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Semiparametric neural networks

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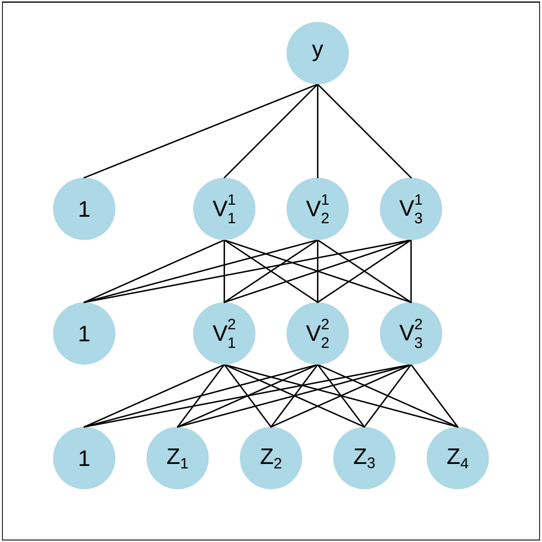
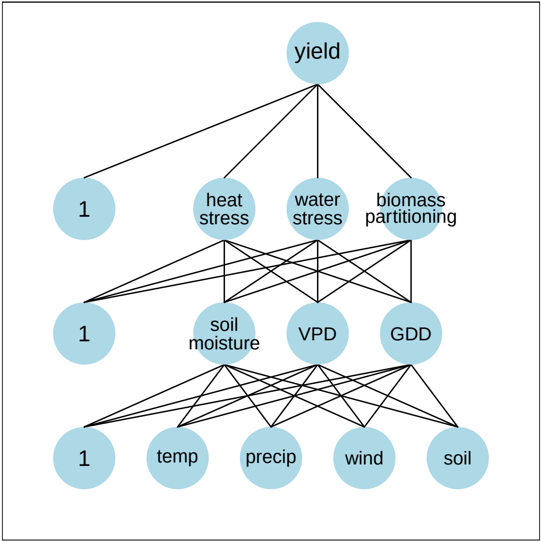
Neural networks



Representation Learning



Neural networks

$$
\begin{aligned}
y &= \gamma^1 + \boldsymbol{V}^1\Gamma^1 + \epsilon \\
\boldsymbol{V}^1 &= a\left(\gamma^2 + \boldsymbol{V}^2\boldsymbol{\Gamma}^2\right) \\
\boldsymbol{V}^2 &= a\left(\gamma^3 + \boldsymbol{V}^3\boldsymbol{\Gamma}^3\right) \\
&\vdots \\
\boldsymbol{V}^L &= a\left(\gamma^L + \boldsymbol{Z}\boldsymbol{\Gamma}^L\right)
\end{aligned}
$$

- y – a (continuous) outcome
- ϵ – additive error
- $\boldsymbol{Z}$ – data
- $\boldsymbol{V}^l$ – “nodes”: derived variables
- $a()$ – the “activation function”. Maps the real line to some subset of it. Modern nets use variants of the ReLU: $a(x) = max(0, x)$
- Dimension of $\boldsymbol{\Gamma}^{1:L}$ controls number of nodes per layer

Semiparametric neural nets

- The top layer of a neural net is an OLS regression in derived variables $\boldsymbol{V}$

