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Feedforward neural networks from a statistical-modelling perspective

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IWSM, 19 July 2023

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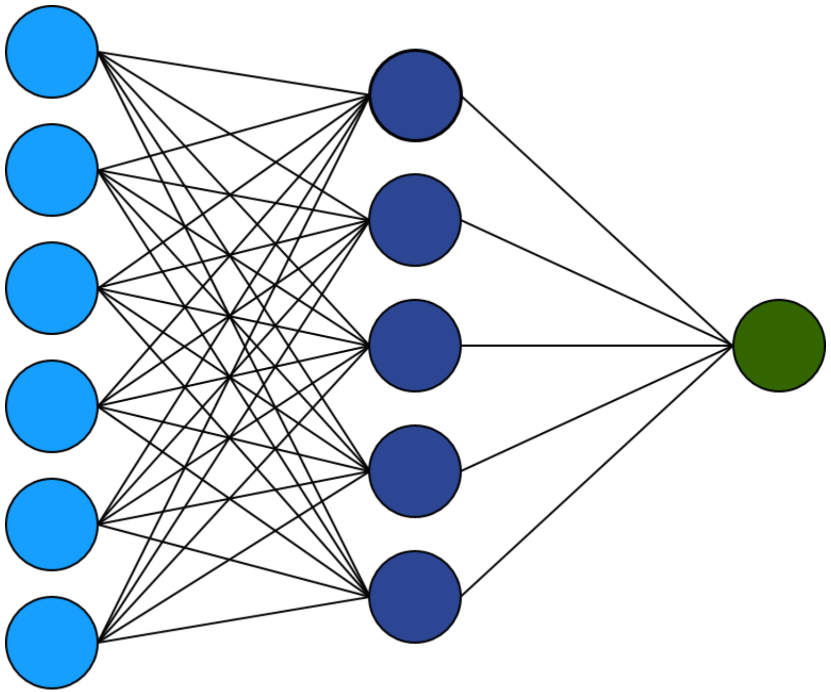
Feedforward Neural Networks



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

Data Application

Insurance Data (Kaggle)

1,338 beneficiaries enrolled in an insurance plan

Response: `charges`

6 Explanatory Variables:

- `age`
- `sex`
- `bmi`
- `children`
- `smoker`
- `region`

R Implementation

Many packages available to fit neural networks in R.

Some popular packages are:

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

R Implementation: nnet

```
library(nnet)
nn <- nnet(charges ~ ., data = insurance, size = 2, maxit = 2000,
           linout = TRUE)
summary(nn)
```

```
## a 8-2-1 network with 21 weights
##  b->h1 i1->h1 i2->h1 i3->h1 i4->h1 i5->h1 i6->h1 i7->h1 i8->h1
##   1.39  -0.43   0.08   0.03  -0.08  -3.16   0.07   0.11   0.15
##  b->h2 i1->h2 i2->h2 i3->h2 i4->h2 i5->h2 i6->h2 i7->h2 i8->h2
##   6.31   0.04   0.13   2.19  -0.11  -6.19   0.15   0.12   0.14
##  b->o h1->o h2->o
##  1.08 -4.82  2.45
## [...]
```

Proposed Solution: interpretnn

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

Statistical Perspective

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

where

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

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

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.

