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Feedforward Neural Networks as Statistical Models

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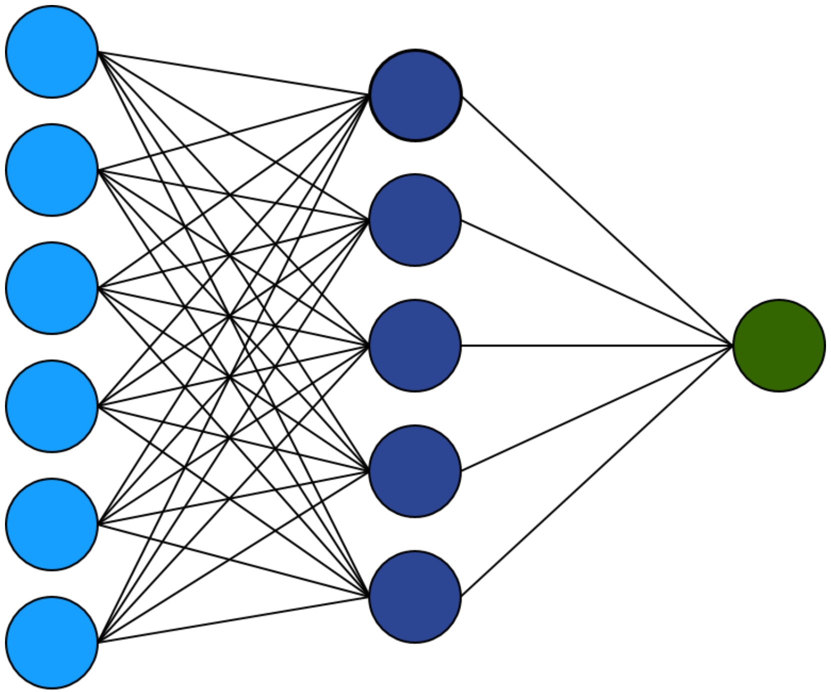
Feedforward Neural Networks



$$\text{NN}(x_i) = \gamma_0 + \sum_{k=1}^{q} \gamma_k \phi \left(\sum_{j=0}^{p} \omega_{jk} x_{ji} \right)$$

Data Application

Boston Housing Data (Kaggle)

506 communities in Boston, MA.

Response:

- `medv` (median value of owner-occupied homes)

12 Explanatory Variables:

- `rm` (average number of rooms per dwelling)
- `lstat` (proportion of population that are disadvantaged)

R Implementation

Many packages available to fit neural networks in R.

Some popular packages are:

- `nnet`
- `neuralnet`
- `keras`

R Implementation: nnet

```r
library(nnet)
nn <- nnet(medv ~ ., data = Boston, size = 8, maxit = 5000,
              linout = TRUE)
summary(nn)
```

```
## a 11-8-1 network with 105 weights
## options were - linear output units
##   b->h1  i1->h1  i2->h1  i3->h1  i4->h1  i5->h1  i6->h1  i7->h1  i8->h1  i9->
##    2.79    5.92    0.34    1.31    0.23   -1.31   -2.67    0.77   -0.22    1.
## i10->h1 i11->h1
##    1.20    1.26
##   b->h2  i1->h2  i2->h2  i3->h2  i4->h2  i5->h2  i6->h2  i7->h2  i8->h2  i9->
##   20.53    5.59    3.52   -0.64   12.64   -5.25   -4.12    0.24    2.64    0.
## i10->h2 i11->h2
##  -21.17    4.03
## [...]
```

Statistical Perspective

$$y_i = \mathrm{NN}(x_i) + \varepsilon_i,$$

where

$$\varepsilon_i \sim N(0, \sigma^2)$$

$$\ell(\theta) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mathrm{NN}(x_i))^2$$

Uncertainty Quantification

Then, as $n \to \infty$

$$\hat{\theta} \sim N[\theta, \Sigma = \mathcal{I}(\theta)^{-1}]$$

Estimate Σ using

$$\hat{\Sigma} = I_o(\hat{\theta})^{-1}$$

However, inverting $I_o(\hat{\theta})$ can be problematic in neural networks.

