Lifting the Curtain on Machine Learning

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SatRday
UCLA, April 6, 2019

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

Outline of Talk

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- Both are "machine learning (ML) alternatives."
- Taking a critical look at certain aspects of ML:
  - neural networks (NNs)
  - t-sne (a "nonlinear PCA")

Sources of Confusion

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  AI = machine learning = neural networks
- Not true, of course, but the NN people have a knack for getting into the press. :-)
- The very term *machine learning* already sounds science fiction-ish, and *neural networks* really does.

Sources of Confusion (cont'd)

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The NN/ML people tend to invent their own terminology. E.g

statistics-ese	ML-ese
observations	cases
predictors	features
covariates	side information
β_0/intercept	bias
prediction	inference
inference	statistics

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- Show what NNs are actually doing.
- Suggest a more straightforward alternative to NNs, that performs as well or better than NNs yet it is simpler and easier to use.
- Present a "spinoff" visualization package that serves as an alternative to a popular ML one.

Neural Networks

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- Outputs of each layer run through an *activation function*, e.g. logistic, to allow for nonlinearity.

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- Predict one of 3 classes, DH, NO, SL. (E.g. NO = normal.)
- Many R packages, e.g. **kerasformula**, **MXNet**.

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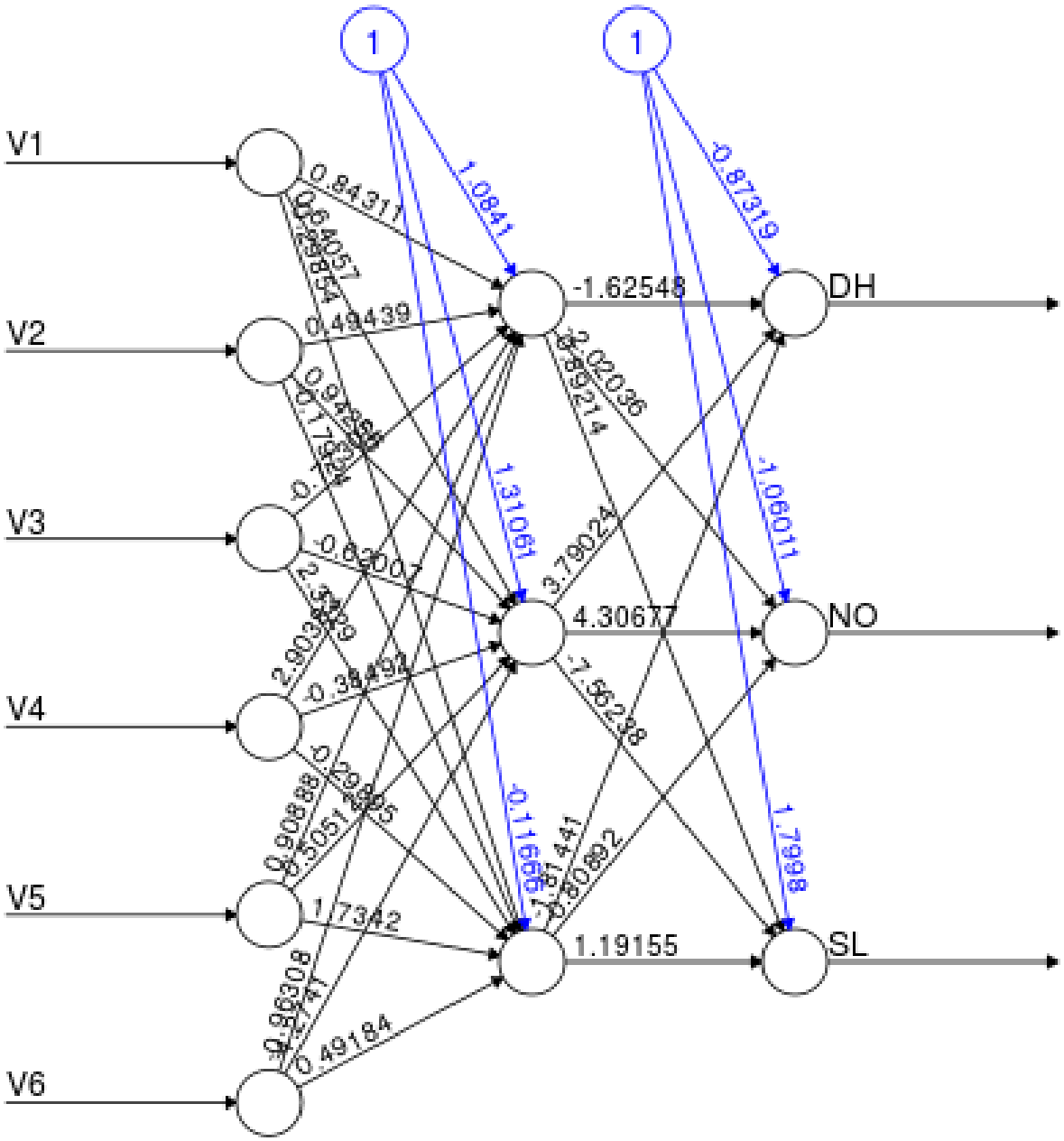
UCI Vert. (cont'd.)



