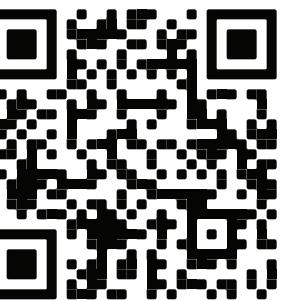


DeepROCK: Error-controlled interaction detection in deep neural networks



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Paper

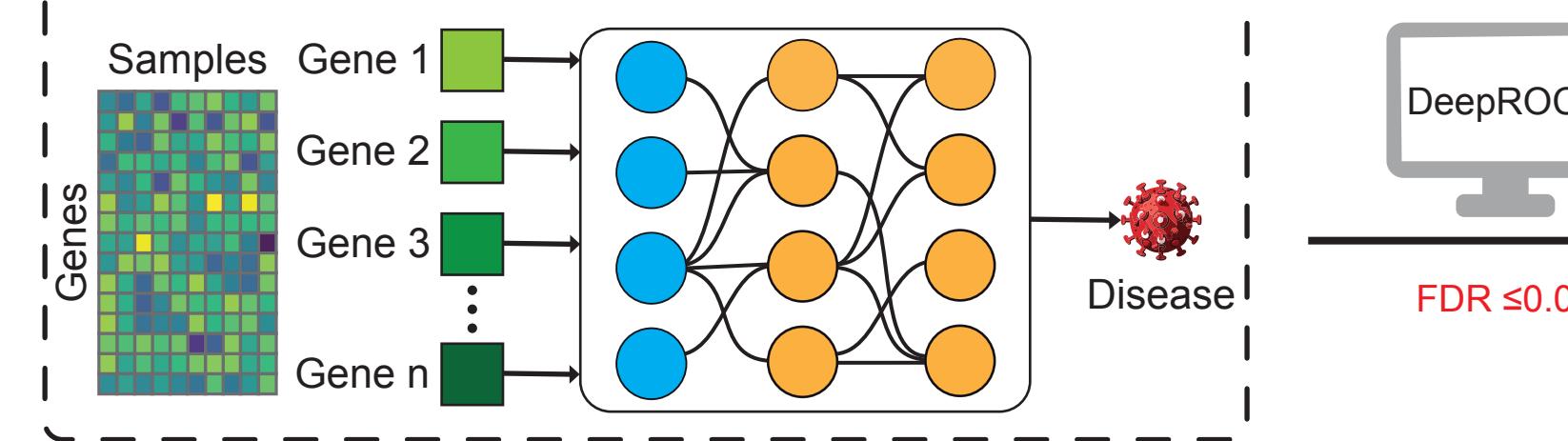
Code

Motivation

Detecting interactions with false discovery rate (FDR) control is crucial for scientific discovery

What is FDR?

