A Surprising Connection: Neural Networks and Polynomial Regression

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BARUG
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These slides will be available at
`http://heather.cs.ucdavis.edu/polygrail.pdf`

Neural Networks

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- Series of *layers*, each consisting of *neurons*.
- First layer consists of the predictor variables.
- Each neuron has inputs from the previous layer.
- Each neuron has output: Linear combination of inputs, then fed through a nonlinear *activation function*.
- Final layer output: The prediction, either regression or classification.

Example

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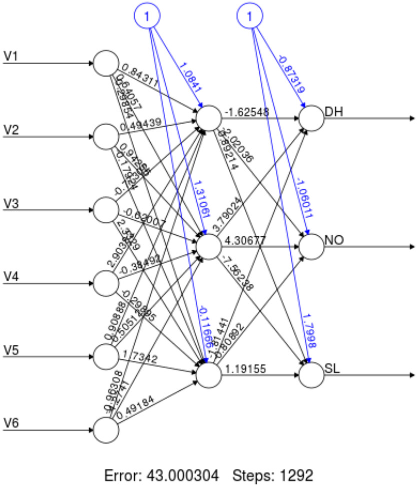
UCI vertebrae data; predict one of 3 classes from 6 predictors.



History of NNs

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- Treated largely as a curiosity through the 1990s.
- Then in the 2000s, "NN+" models won a number of major competitions, a huge boost to their popularity.
- But also many dismiss them as hype.
- Some say NNs work poorly on their data; others counter, "You're not using them right."

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(g) Developed many-featured R pkg., **polyreg**.

Notation and Acronyms

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- n cases; p predictors
- polynomials of degree d
- *PR*: polynomial regression
- *NNAEPR* Neural Networks Are Essentially Polynomial Regression

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- Etc.
- Polynomial regression!
- **Important note:** The degree of the fitted polynomial in NN grows with each layer.

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    - Etc.
- Hence NNAEPR.

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- We consider this an orthogonal issue to NNs. E.g. random forests versions of CNNs have been developed.
- But it is a topic of future research.

Implications of NNAEPR

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- Use our understanding of PR to gain insights into NNs.
- Heed the "advice" of NNAEPR, and use PR instead of NNs!

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- Is it true? Yes!

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layer	% VIFs > 10	mean VIF
1	0.0078125	4.3537
2	0.9921875	46.84217
3	1	5.196113×10^{13}

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  - No convergence problems.

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  - KF: **kerasformula**, R NN pkg.
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- Calculated accuracy (mean abs. prediction error, prop. of correct classification).
- In every single dataset, **PR matched or exceeded the accuracy of NNs**.

Programmer/Engineer Wages

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setting	accuracy
PR, 1	25595.63
PR, 2	24930.71
PR, 3,2	24586.75
PR, 4,2	24570.04
KF, default	27691.56
KF, layers 5,5	26804.68
KF, layers 2,2,2	27394.35
KF, layers 12,12	27744.56

Prog./Eng. Occupation

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setting	accuracy
PR, 1	0.3741
PR, 2	0.3845
KF, default	0.3378
KF, layers 5,5	0.3398
KF, layers 500	0.3401
KF, layers 5,5; dropout 0.1	0.3399
KF, layers 256,128; dropout 0.8	0.3370

Million Song Data, predict year

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setting	accuracy
PR, 1, PCA	7.7700
PR, 2, PCA	7.5758
KF, default	8.4300
KF, layers 5,5	7.9381
KF, layers 2,2	8.1719
DN, layers 2,2	7.8809
DN, layers 3,2	7.9458
DN, layers 3,3	7.8060
DN, layers 2,2,2	8.7796

UCI Forest Cover Data, predict type

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setting	accuracy
PR, 1	0.6908
PR, 2	-
KF, layers 5,5	0.7163

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KF, layers 5,5	0.7163

PR,2: out of memory

UCI Concrete Strength

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method	correlation (pred. vs. actual)
neuralnet	0.608
kerasformula	0.546
PR, 2	**0.869**

MOOCs Data, predict cert.

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setting	accuracy
PR, 1	0.9871
PR, 2	0.9870
KF, layers 5,5	0.9747
KF, layers 2,2	0.9730
KF, layers 8,8; dropout 0.1	0.9712

Cancer/Genetics, predict Alive

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model	brain cancer	kidney cancer
deepnet	0.6587	0.5387
nnet	0.6592	0.7170
PR (1, 1)	0.6525	0.8288
PR (1, 2)	0.6558	0.8265
PR (PCA, 1, 1)	0.6553	0.8271
PR (PCA, 2, 1)	0.5336	0.7589
PR (PCA, 1, 2)	0.6558	0.8270
PR (PCA, 2, 2)	0.5391	0.7840

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Crossfit Data, predict Rx rank

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model	accuracy	range among 5 runs
KF	0.081	0.164
PR, 1	0.070	0.027
PR, 2	0.071	0.069
PR, 3	0.299	7.08
PR, 4	87.253	3994.5

NYC Taxi Data, predict trip time

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setting	accuracy
PR, 1	**580.6935**
PR, 2	591.1805
DN, layers 5,5	592.2224
DN, layers 5,5,5	623.5437
DN, layers 2,2,2	592.0192

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- Default values for number of layers etc. in NN software likely much too large.
- All NN software should monitor multicollinearity. Likely causes the convergence problems.
- See full paper, *https://arxiv.org/abs/1806.06850*.