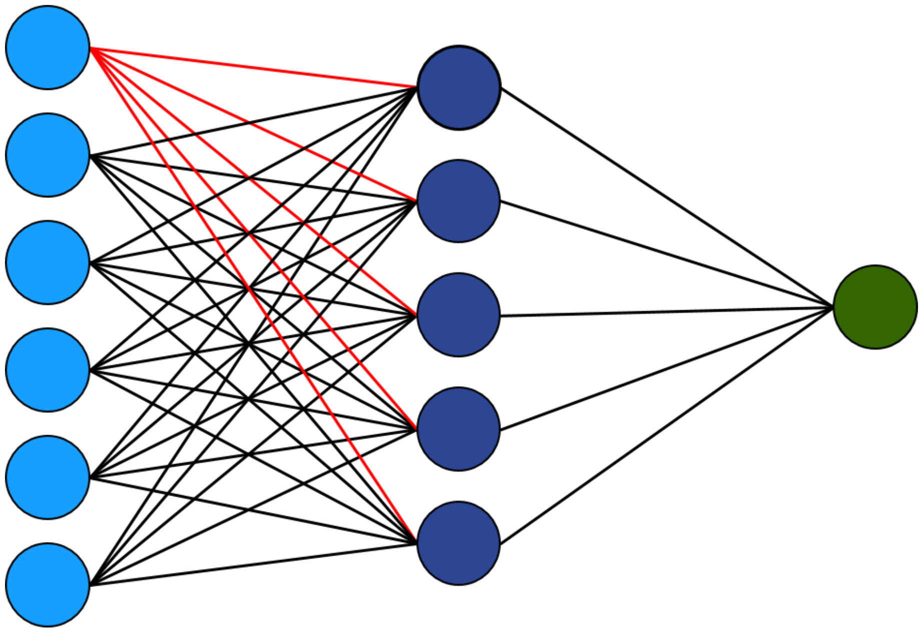
Redundancy

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

Redundant hidden nodes $\implies$ Singular information matrix.

Trade-off between model flexibility and interpretability.

Significance Testing



Wald test:

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

$$H_0 : \omega_j = 0$$

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

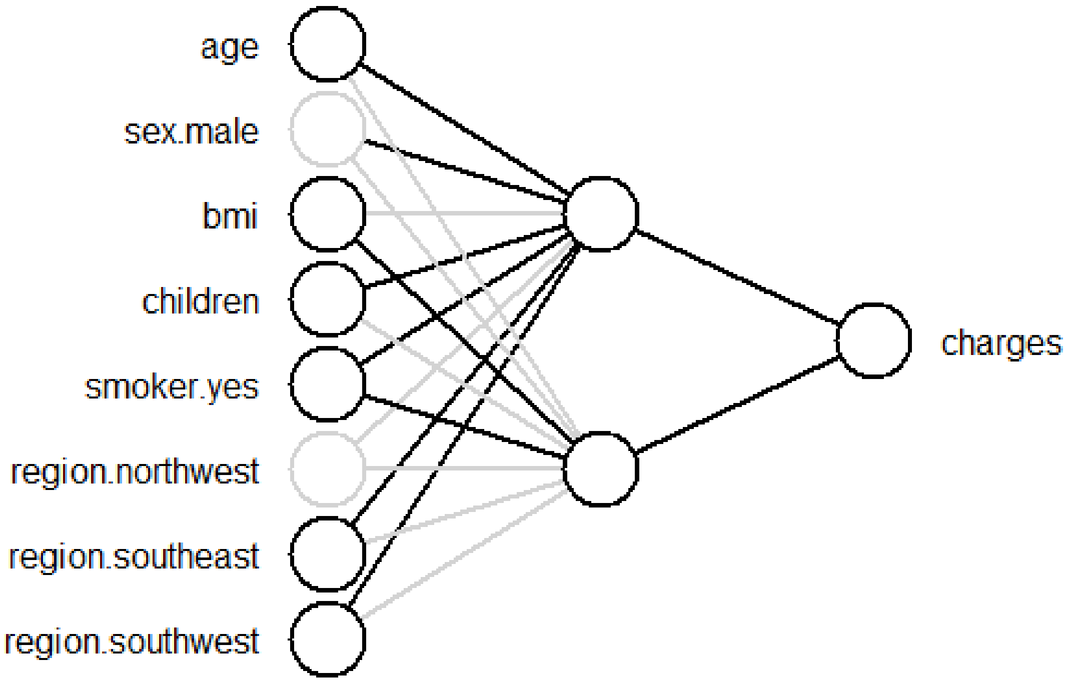
Insurance: Model Summary

```r
intnn <- interpretnn(nn)
summary(intnn)
```

```
## Coefficients:
##                                  Weights |       X^2    Pr(> X^2)
##                 age      (-0.43***, 0.04) |  41.4363 1.01e-09 ***
##            sex.male         (0.08*, 0.13) |   5.5055 6.38e-02 .
##                 bmi       (0.03, 2.19***) | 105.6106 0.00e+00 ***
##            children    (-0.08***, -0.11.) |  19.0146 7.43e-05 ***
##          smoker.yes (-3.16***, -6.19***) | 250.6393 0.00e+00 ***
##    region.northwest         (0.07., 0.15) |   2.8437 2.41e-01
##    region.southeast         (0.11*, 0.12) |   6.2560 4.38e-02 *
##    region.southwest        (0.15**, 0.14) |  10.8218 4.47e-03 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Insurance: Model Summary

