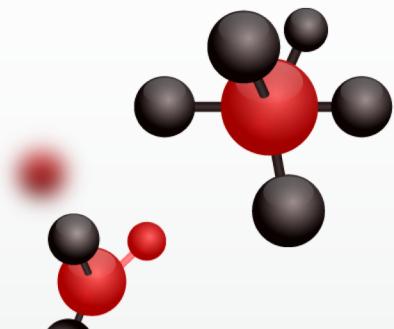


Predicting Toxicity With Deep Learning

By Sean Davern



30% of Drugs Fail Clinical Trials due to Toxicity

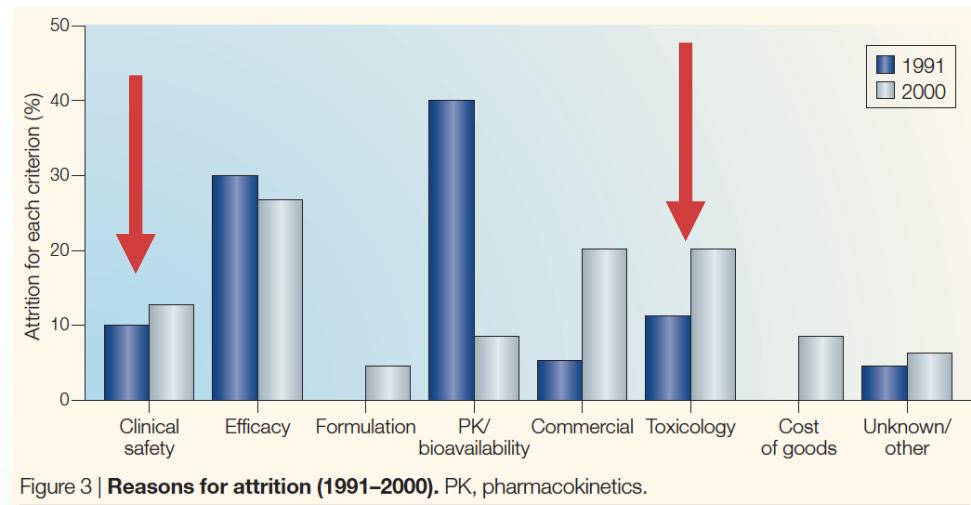
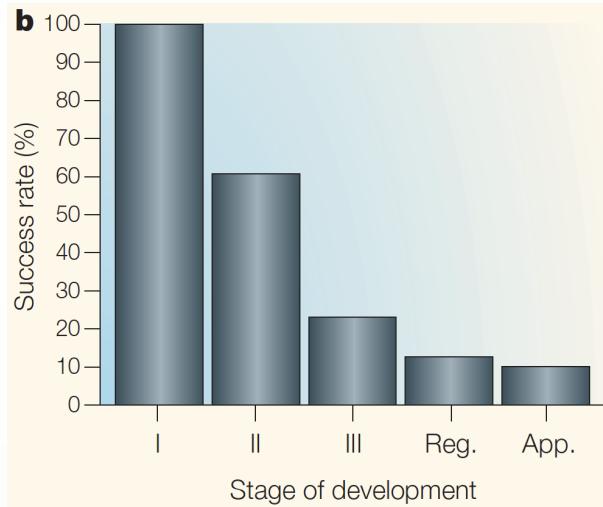


Figure 3 | Reasons for attrition (1991–2000). PK, pharmacokinetics.



Data

Obtain Data > Scrub > Explore > Model > Use



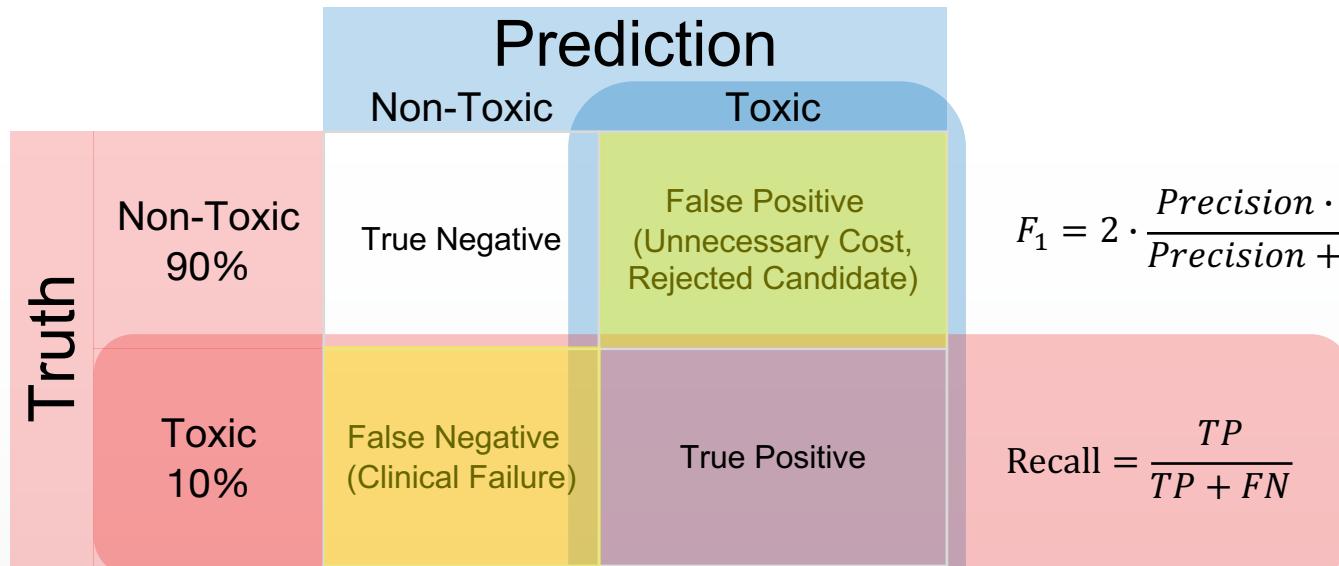
[» Home](#) [About](#) [Registration](#) [Data/Resources](#) [Submissions](#) [Leaderboard](#) [Contact Us](#) [Survey](#)

