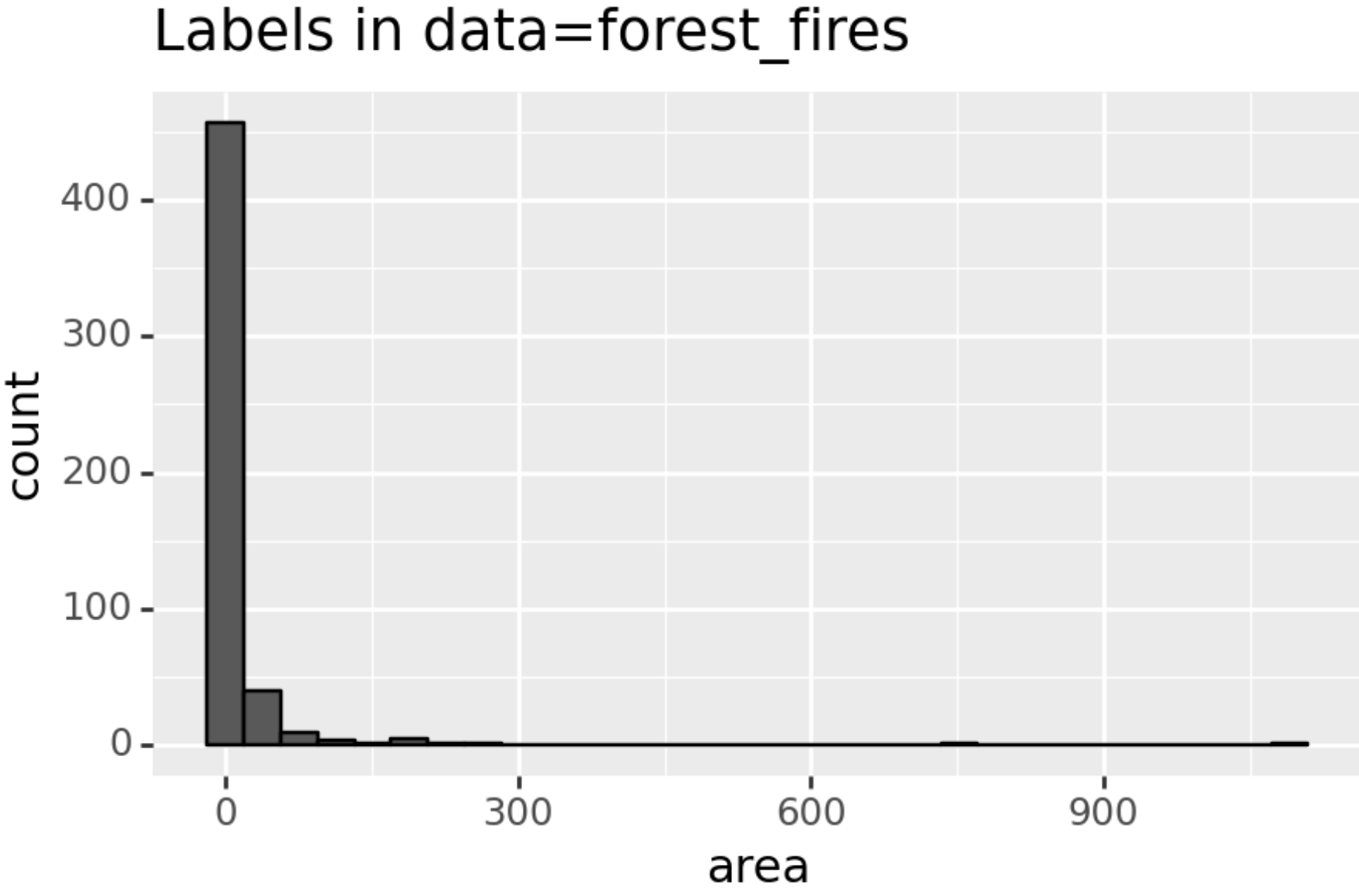

Labels in data=air_foil
120
90
60
30
0
count
0
0.25
0.50
0.75
1
norm01(decibels)

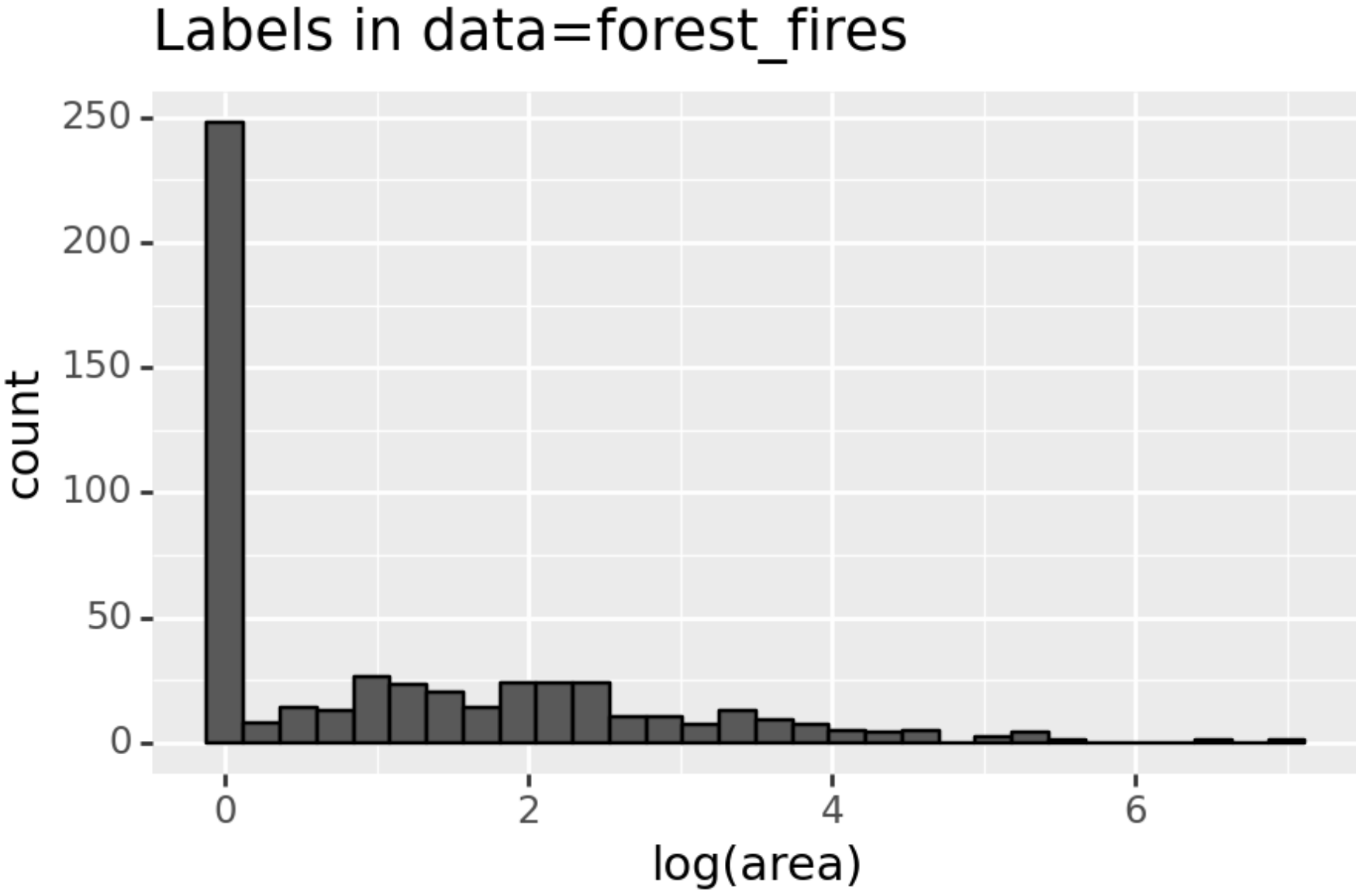

Labels in data=air_foil
300
200
100
0
count
0
1
2
3
log(decibels)