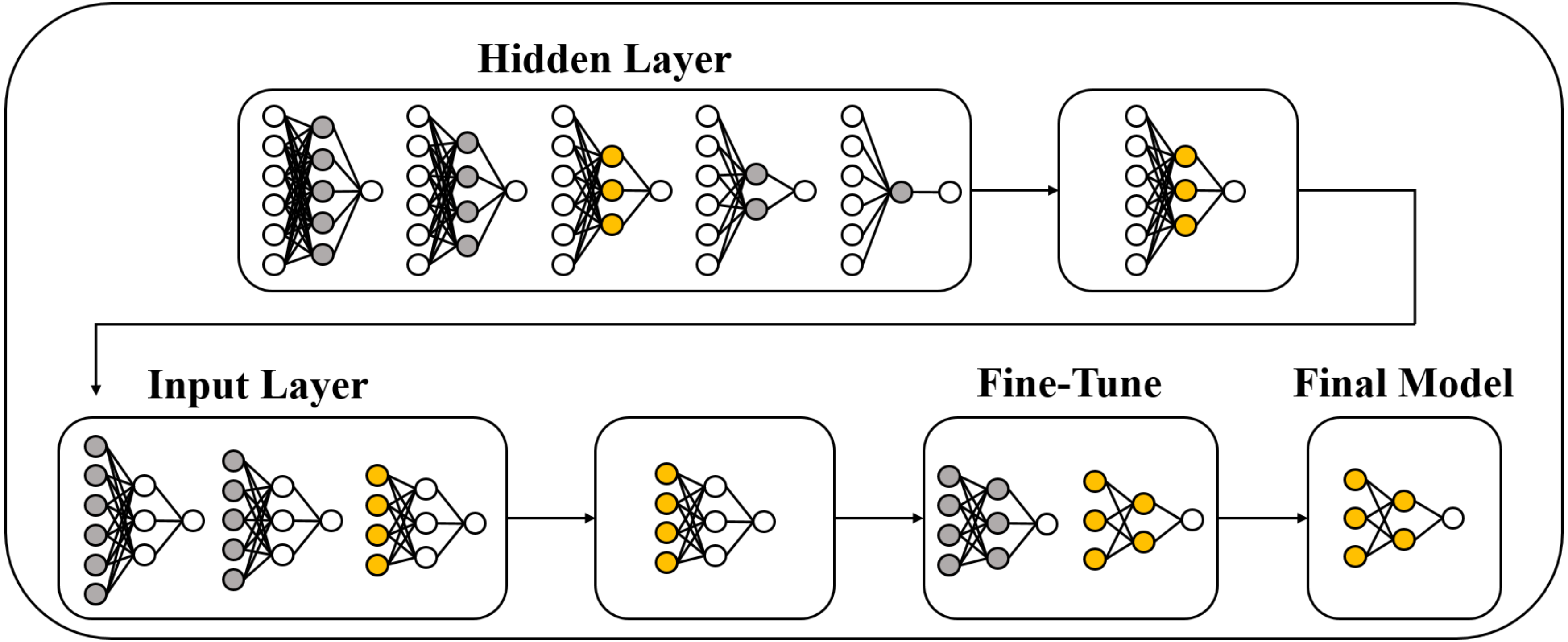
Redundancy

Redundant hidden nodes can lead to issues of unidentifiability for some of the parameters (Fukumizu 1996).

Redundant hidden nodes $\implies$ Singular information matrix.