```
plotnn(intnn)
```



Covariate-Effect Plots

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

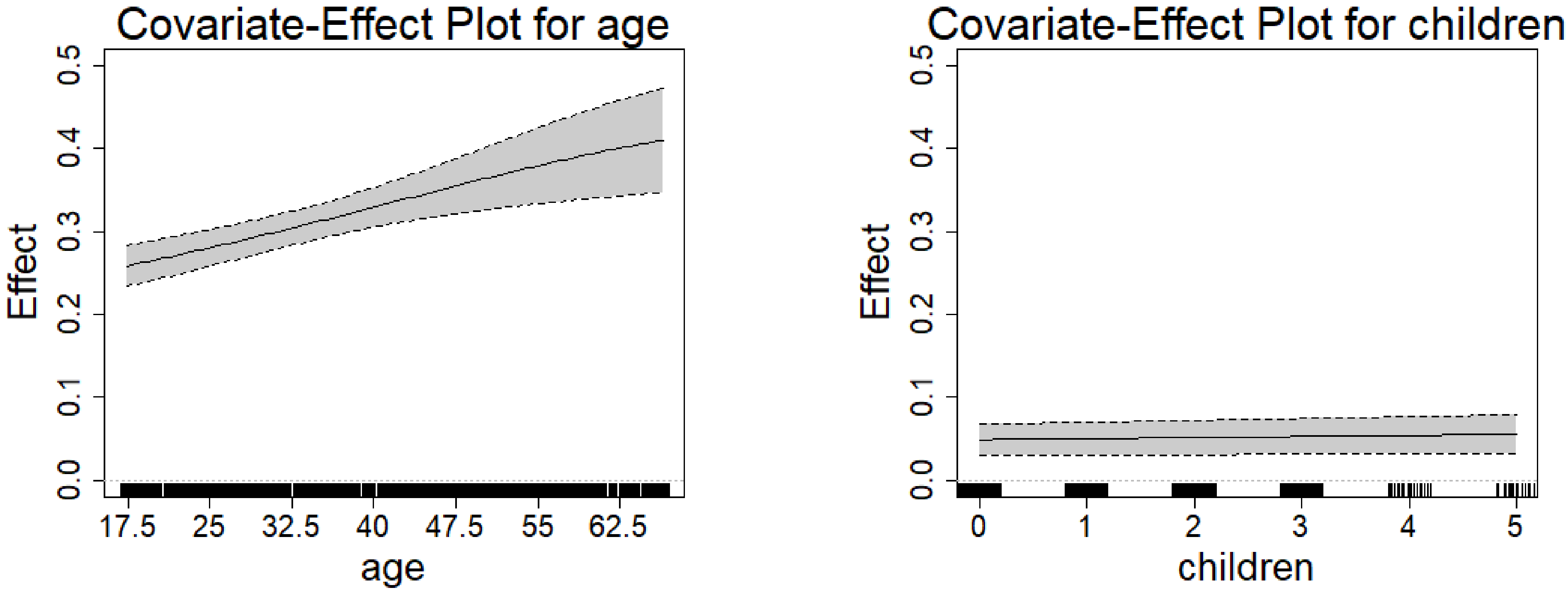
Propose covariate-effect plots of the following form:

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

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

Insurance: Covariate Effects

```
plot(intnn, conf_int = TRUE, which = c(1, 4))
```



References

- McInerney, A., & Burke, K. (2022). A statistically-based approach to feedforward neural network model selection. arXiv preprint arXiv:2207.04248.
- McInerney, A., & Burke, K. (2023). Interpreting feedforward neural networks as statistical models. In Preparation.

R Package

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