$$y = \gamma + \boldsymbol{V}\Gamma + \epsilon$$

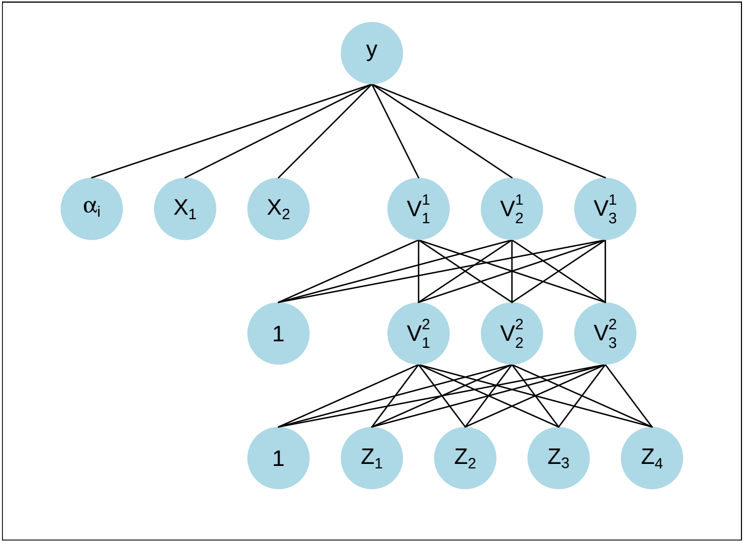
- It is simple to add linear terms to the model, where a linear-in-parameters relationship is known to be appropriate:

$$y = \gamma + \boldsymbol{X}\beta + \boldsymbol{V}\Gamma + \epsilon$$

- Likewise, panel structure can be accounted-for by adding unit-specific intercepts at the top level:

$$y_{it} = \alpha_i + \boldsymbol{X}_{it}\beta + \boldsymbol{V}_{it}\Gamma + \epsilon_{it}$$

Semiparametric and panel neural nets



Why might you want to do this?

- **Statistical efficiency**
- When the goal is to do prediction, but you're working in a topic area in which people have been doing inference and understand the data-generating process somewhat
- When a purely nonparametric model has a hard time representing specific kinds of structure:
  - Longitudinal structure
  - Secular trends
  - Response heterogeneity by specific, known features
- (With caveats) for certain sorts of causal inference tasks
  - 2SLS first stages
  - For predictive models that need a few interpretable marginal effects (maybe)

The method

- It has been implemented in the R package `panelNNET`, and a paper on the method has been published in *Environmental Research Letters*

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Environmental Research Letters

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Machine learning methods for crop yield prediction and climate change impact assessment in agriculture

Andrew Crane-Droesch[1]

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- It achieves state-of the art predictive skill in its domain, outperforming fully-nonparametric neural nets as well as parametric statistical models

Environmental Research Letters

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Machine learning methods for crop yield prediction and climate change impact assessment in agriculture

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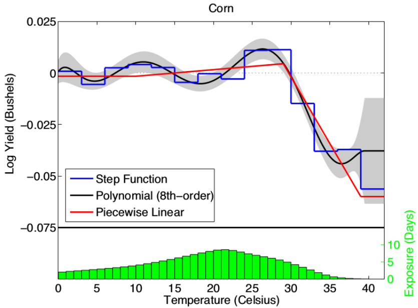
Model	Bagged	$\widehat{\mathrm{MSE}}_{oob}$
Parametric	no	367.9
Semiparametric neural net	no	292.8
Parametric	yes	334.4
Fully-nonparametric neural net	yes	638.6
Semiparametric neural net	yes	251.5

Baseline parametric yield model

$$y_{it} = \alpha_i + \sum_r \mathrm{GDD}_{rit}\beta_r + \boldsymbol{X}_{it}\boldsymbol{\beta} + \epsilon_{it}$$

- Pioneered by Schlenker & Roberts (2009)



→ small shifts in heat have severe impacts on yields

Semiparametric Specification

$$
\begin{aligned}
y_{it} &= \alpha_i + \sum_r \mathrm{GDD}_{rit}\beta_r + \boldsymbol{X}_{it}\boldsymbol{\beta} + \boldsymbol{V}_{it}\boldsymbol{\Gamma} + \epsilon_{it} && \boldsymbol{\Gamma}\text{: } 100 \times 1 \\
\boldsymbol{V}_{it}^1 &= a\left(\gamma^2 + \boldsymbol{V}_{it}^2\boldsymbol{\Gamma}^2\right) && \boldsymbol{\Gamma}^2\text{: } 100 \times 100 \\
&\vdots \\
\boldsymbol{V}_{it}^{10} &= a\left(\gamma^{10} + \boldsymbol{W}_{it}\boldsymbol{\Gamma}^{10}\right) && \boldsymbol{\Gamma}^{10}\text{: many } \times 100 \\
\boldsymbol{W}_{it} &= \left[\boldsymbol{Z}^{fixed}, \mathcal{C}\left(\boldsymbol{Z}^{daily}\right)\right]
\end{aligned}
$$