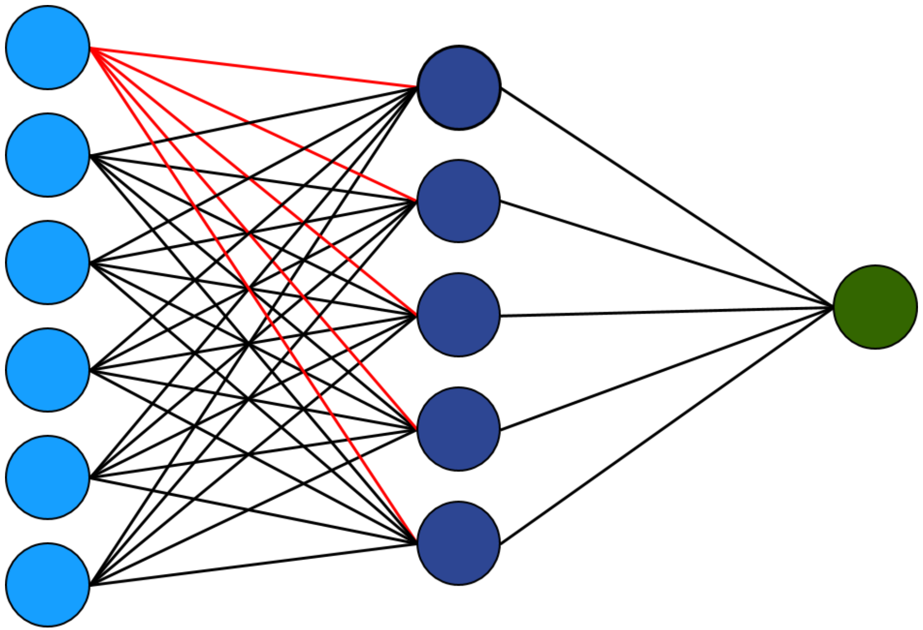
Model selection is required.

Model Selection



A Statistically-Based Approach to Feedforward Neural Network Model Selection (arXiv:2207.04248)

Hypothesis Testing



Wald test:

$$\omega_j = (\omega_{j1}, \omega_{j2}, \ldots, \omega_{jq})^T$$

$$H_0 : \omega_j = 0$$

$$(\hat{\omega}_j - \omega_j)^T \Sigma_{\hat{\omega}_j}^{-1} (\hat{\omega}_j - \omega_j) \sim \chi_q^2$$

Covariate-Effect Plots

$$\overline{\mathrm{NN}}_j(x) = \frac{1}{n}\sum_{i=1}^{n} \mathrm{NN}(x_{i,1}, \ldots, x_{i,j-1}, x, x_{i,j+1}, \ldots)$$

Propose covariate-effect plots of the following form:

$$\hat{\beta}_j(x, d) = \overline{\mathrm{NN}}_j(x + d) - \overline{\mathrm{NN}}_j(x)$$

Usually set $d = \mathrm{SD}(x_j)$

Associated uncertainty via delta method.

R Implementation

```r
# install.packages("devtools")
library(devtools)
install_github("andrew-mcinerney/statnn")
```

Data Application (Revistied)

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Boston Housing: Model Selection

```r
library(statnn)
nn <- selectnn(medv ~ ., data = Boston, Q = 10,
               n_init = 10, maxit = 5000)
summary(nn)
```

```
## Call:
## selectnn.formula(formula = medv ~ ., data = Boston, Q = 10, n_init = 10,
##     maxit = 5000)
##
## Number of input nodes: 8
## Number of hidden nodes: 4
##
## Inputs:
##  Covariate Selected Delta.BIC
##         rm      Yes   236.907
##      lstat      Yes   168.023
## [...]
```