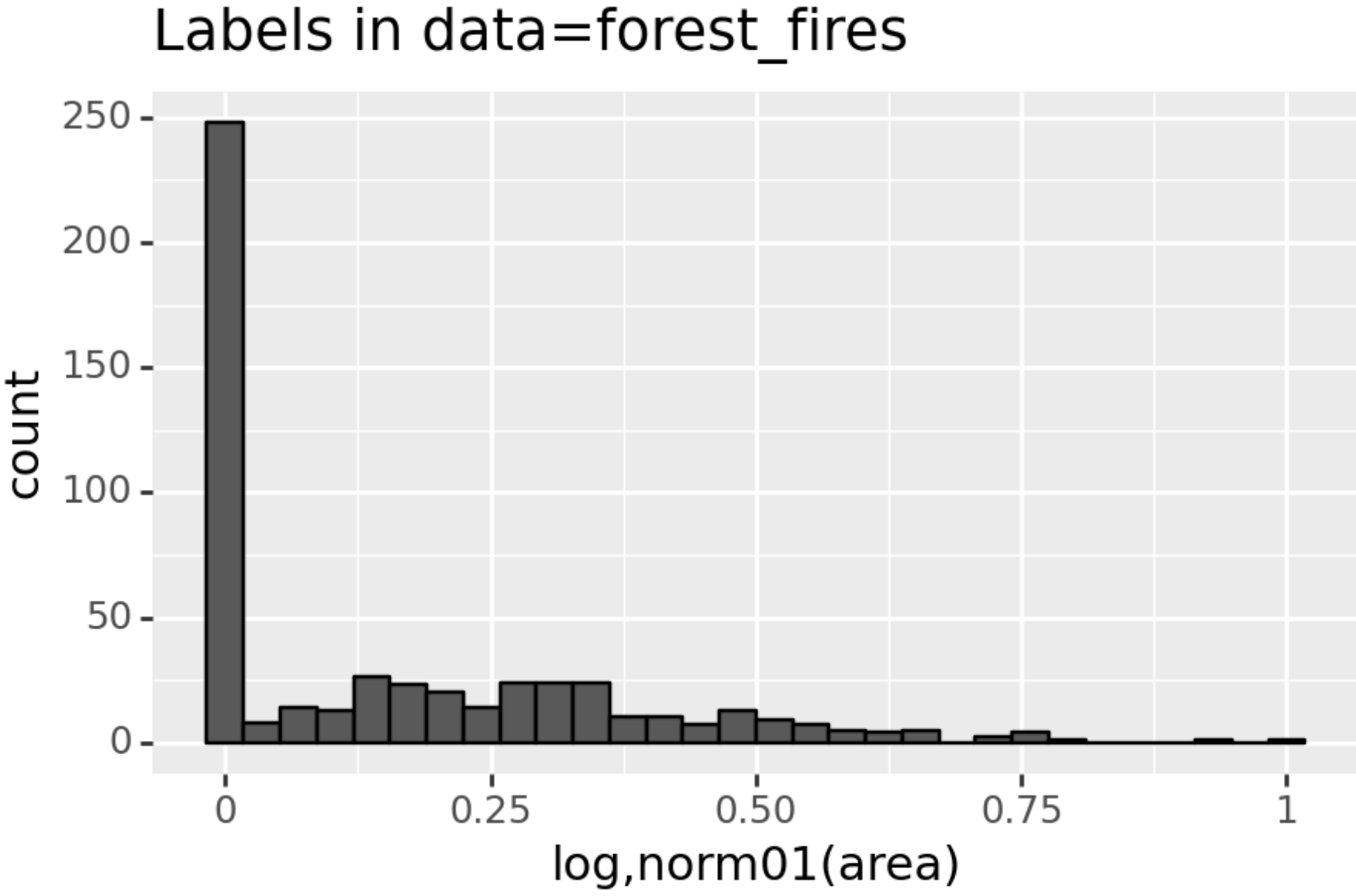
forest fires data

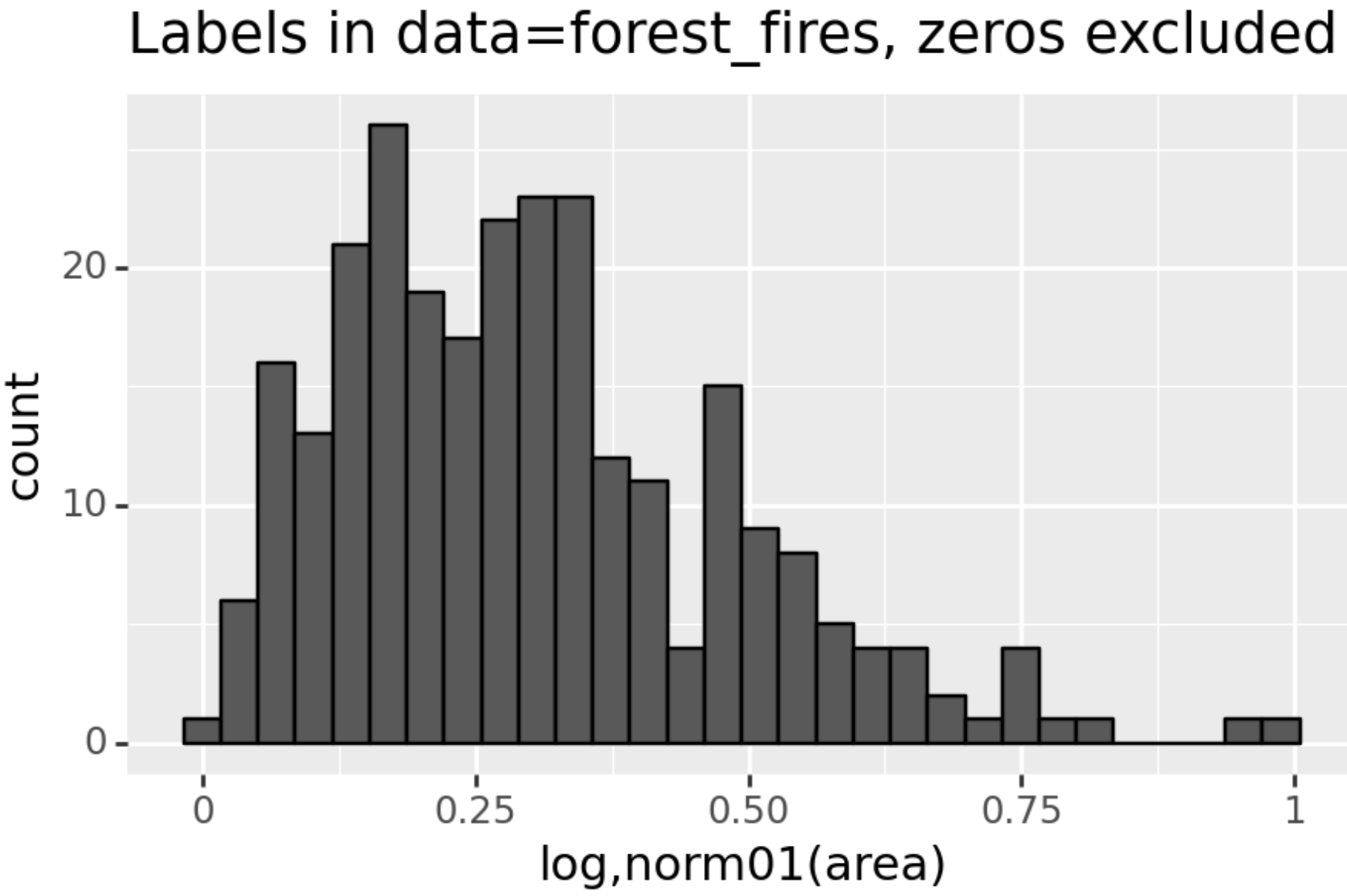
```
##       X  Y month  ... wind  rain   area
## 0     7  5   mar  ...  6.7   0.0   0.00
## 1     7  4   oct  ...  0.9   0.0   0.00
## 2     7  4   oct  ...  1.3   0.0   0.00
## 3     8  6   mar  ...  4.0   0.2   0.00
## 4     8  6   mar  ...  1.8   0.0   0.00
## ..   .. ..   ...  ...  ...   ...    ...
## 512   4  3   aug  ...  2.7   0.0   6.44
## 513   2  4   aug  ...  5.8   0.0  54.29
## 514   7  4   aug  ...  6.7   0.0  11.16
## 515   1  4   aug  ...  4.0   0.0   0.00
## 516   6  3   nov  ...  4.5   0.0   0.00
##
## [517 rows x 13 columns]
```