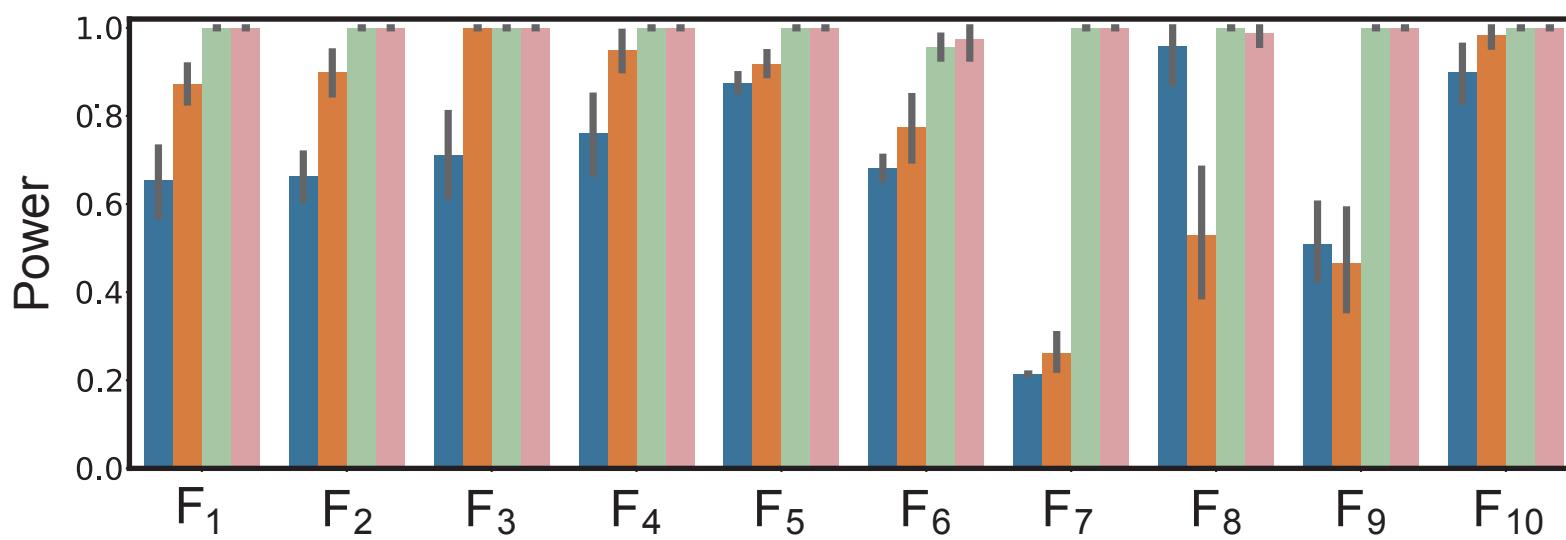
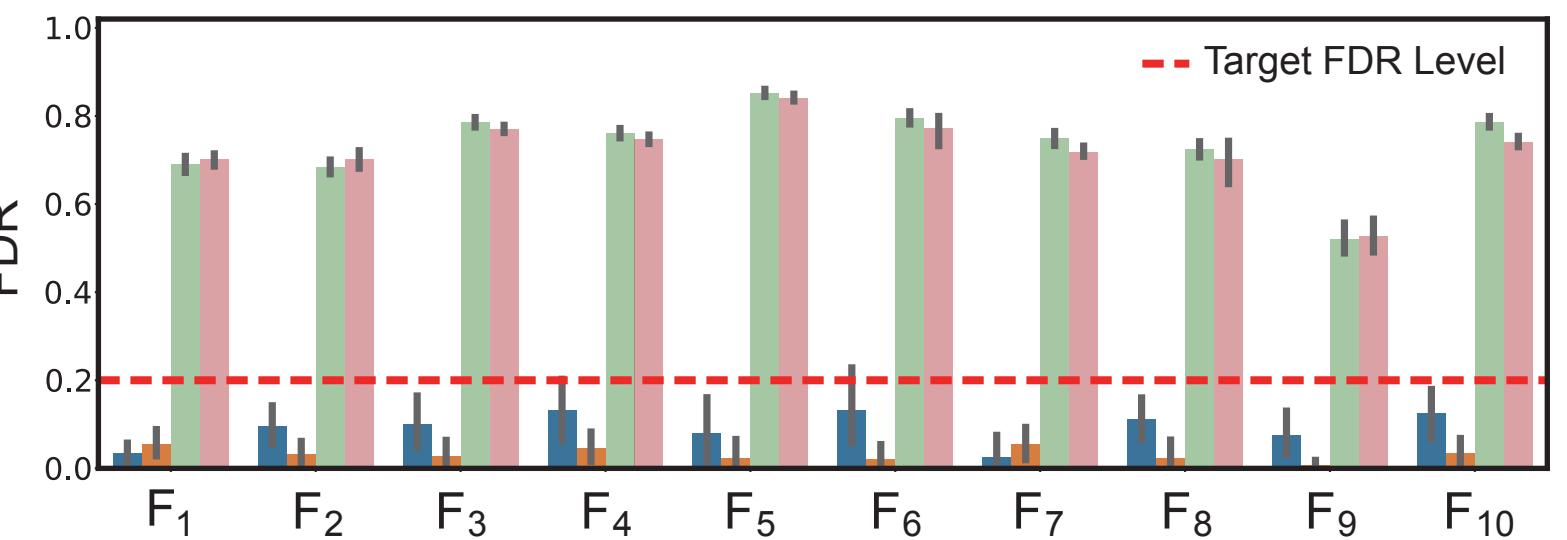
$$FDR = E \left[\frac{\# \text{ false selected interactions}}{\# \text{ total selected interactions}} \right]$$