Tox21 Data Challenge 2014

The image shows a laboratory setting with a yellow robotic arm positioned over a workbench. In the foreground, there is a white rectangular panel with the "Tox21" logo, which consists of a stylized triangle above the word "Tox21".

- 12,700 Compounds
- 800 Physiochemical and 844 Structural Features
- 12 Toxicity measures

Business Should Drive Metrics



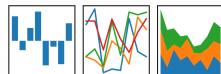
$$Precision = \frac{TP}{TP + FP}$$

Modeling



Data Handling, Pre-Processing

pandas
 $y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$



NumPy

SciPy

imblearn

Neural Network Design & Training



Hyperparameter Tuning
(Bayesian Optimization)

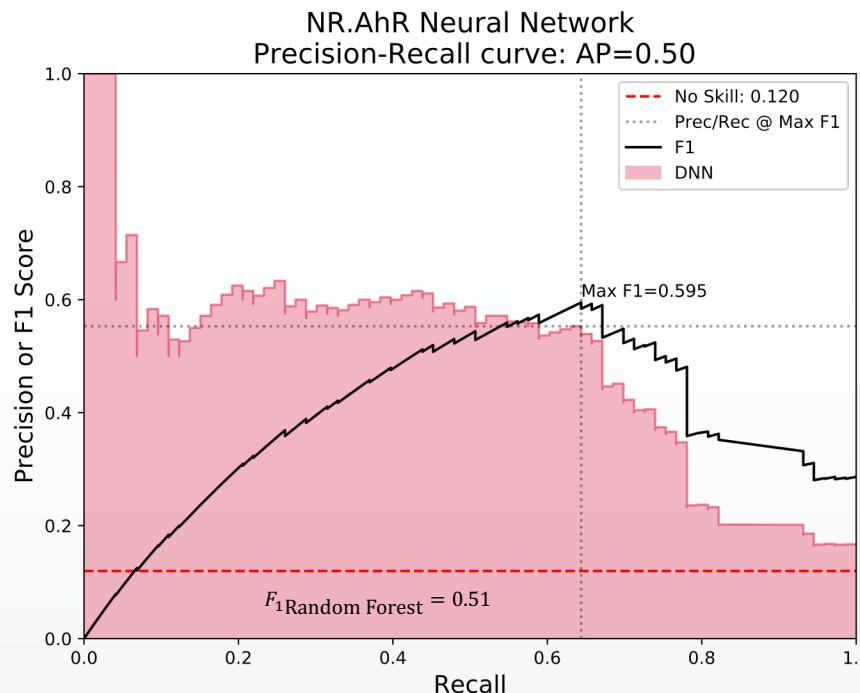


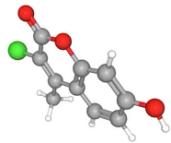
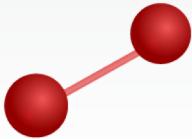
Metrics, Visualization



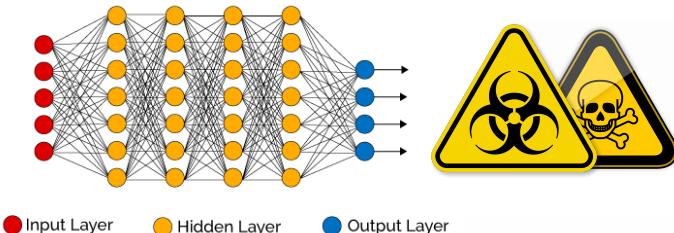
Using Results

Obtain Data > Scrub > Explore > Model > Use





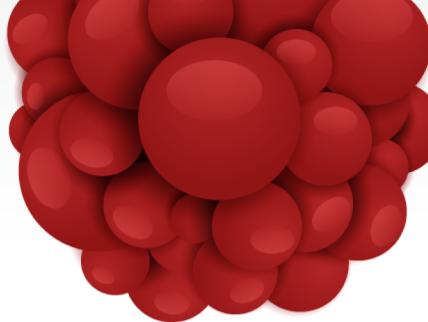
Dense Neural Networks



● Input Layer

● Hidden Layer

● Output Layer



THANKS



Please contact me with any questions?

Sean Davern
sean@lizandsean.com
(206) 919-2026



@seandavern