Closeup: 2nd Neuron in 2nd Layer

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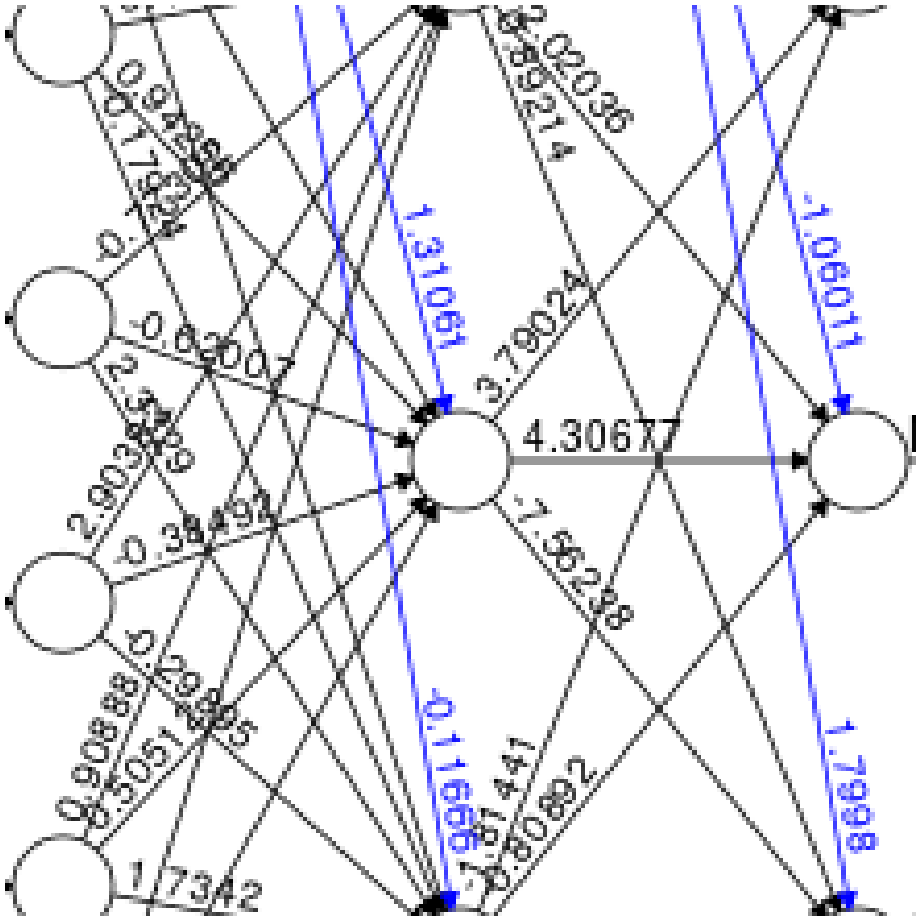

Input to this neuron: $\ldots + 0.94V2 - 0.62V3 - 0.38V4 + \ldots$

This neuron then feeds that lin. comb. into logistic, which is then input to all neurons in next layer, with weights 3.79, 4.31 and 7.56.

History of NNs

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- Treated largely as a curiosity through the 1990s.
- Then in the 2000s, "NN+" models, e.g. CNN, 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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- NN=PR suggests that one might simply fit a polynomial model in the first place, bypassing NNs.
- Thus avoid NN's problems, e.g. choosing numerous hyperparameters, nonconvergence and so on.
- Tried many datasets. In all cases, **PR meets or beats NNs in predictive accuracy**.
- Developed many-featured R pkg., **polyreg**.