For categorical variables like month, need to ignore, or re-encode (ordinal or one-hot encoding).

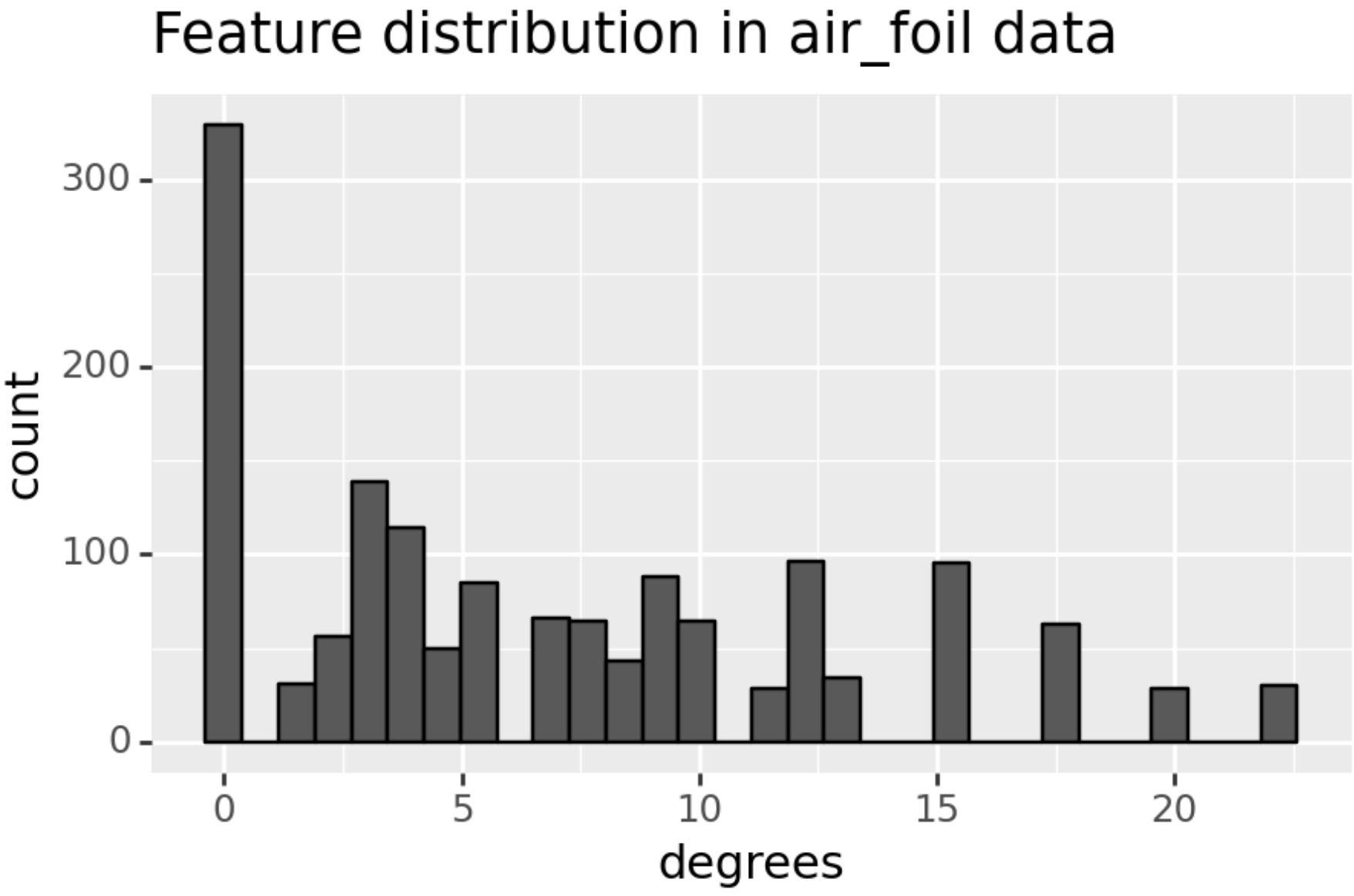

Labels in data=forest_fires
400
300
200
100
0
count
0
300
600
900
area


Labels in data=forest_fires
250
200
150
100
50
0
count
0
2
4
6
log(area)