Rank	Interaction	FDR
#1	Gene 1 - Gene 8	0.01 ✓
#2	Gene 4 - Gene 2	0.02 ✓
#3	Gene 2 - Gene 3	0.05 ✓
#4	Gene 9 - Gene 7	0.10 ✗
:	:	:

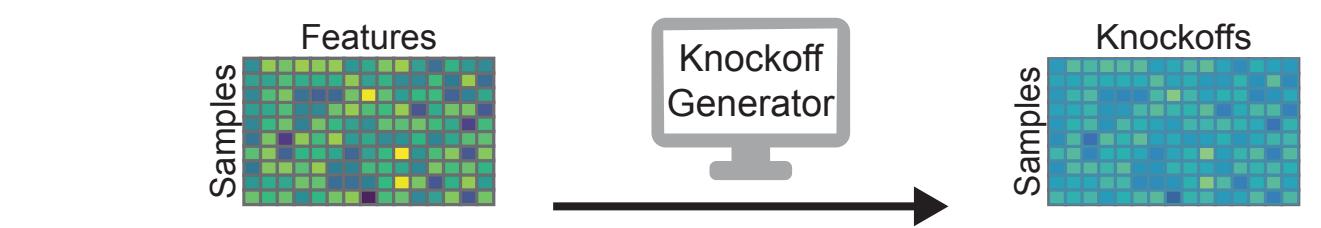
Simulation Experiments

DeepROCK exhibits strong statistical power and effectively controls FDR across 10 simulation functions [1]



Method

DeepROCK controls FDR using knockoffs



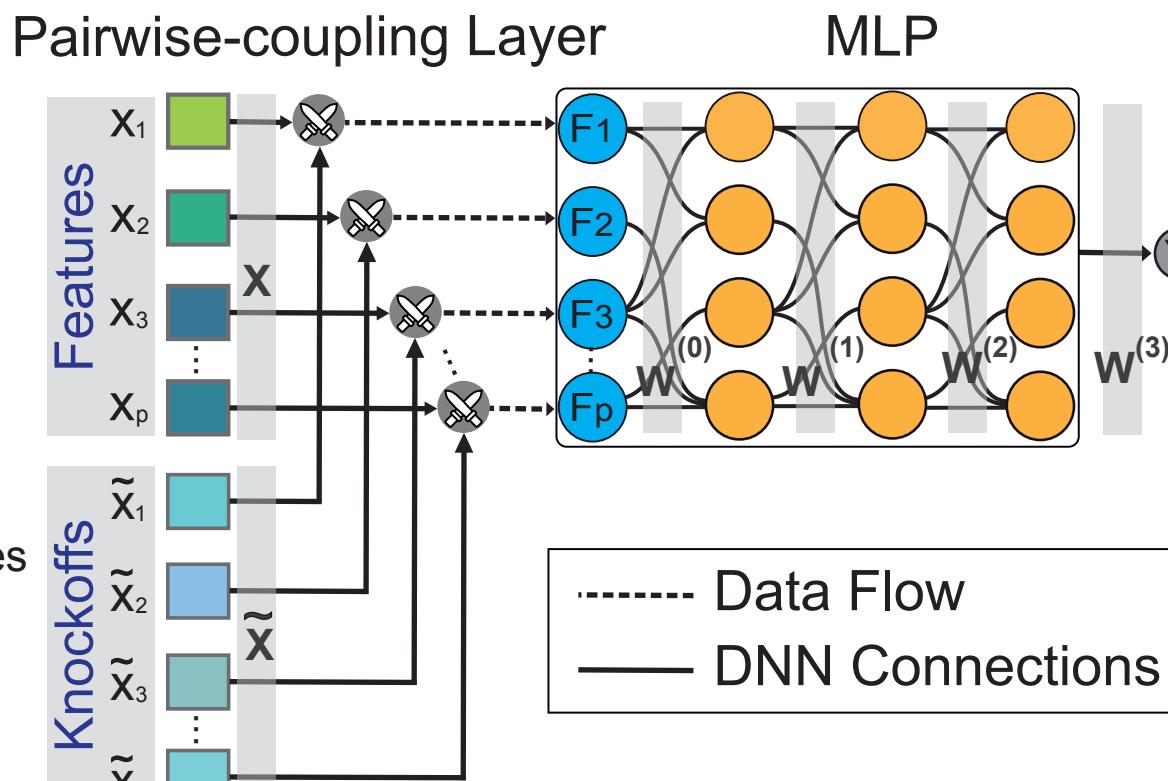
Knockoffs replicate the correlation structure between features