- *Identical* to parametric model, with addition of 100-node neural network layer
- 10 layers, 50 nodes each. **MANY parameters (>>N!)** Regularization is extremely important.
- $\mathcal{C}()$ represents a 1D **convolutional** layer
  - In this application, convolutional layers constrain the nonlinear interactions of daily weather to adjacent days

Training: backpropagation

Typical loss function for continuous-variable prediction problems is the L2-penalized squared error loss:

$$\underset{\boldsymbol{\theta}}{argmin}\left((y-\hat{y})^2+\lambda\boldsymbol{\theta}^{\boldsymbol{T}}\boldsymbol{\theta}\right)$$

where $\boldsymbol{\theta} \equiv vec(\Gamma^1, \Gamma^2, ..., \Gamma^L)$ and λ is a tunable hyperparameter controlling model complexity

Other hyperparameters include dropout rate, batch size, learning rate, etc.

No closed-form solution! Instead, training is done by (mini-batch) gradient descent

Goal is a parameter set ($\boldsymbol{\theta}$) that predicts yields of years that were withheld from the training sample

The OLS trick

Loss function can be recast as

$$\underset{\boldsymbol{\theta}}{argmin} \, (y - \hat{y})^2 \text{ s.t. } \hat{\boldsymbol{\theta}}^{\boldsymbol{T}} \hat{\boldsymbol{\theta}} \leq c$$

- λ thus implies a "budget" for deviation from zero within of $\hat{\boldsymbol{\theta}}$
- Because gradient descent is inexact, top-level parameters of neural net are not those that minimize loss function

$$\underset{\Psi}{min} \, (\boldsymbol{y} - \boldsymbol{W}\Psi)^T (\boldsymbol{y} - \boldsymbol{W}\Psi) + \tilde{\lambda}\Psi^T\Psi$$

- where
  - $\boldsymbol{W} \equiv [X, V]$
  - Ψ indicates the portion of $\hat{\boldsymbol{\theta}}$ corresponding to the top level of the network
  - $\tilde{\lambda} > \lambda$ is the penalty corresponding to the "budget" that is "left over" after fitting the lower level parameters which generate $\boldsymbol{V}$

The OLS trick

Can calculate the implicit $\tilde{\lambda}$ for the top level of the neural network by minimizing

$$\underset{\tilde{\lambda}}{min}\left(\mathcal{B}^T\mathcal{B} - \Psi^{mT}\Psi^m\right)^2$$

where

$$\mathcal{B} = (\boldsymbol{W}^{\boldsymbol{T}}\boldsymbol{W} + \tilde{\lambda}I)^{-1}\boldsymbol{W}^T\boldsymbol{y}$$

- Replacing Ψ^m with $\mathcal{B}$ ensures that the sum of the squared parameters at the top level of the network remains unchanged
- The (top level of the) penalized loss function reaches its minimum subject to that constraint.
- Alternatively, separate λ's can be specified for each layer, and the OLS trick can pick the optimal value of λ for the top layer as often as desired.

Fixed and random effects

- Heterogeneous intercepts can be implemented in Keras by concatenating a tensor of dummies, and penalizing their weights if random effects are desired
    - Recall that ridge regression on cross-sectional dummies is equivalent to a random effects model (Harville 1977, 1978)
    - Keras/Tensorflow can handle estimation of thousands of dummy effects without issue on a standard laptop
- For the fixed-effects model (i.e.: where α_i is unpenalized), the closed form solution is faster and more precise:

$$\hat{\alpha} = (y_{it} - \bar{y}_i) - \left(\boldsymbol{X}_{it} - \bar{\boldsymbol{X}}_i\right)\hat{\beta} - \left(\boldsymbol{V}_{it} - \bar{\boldsymbol{V}}_i\right)\hat{\Gamma}$$

    - Like the OLS trick, these can be computed every few iterations and inserted into the model, short-circuiting gradient descent, and speeding convergence.