Notation and Acronyms

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

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- Has dimension reduction options.
- *github.com/matloff/polyreg*

Key polyreg functions

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```
polyFit(function (xy, deg, maxInteractDeg = deg,
    use = "lm", pcaMethod = NULL, pcaLocation =
    "front", pcaPortion = 0.9, glmMethod = "one",
    return_xy = FALSE, returnPoly = FALSE)

predict.polyFit(object, newdata, ...)
```

E.g. if choose dimension reduction by PCA in **polyFit()**, **predict()** will automatically take care of it.

Various other dim. reduction, helper functions.

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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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- Even without Taylor series etc.] any reasonable activation function is "close" to a polynomial.
- Hence NN=PR.

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- **Warning:** Beware of "p-hacking" effects. Don't take timings rankings overly seriously.

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

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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	0.69
PR, 3	**0.80**
KF, layers 5,5	0.72
reader report, NN	0.75

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

Note: Sorely needs data cleaning.

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- So in principle PR should perform as well.
- But so far we have not had a chance to do much with "C."
- Have just done non="C", using PCA for dimension reduction.
- Respectable, e.g. 98.7% on MNIST, but need to do serious use of "C."

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- *github.com/matloff/prVis*

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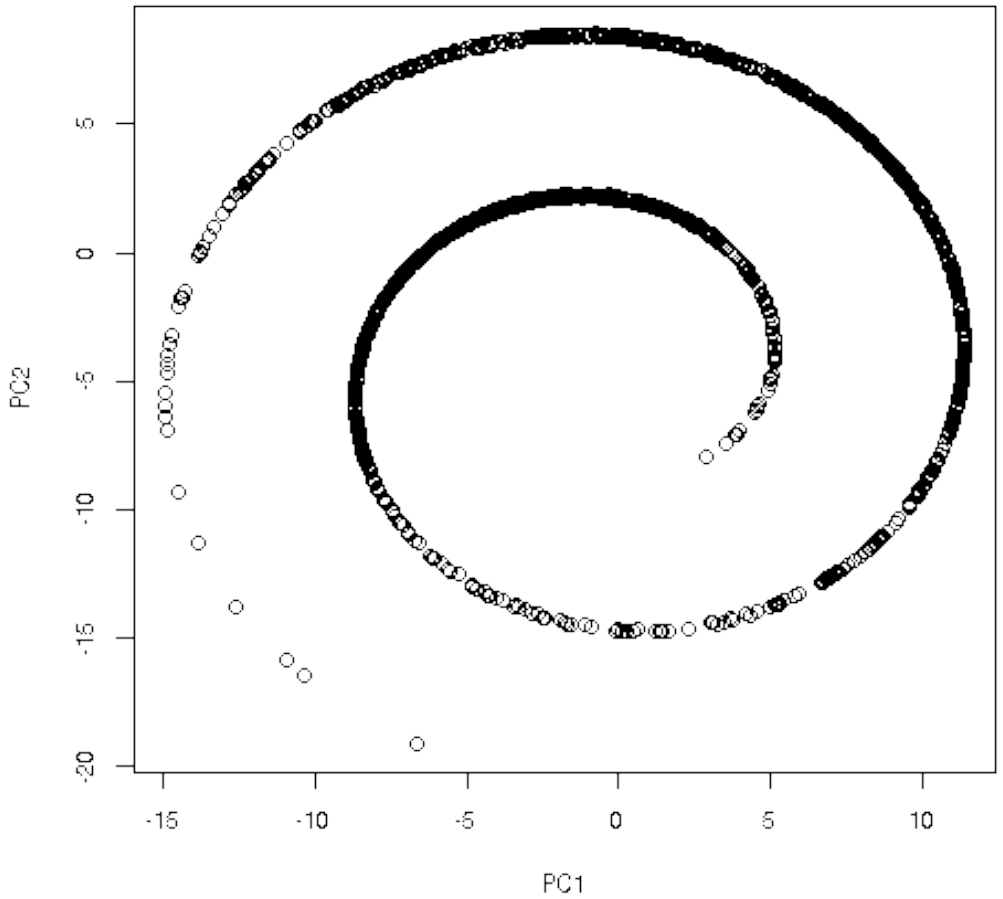
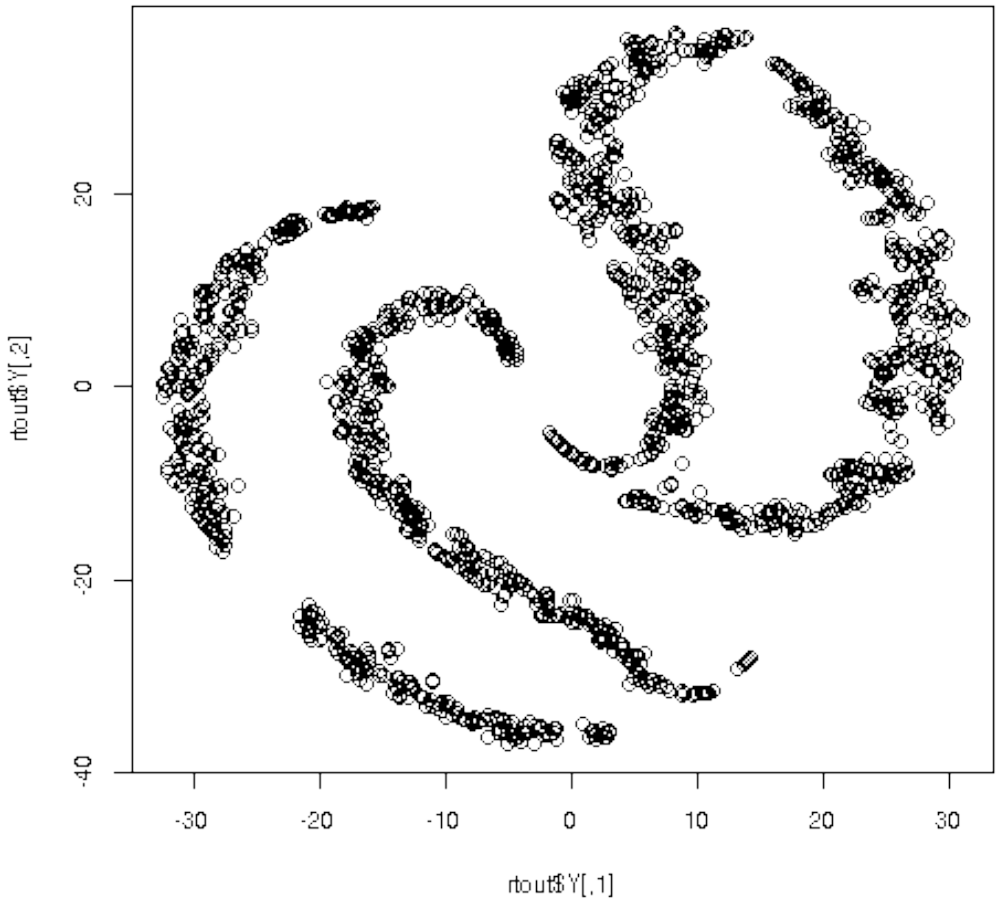
- Designed to be a mixture of 4 components.
- **The Test**: Will any of these visualization tools detect that?
- Let's temporarily pretend we don't know there are 4.