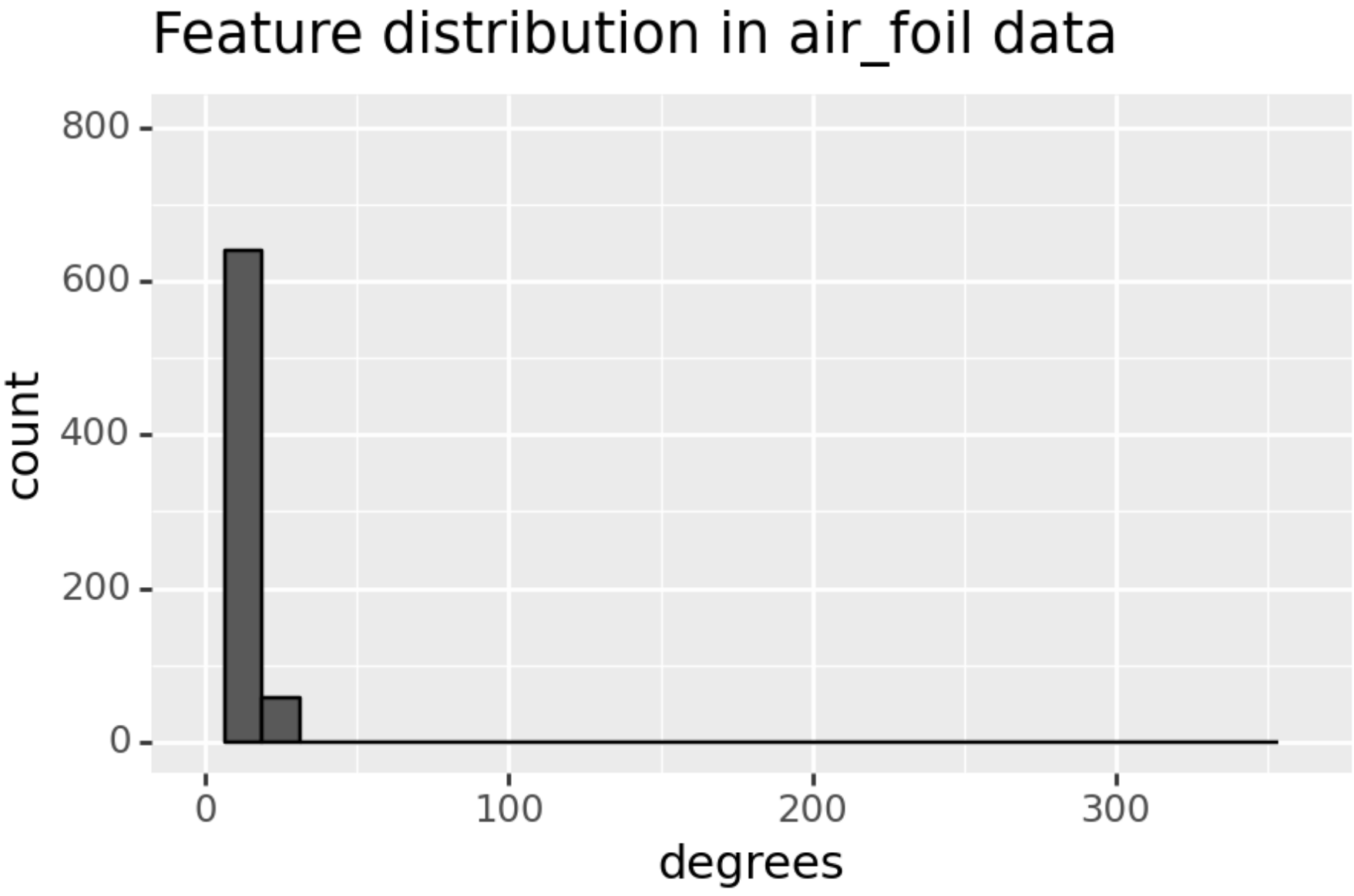

Labels in data=forest_fires
250
200
150
100
50
0
count
0
0.25
0.50
0.75
1
log,norm01(area)


Labels in data=forest_fires, zeros excluded
count
20
10
0
0
0.25
0.50
0.75
1
log,norm01(area)