Implementation in Keras/Tensorflow/R

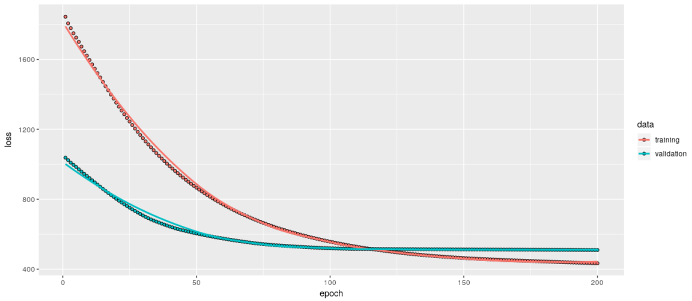
- Keras is a high-level API for various deep learning libraries
- Tensorflow is Google's deep learning library. Keras calls it "under the hood," and can run with others (Torch, Theano, CTNK, etc).
- RStudio has recently implemented a wrapper for Keras. It seems to just call Python from R.
- Most of the user community works in Python – more resources and support in that ecosystem

See `https://github.com/cranedroesch/SNN_python/blob/master/SNN_python.ipynb` for a fixed-effects implementation in python

Fitting a basic neural net in Keras through R

```r
library(keras)
library(dplyr)
X <- mtcars[,-1] %>% as.matrix
y <- mtcars[,1] %>% as.matrix
inp <- layer_input(shape = ncol(X))
# note mutability! not common in R
layers <- inp %>%
  layer_dense(units = 3, activation = "relu") %>%
  layer_dense(units = 1, activation = "linear")
model <- keras_model(inputs = inp, outputs = layers)
model %>% compile(
  loss = 'mean_squared_error',
  optimizer = optimizer_nadam()
)
```


```
history <- fit(model,
               x = X,
               y = y,
               verbose = 1,
               epochs = 200,
               validation_split = .2
)
plot(history)
```



Representing parametric structure in Keras

Say I wanted to include a parametric term in weight and cylinders, and let the rest get squashed into a single term

```
> head(mtcars)
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

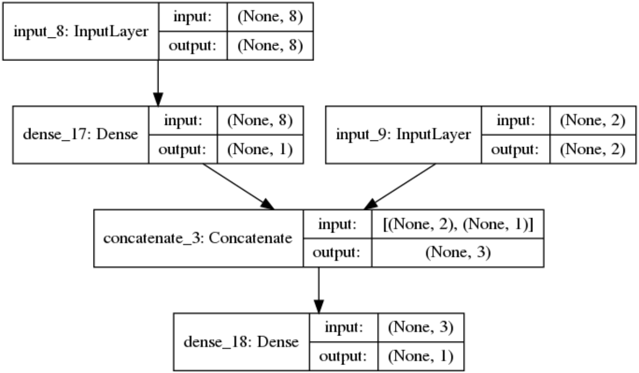
Representing parametric structure in Keras

```
"%ni%" <- Negate("%in%")
Xp <- mtcars[,c("wt", "cyl")] %>% as.matrix
Xnp <- mtcars[,colnames(mtcars) %ni% c("mpg", "cyl", "wt")] %>%
  as.matrix
npinp <- layer_input(shape = ncol(Xnp))
pinp <- layer_input(shape = ncol(Xp))
nplayers <- npinp %>%
  layer_dense(units = 3, activation = "relu")
merged <- layer_concatenate(list(pinp, nplayers)) %>%
  layer_dense(units = 1, activation = "linear")