PCA



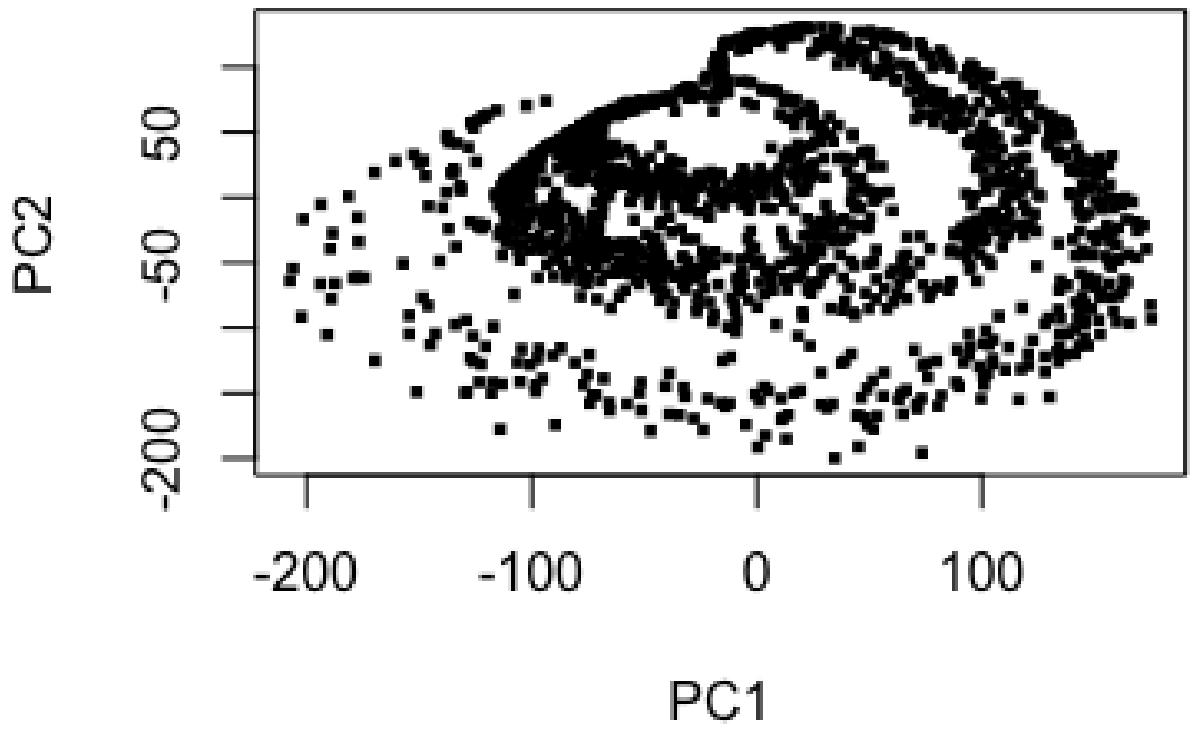
No clue at all that there are 4 components.

t-sne



3 components? 4? 5? Even 1? Not clear.

prVis



Fairly clear there are 4 components.

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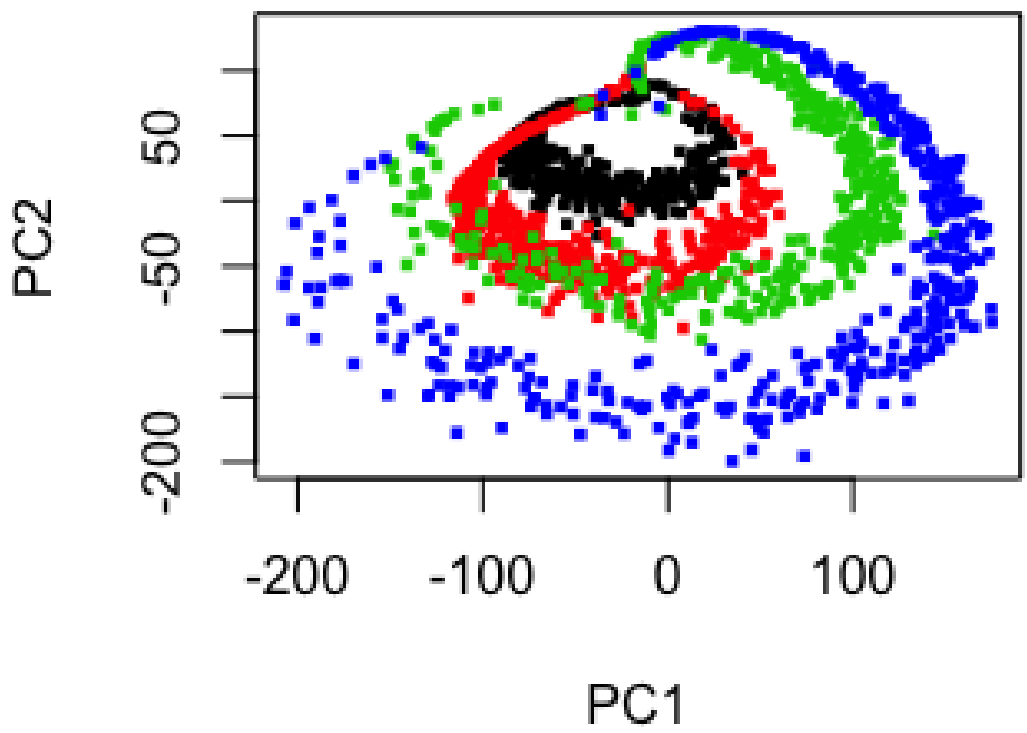

Yep!

The Team!

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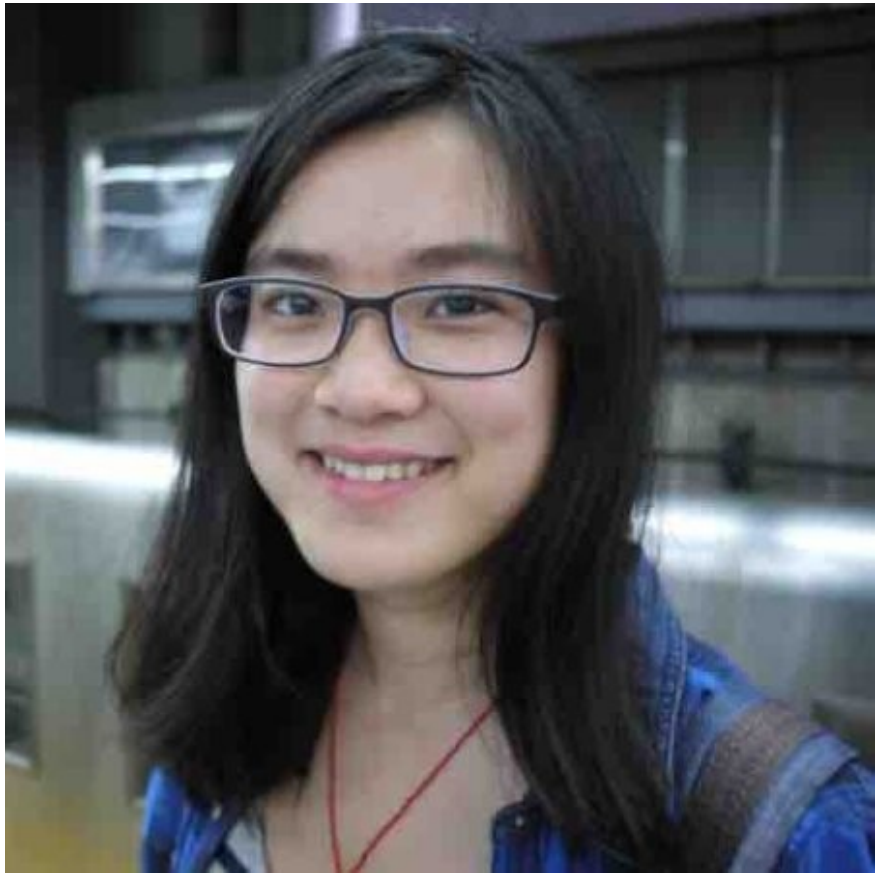
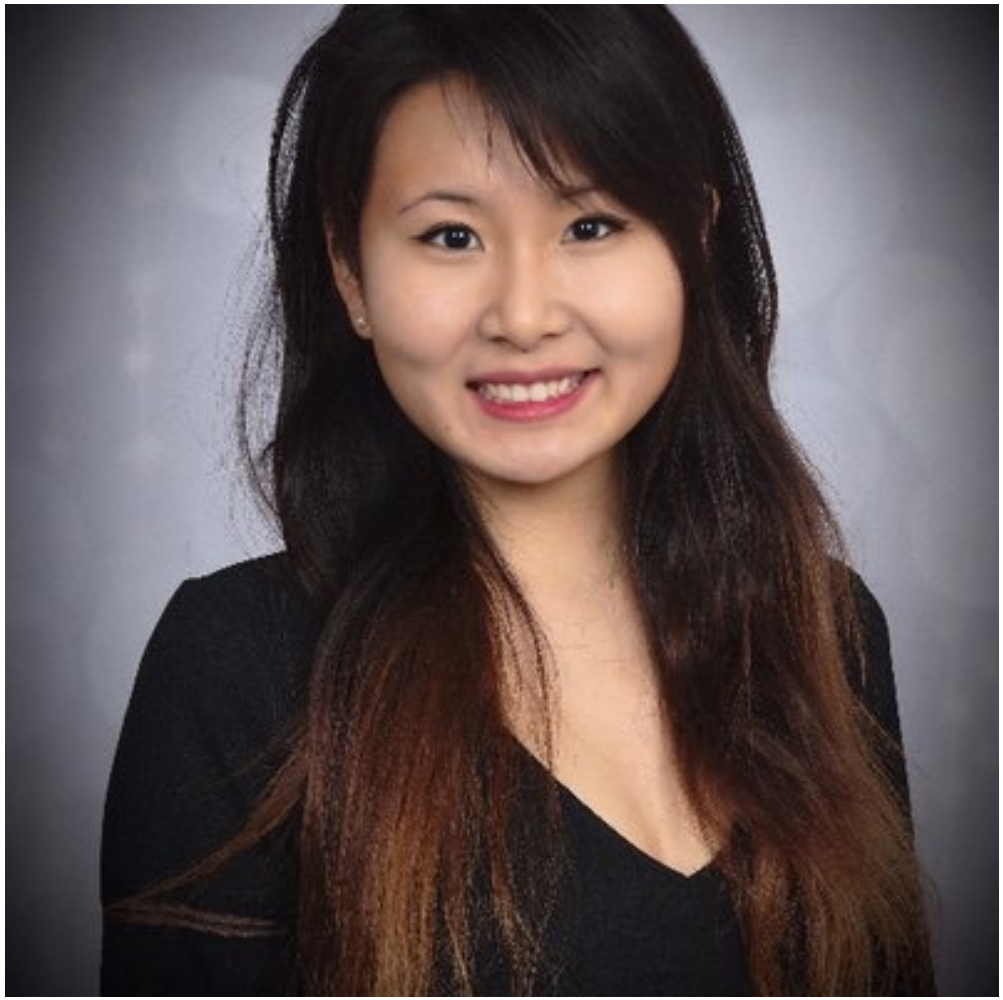


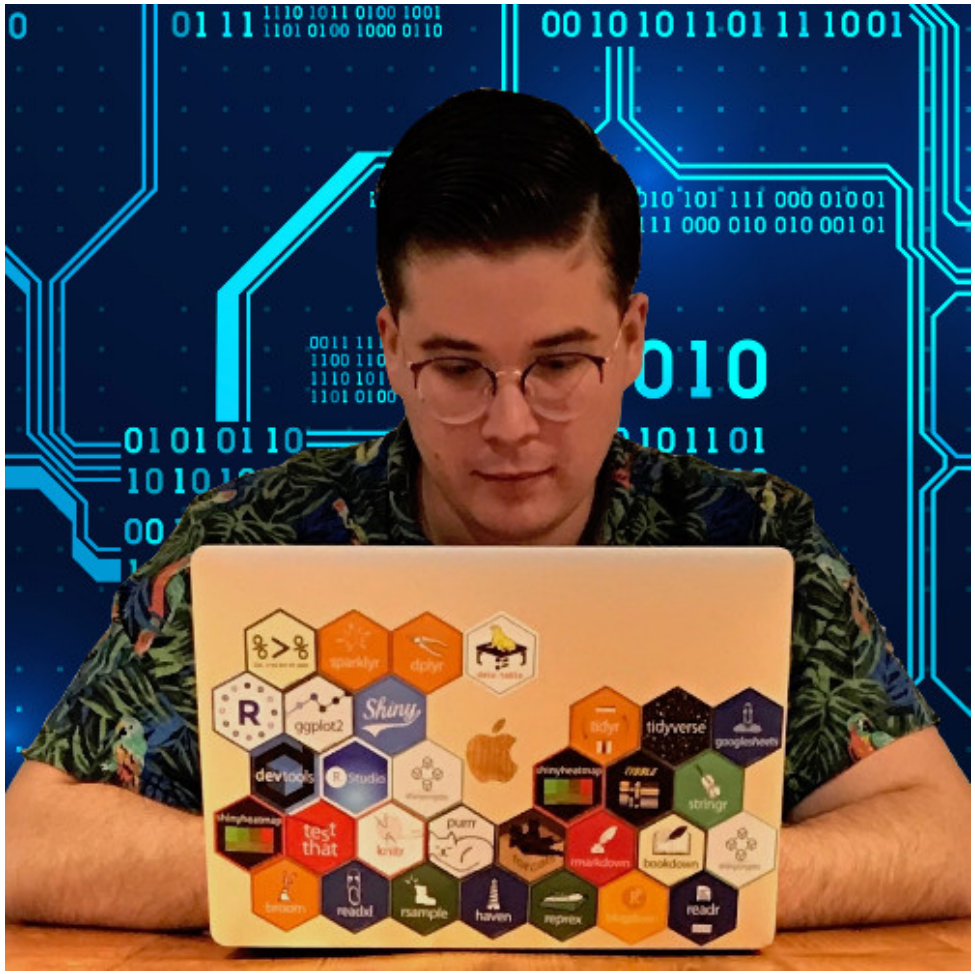
Xi Cheng

The Team! (contd.)