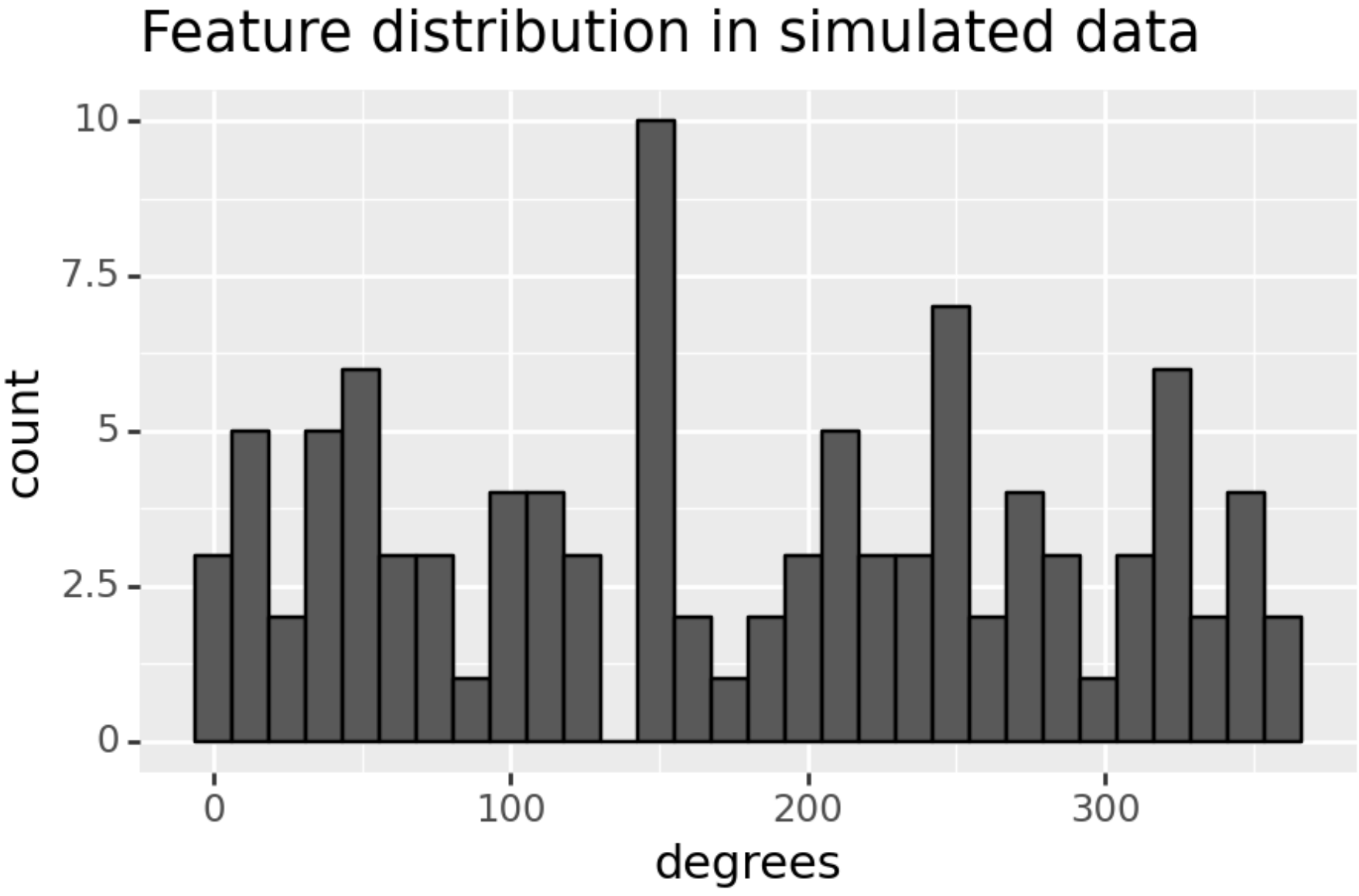
Real data feature distribution



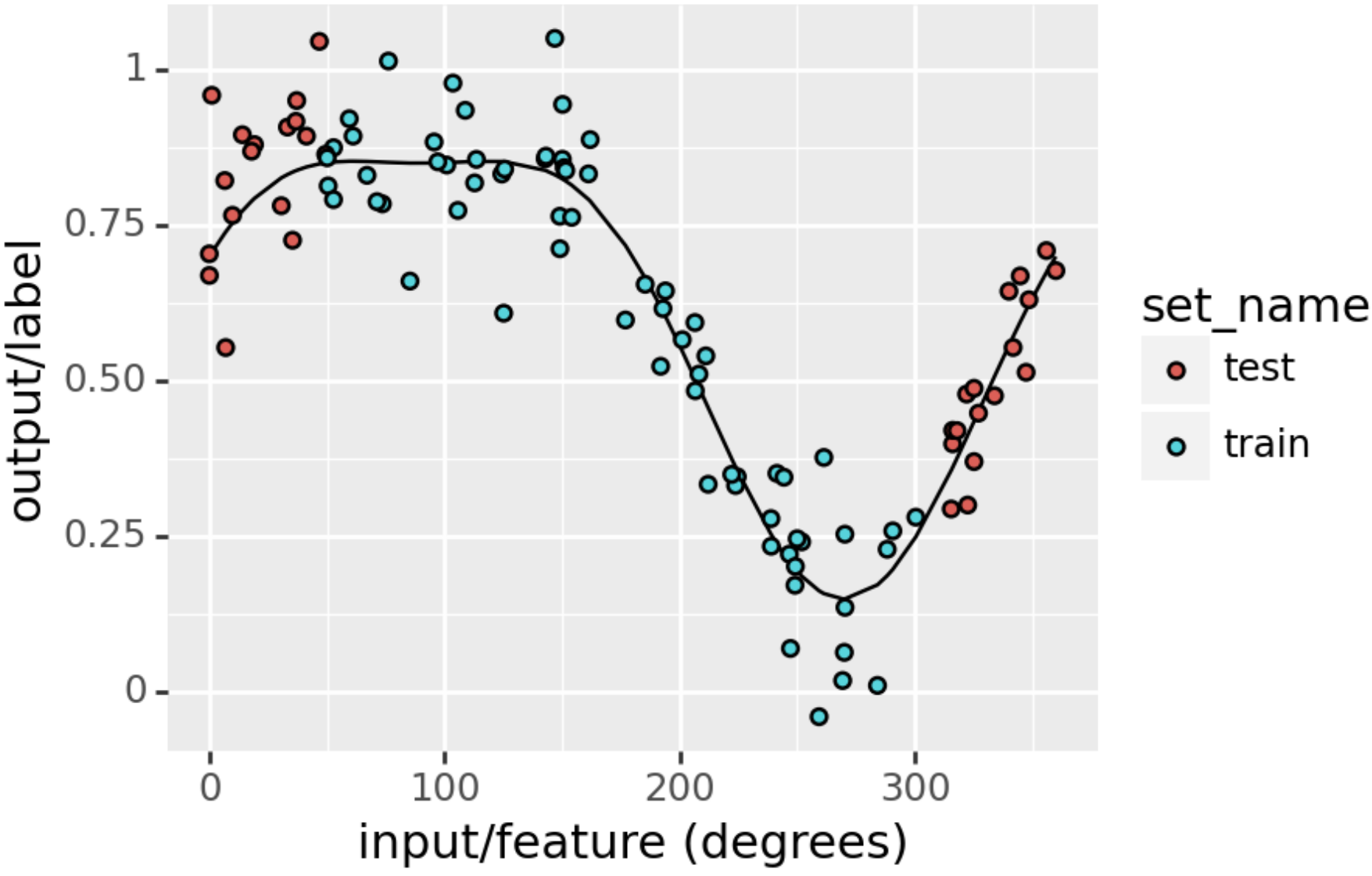
Real data feature distribution