$$\begin{pmatrix} \text{Features} \end{pmatrix}^T \times \begin{pmatrix} \text{Features} \end{pmatrix} = \begin{pmatrix} \text{Knockoffs} \end{pmatrix}^T \times \begin{pmatrix} \text{Knockoffs} \end{pmatrix}$$

Knockoffs replicate the correlation structure between themselves and features

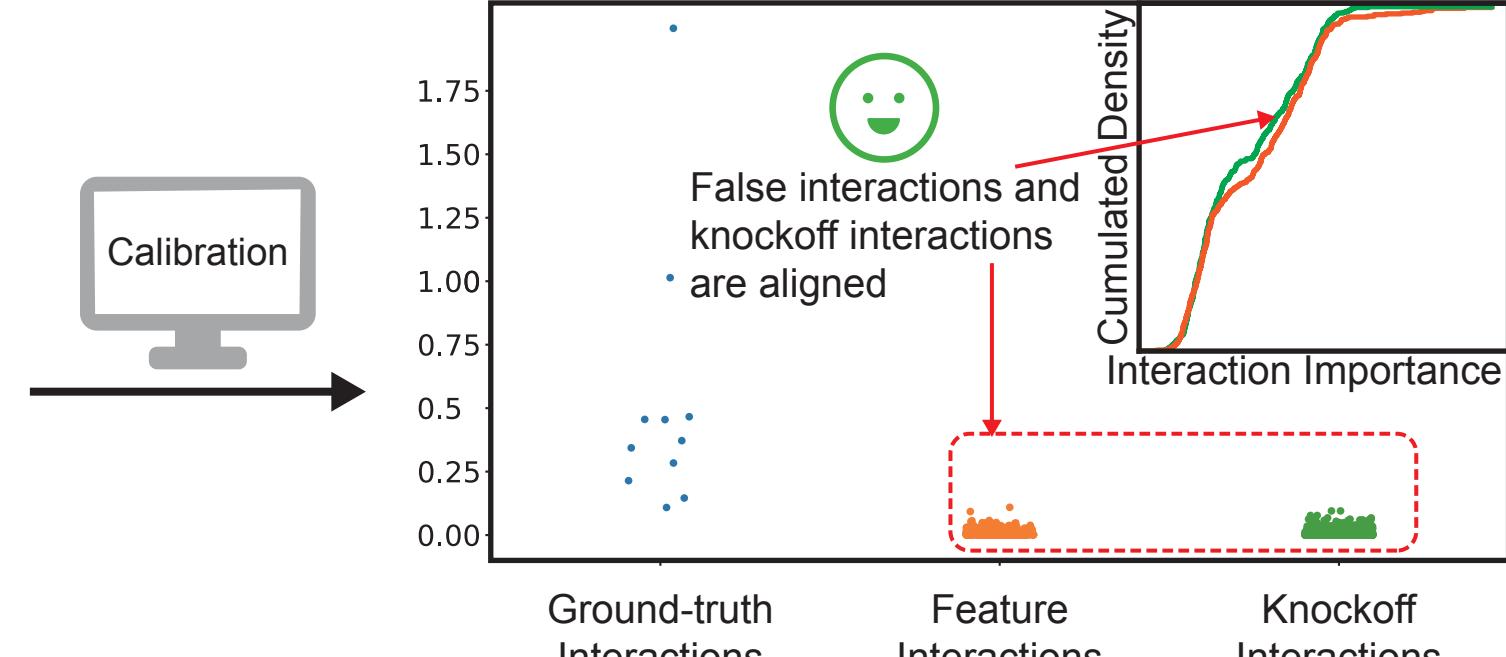
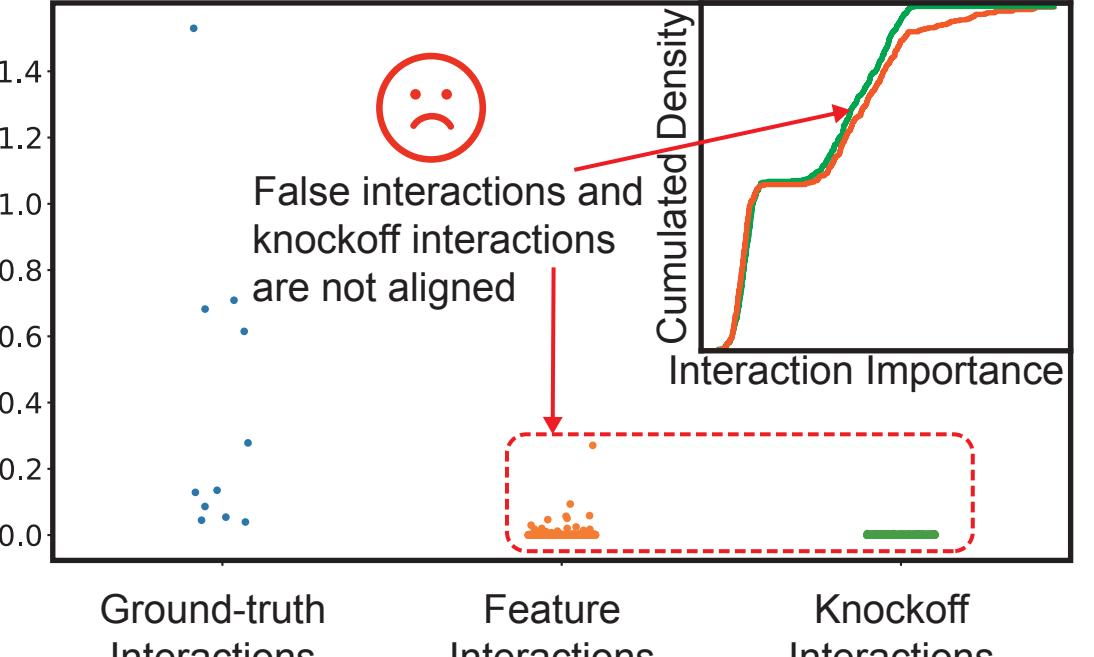
$$\begin{pmatrix} \text{Features} \end{pmatrix}^T \times \begin{pmatrix} \text{Features} \end{pmatrix} = \begin{pmatrix} \text{Knockoffs} \end{pmatrix}^T \times \begin{pmatrix} \text{Features} \end{pmatrix}$$