Tiffany Jiang

The Team! (contd.)



Bohdan Khomtchouk

The Team! (contd.)

Matt Kotila

The Team! (contd.)

Pete Mohanty

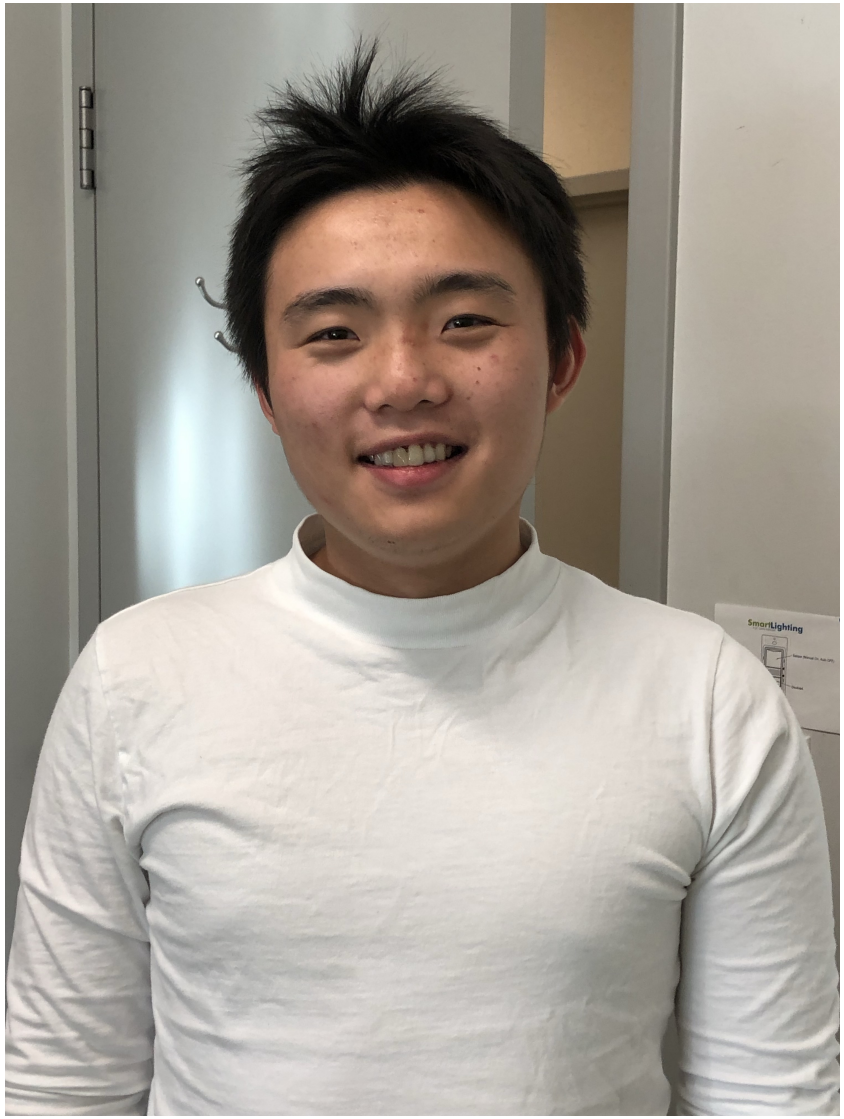
The Team! (contd.)

Robert Tucker

The Team! (contd.)

Robin Yancey

The Team! (contd.)



Allan Zhao

Thanks

Thanks

Thanks to all!

Appendix

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Backup slides:

Multicollinearity in NNs

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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}