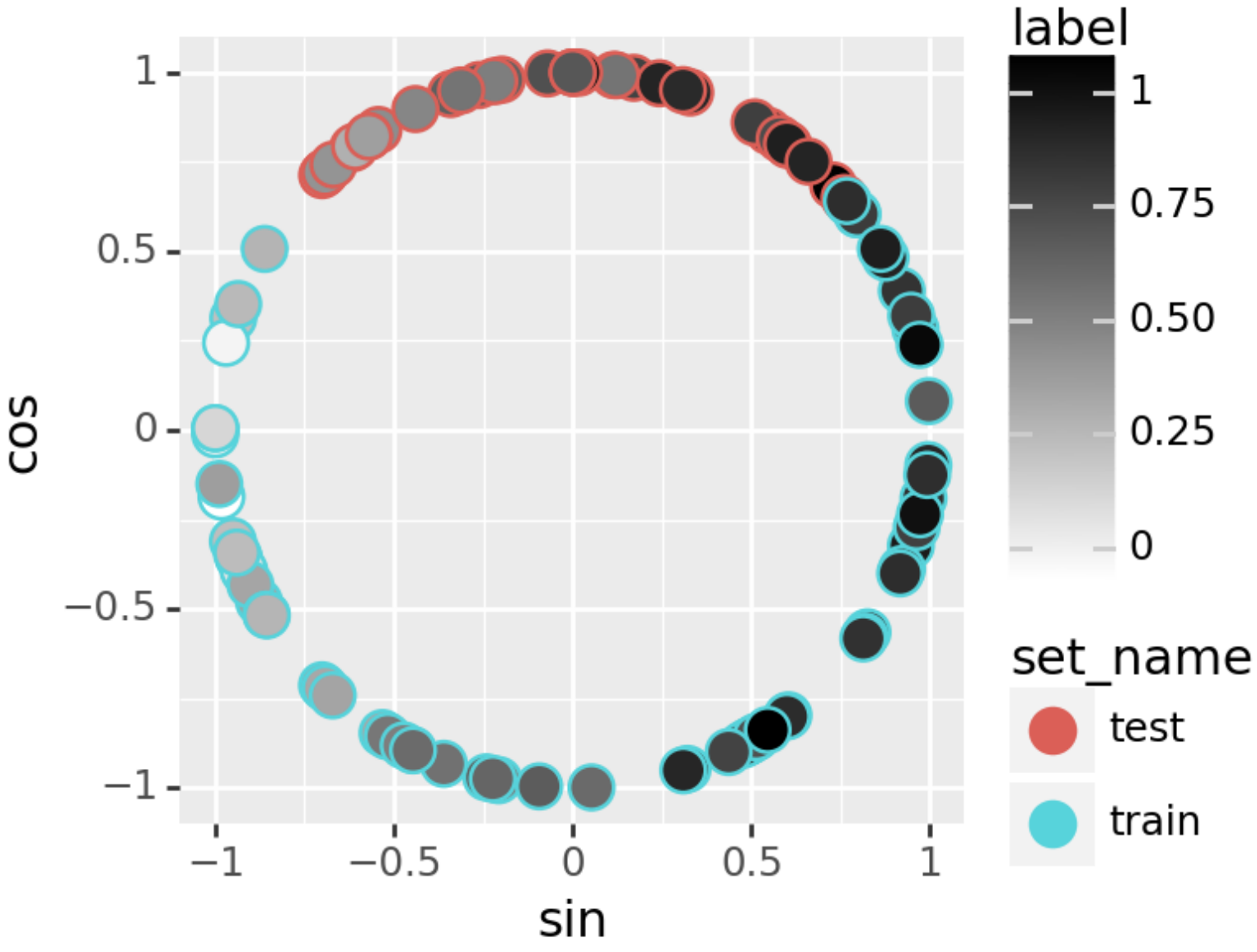
Simulated data feature distribution



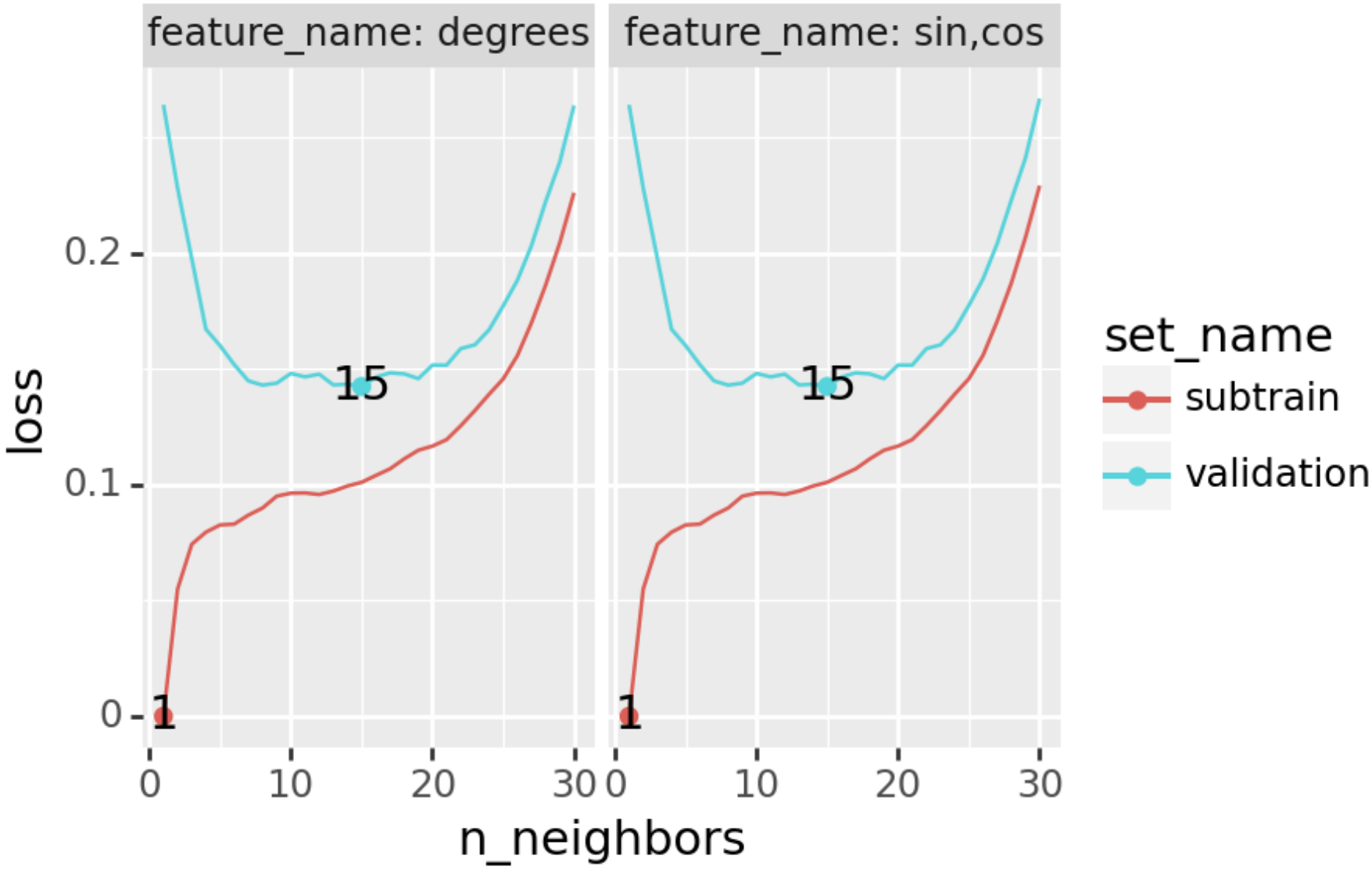
Pattern in simulated data has continuity over 0/360 edge