DeepROCK maximizes power using a novel pairwise-coupling layer



DeepROCK leverages a calibration procedure to correct FDR estimate

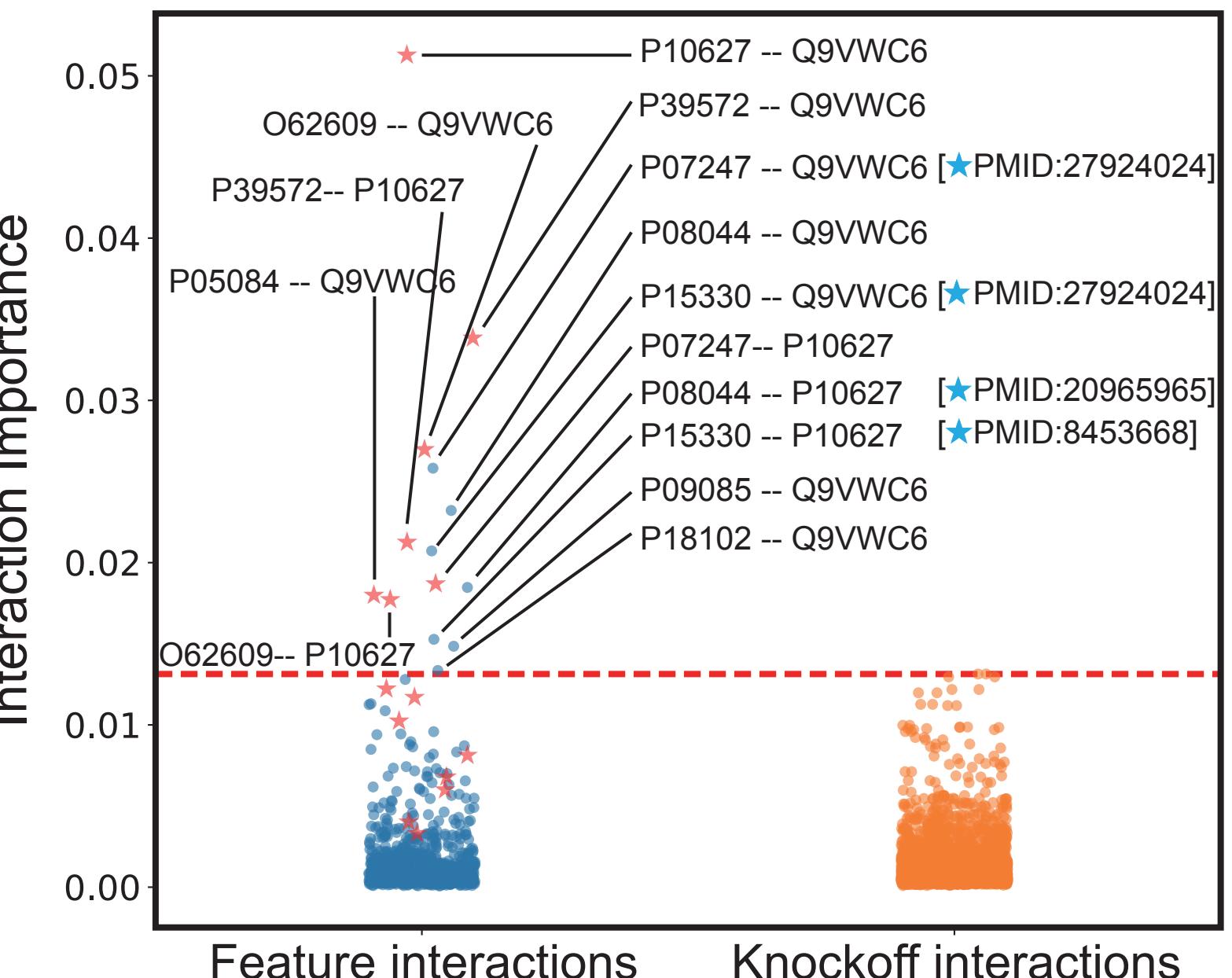
Uncalibrated Importance