model <- keras_model(inputs = c(pinp, npinp), outputs = merged)
model %>% compile(
  loss = ’mean_squared_error’,
  optimizer = optimizer_nadam()
)
```

Representing parametric structure in Keras

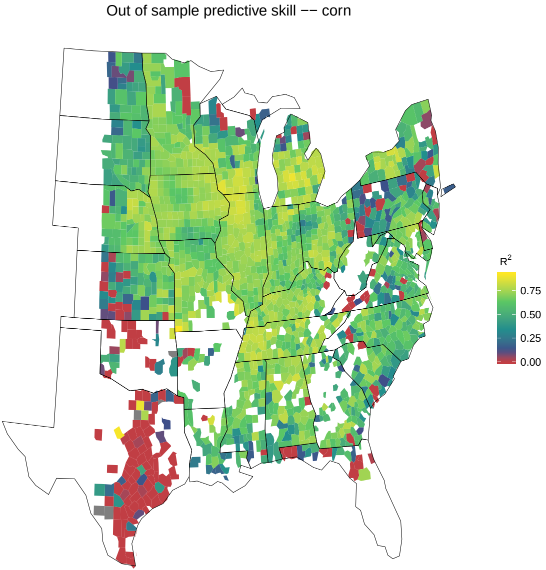
```r
library(kerasR)
plot_model(model, to_file = "model.png", show_shapes = T,
           show_layer_names = TRUE)
```



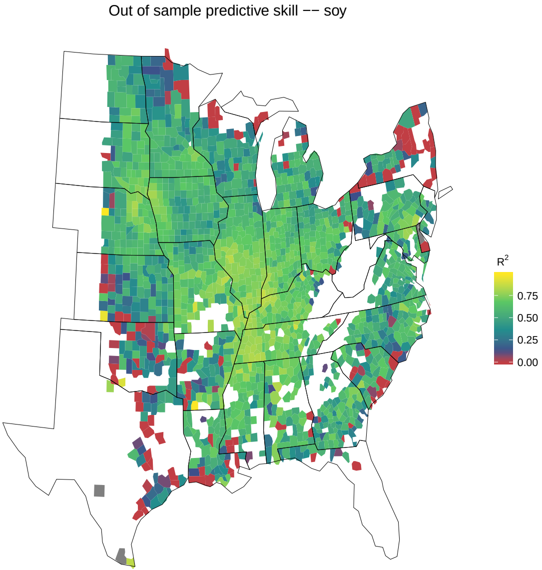
Application: dryland yield prediction

- Maize and soy yield data from the US east of 100W Longitude
- Historical weather data from METDATA (Abatzoglou 2013)
  - Daily observations of min/max temperature, min/max relative humidity, precipitation, wind speed, insolation
  - 4km resolution
  - Aggregated to counties and weighted by agricultural area
- Model is a semiparametric neural net with the following parametric terms
  - random (not fixed) effects
  - GDD variables
  - penalized cubic spline in total annual rainfall, time, and insolation
- Fit in Keras/R, developed to study SRM geoengineering

Model fit – Corn

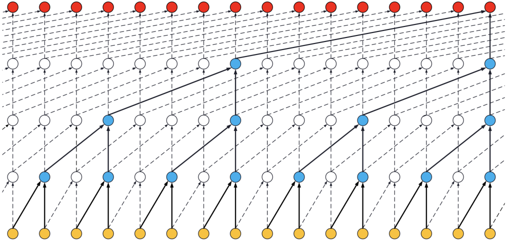


Model fit – Soy



Future work

- Moving beyond feed-forward neural nets: adding parametric time-series structure to Temporal Convolutional Networks



  - Initializing the parametric component using `GETS/IIS`
  - Applying it to spatio-temporal forecasting problems (adaptation?)
- Explicitly modeling response heterogeneity through interactive, multi-headed architectures

Big picture

- Keras and Tensorflow are powerful and well-made
- Neural nets are general: workhorse econometric models are nested within them (with more or less hacking)
- They're a complement to the work that empirical economists have always done

Resources

- See here for a Python/Keras implementation of a SNN: `github.com/cranedroesch/SNN_python/blob/master/SNN_python.ipynb`
- Code for replicating the ERL paper: `github.com/cranedroesch/ML_yield_ERL`
- panelNNET source: `github.com/cranedroesch/panelNNET`