Non-linear basis expansion

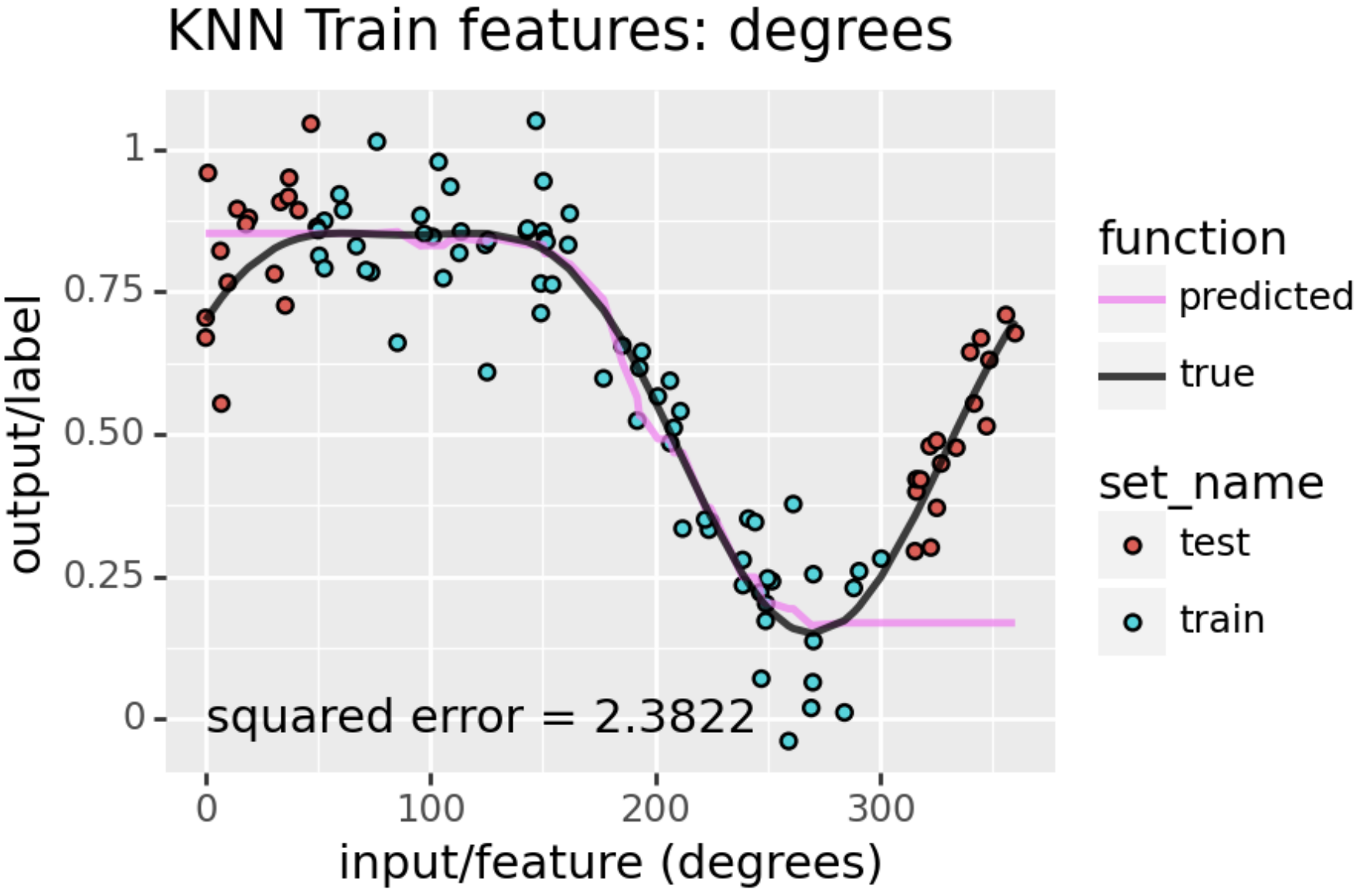


Train nearest neighbor regression

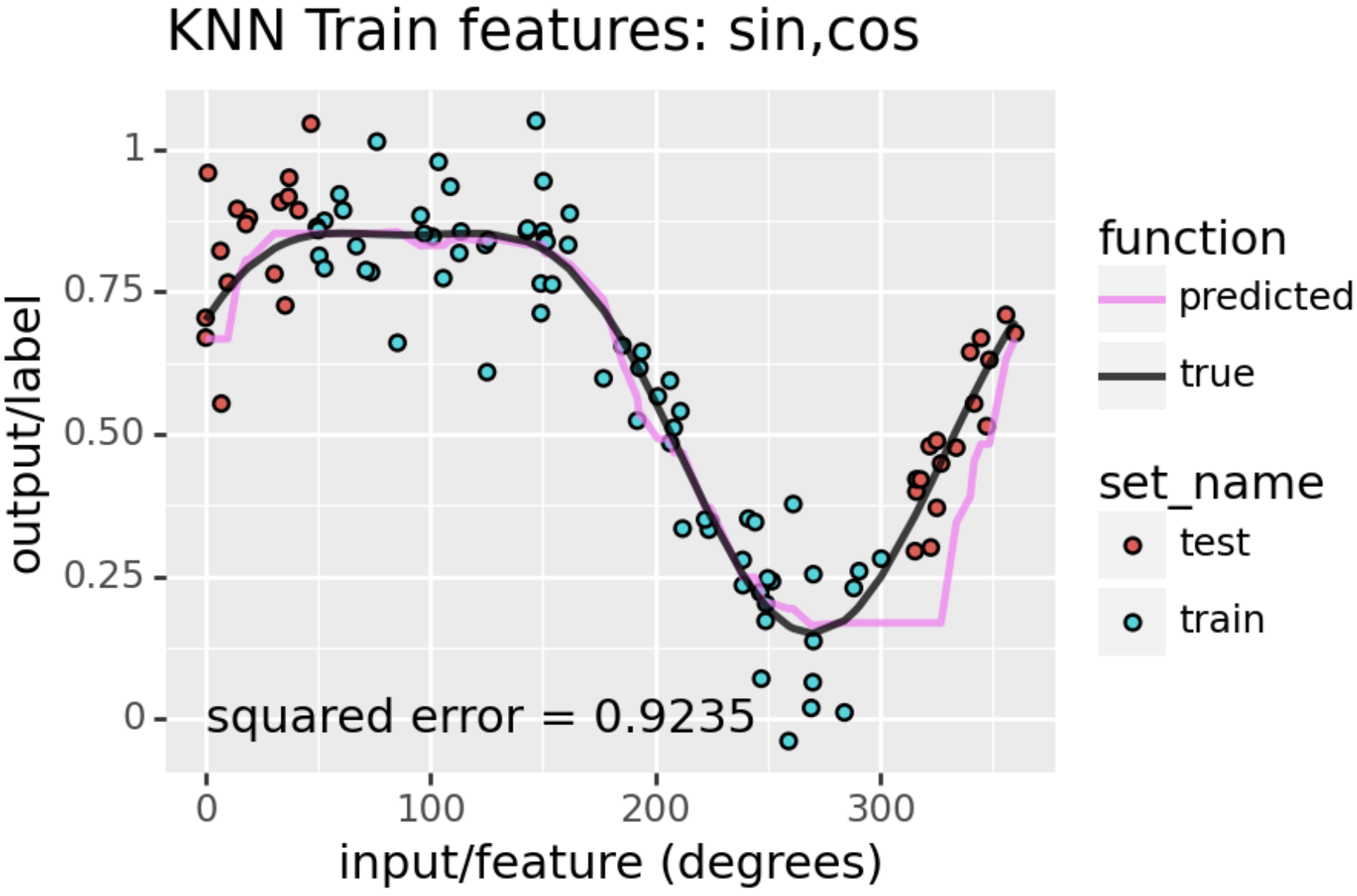


Predict mean of K nearest neighbors.

Learned function not continuous over 0/360

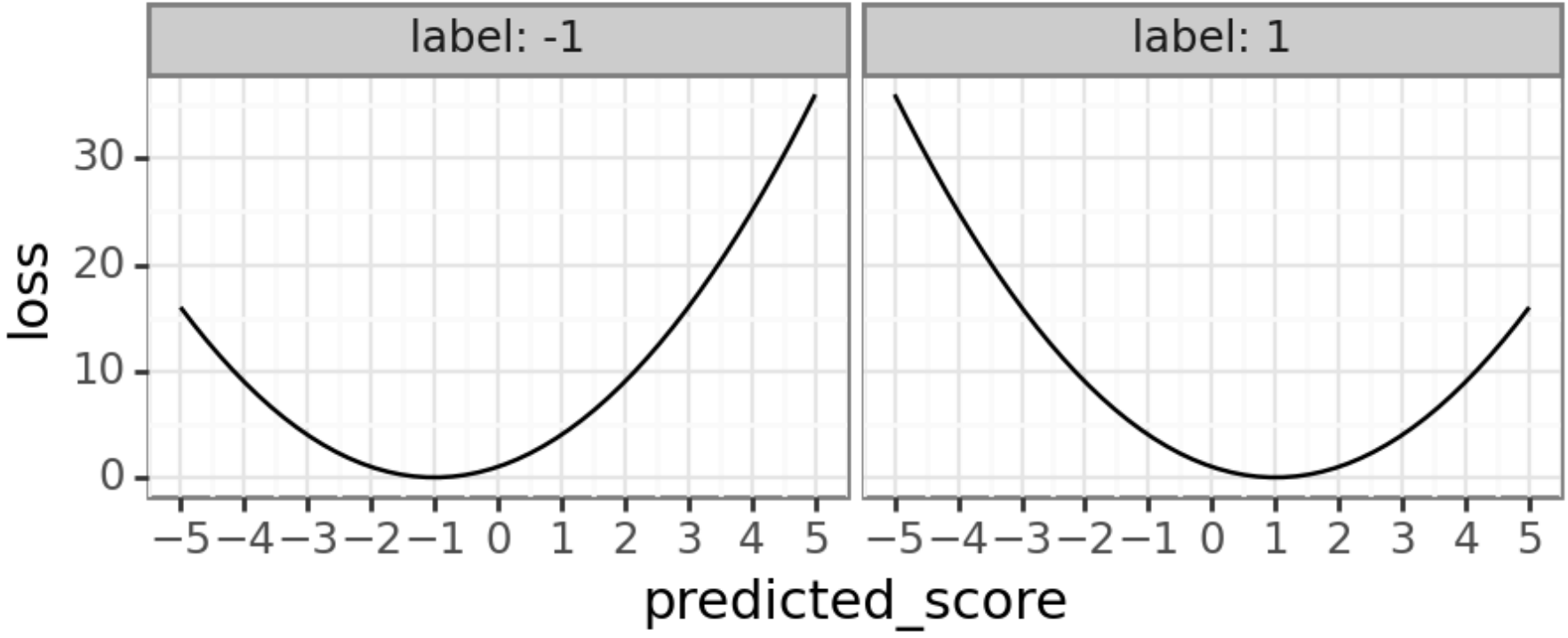


sin/cos features enforce continuity

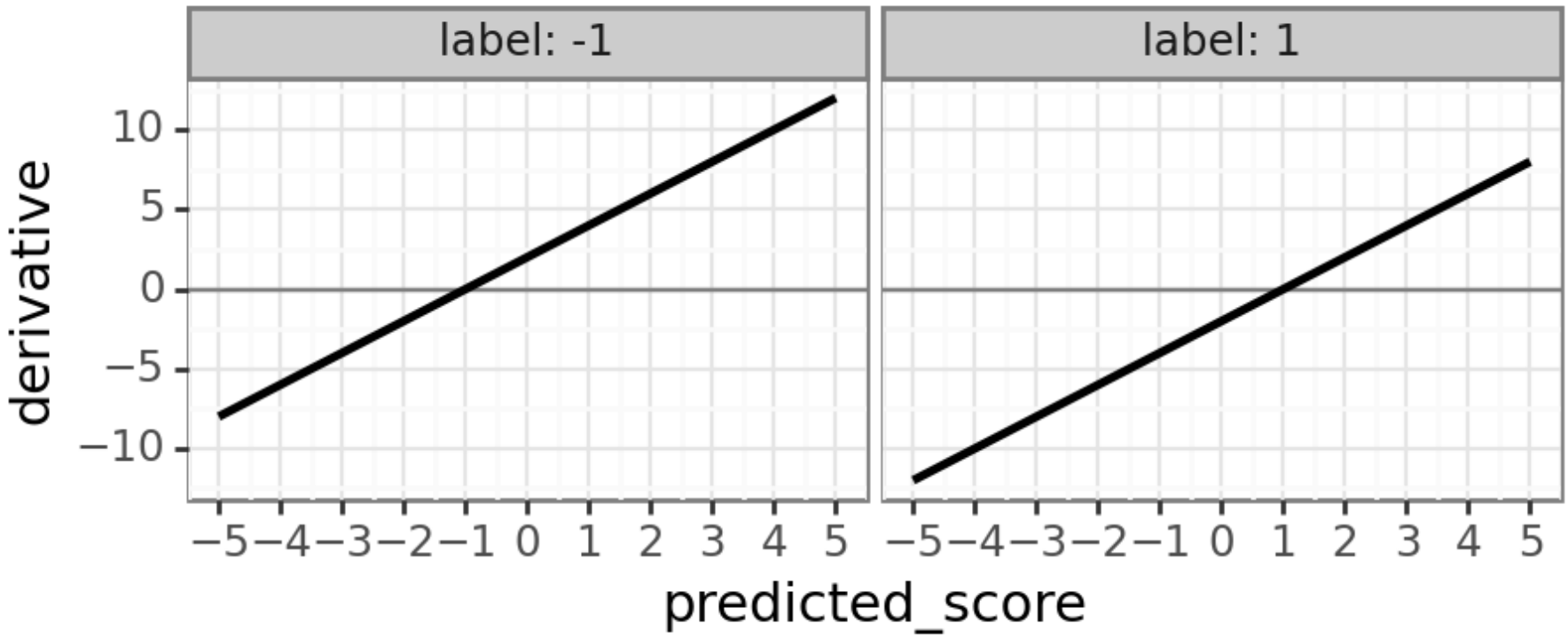


How are the neural network weights learned?