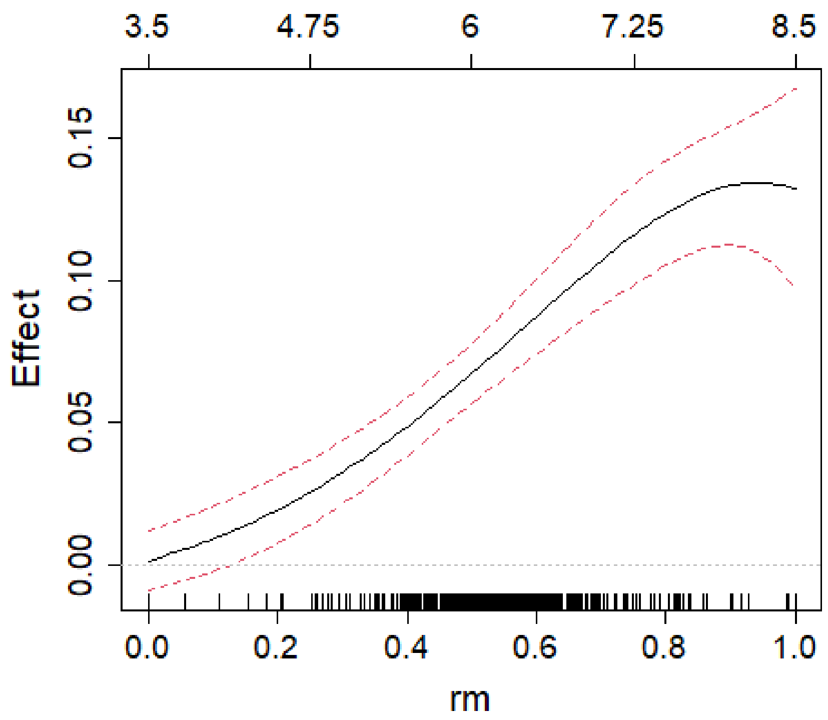
Boston Housing: Model Summary

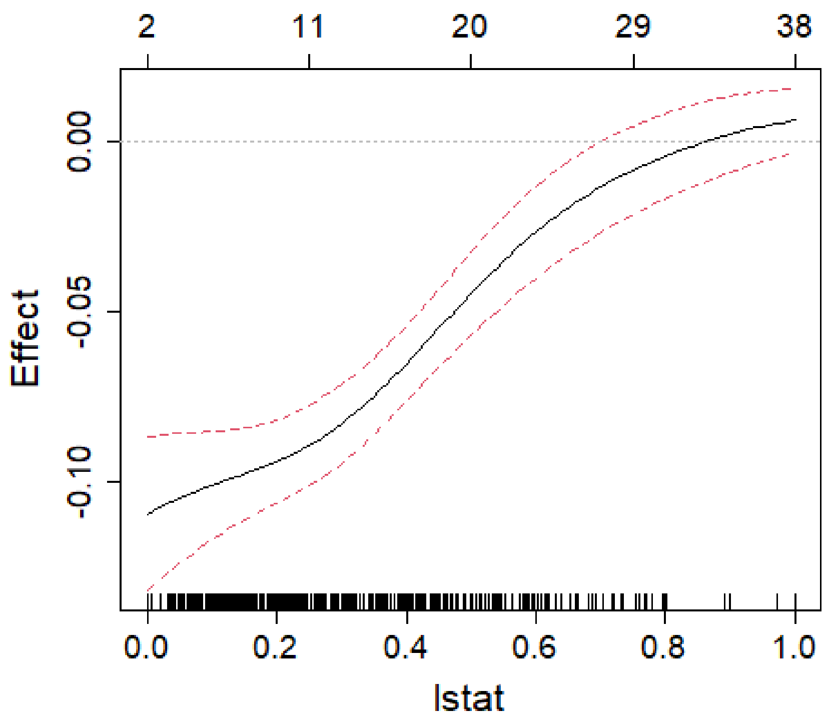
```
stnn <- statnn(nn)
summary(stnn)
```

```
## [...]
## Coefficients:
##                                              Wald
##            Estimate Std. Error |      X^2    Pr(> X^2)
##      crim -0.115769   0.019085 | 109.8369 0.00e+00 ***
##     indus -0.176500   0.018028 |  51.6302 1.65e-10 ***
##       nox -0.163091   0.020639 |  39.4919 5.51e-08 ***
##        rm  0.201211   0.017924 |  45.5051 3.12e-09 ***
##       dis  0.101701   0.022437 |  14.6031 5.60e-03 **
##       rad -0.099667   0.019687 | 107.3354 0.00e+00 ***
##   ptratio -0.192649   0.016672 |   7.8733 9.63e-02 .
##     lstat -0.263402   0.014443 |  50.2500 3.20e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## [...]
```

Boston Housing: Covariate-Effect Plots

```
plot(stnn, conf_int = TRUE, method = "deltamethod", which = c(4, 8))
```





Summary

Feedforward neural networks are non-linear regression models.

Calculation of a likelihood function allows for uncertainty quantification.

Our R package extends existing neural network packages to allow for a more interpretable, statistically-based output.

References

Fukumizu, K. (1996). A regularity condition of the information matrix of a multilayer perceptron network. Neural Networks, 9(5):871–879.

McInerney, A. and Burke, K. (2022). A Statistically-Based Approach to Feedforward Neural Network Model Selection. arXiv preprint arXiv:2207.04248.

R Package

```
devtools::install_github("andrew-mcinerney/statnn")
```

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