- Typically we use some version of gradient descent.
- This algorithm requires definition of a differentiable loss function to minimize on the train set.
- For regression problems ($y \in \mathbb{R}$) we use the square loss, $\ell[f(\mathbf{x}), y) = [f(\mathbf{x}) - y]^2$.



Visualization of square loss gradient/derivative



Enforcing non-negative predictions

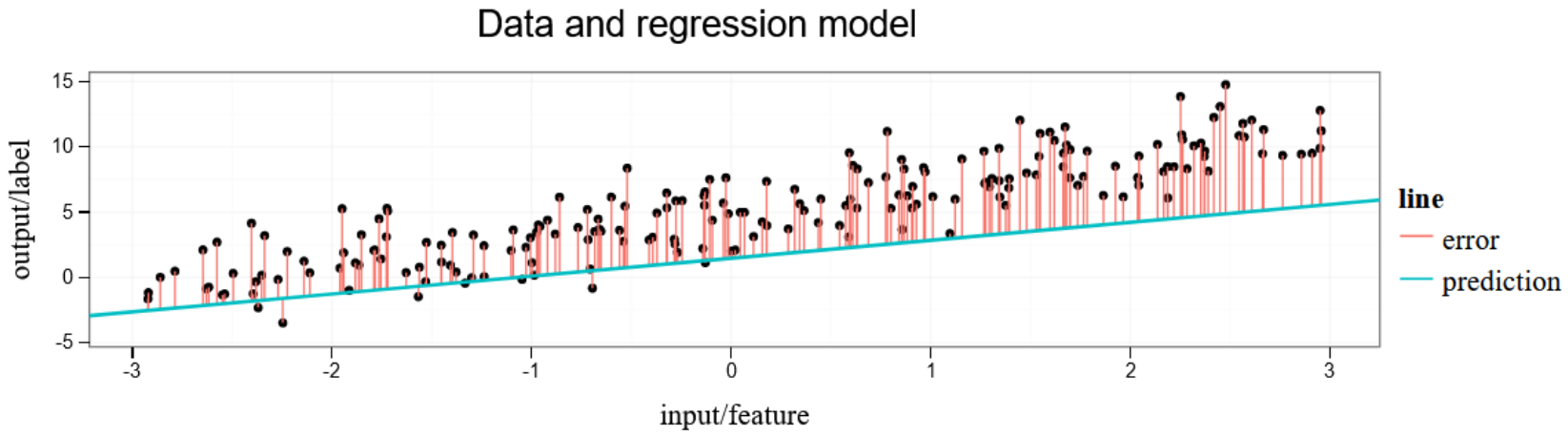
Assume labels $y \geq 0$. How to make sure that the neural network predicts $f(x) \geq 0$?

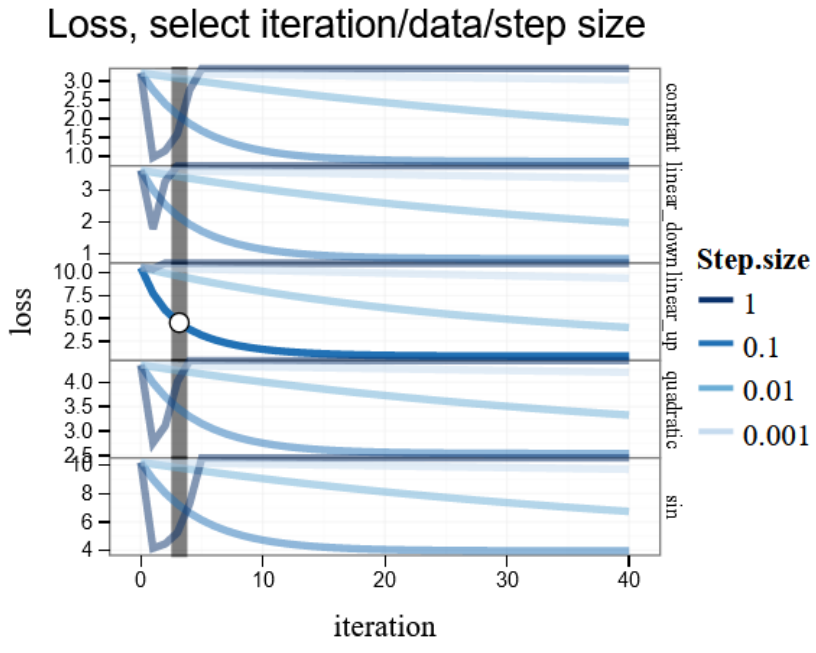
Square loss is defined for all real numbers. Neural network predicts $f(x)$, a real number (maybe negative).

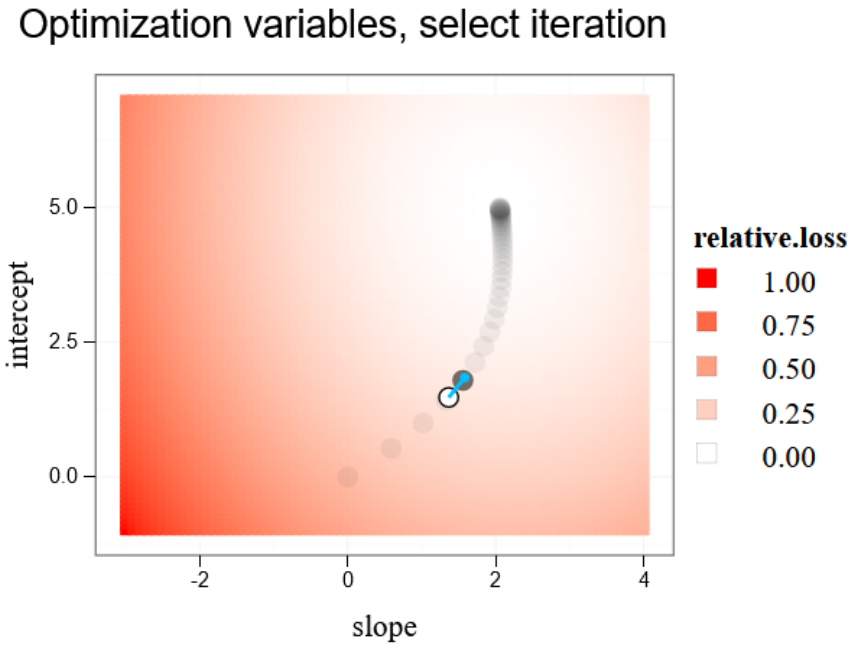
Taking $\exp f(x) > 0$ ensures positive output.

Interactive visualization of gradient descent for regression

http://ml.nau.edu/viz/2022-02-02-gradient-descent-regression/







Possible exam questions

- TODO