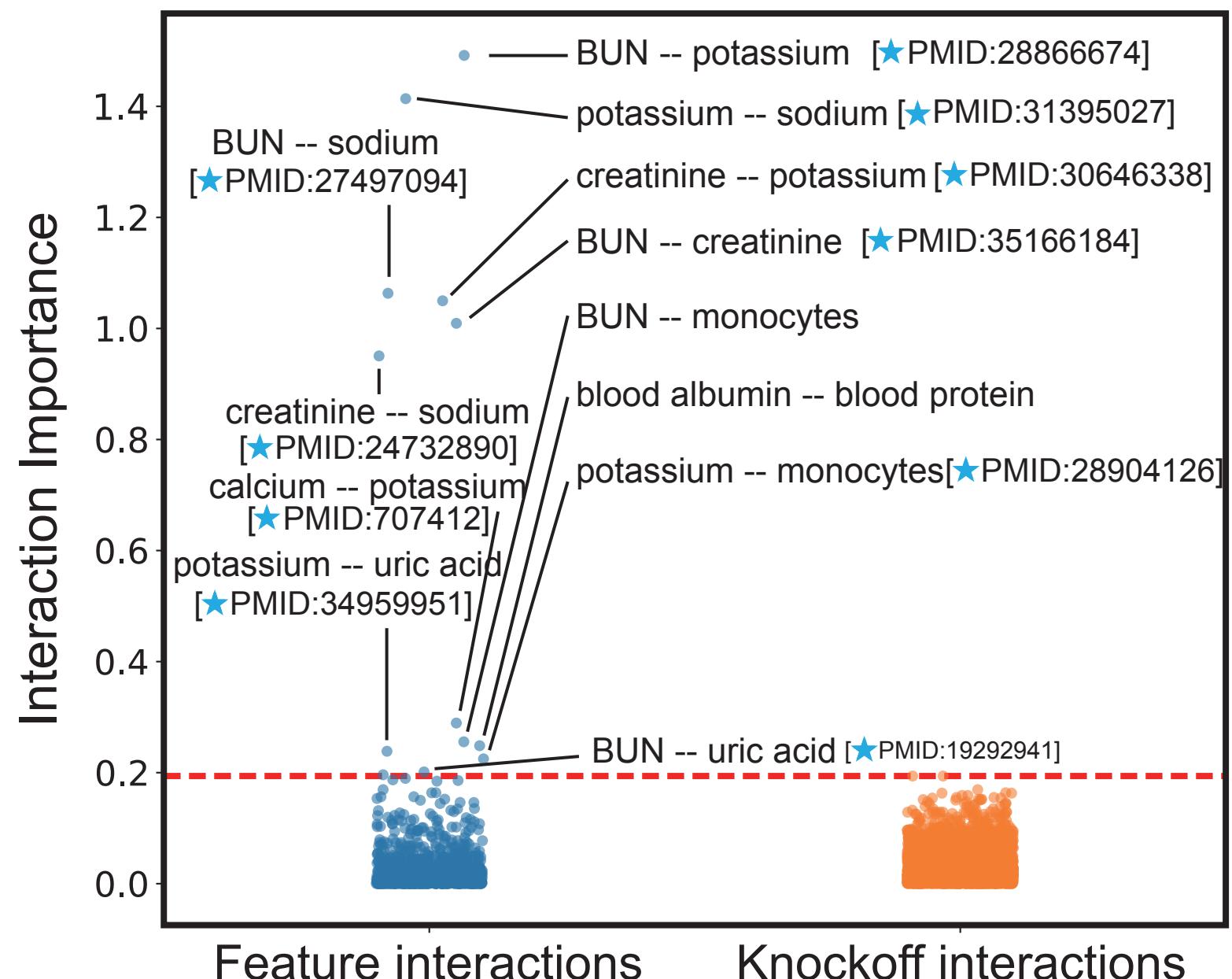
Real Data Experiments

DeepROCK discovers experimentally validated and literature-supported real-world interactions

Transcription Factors Dataset [2]



Mortality Risk Dataset [3]



References

- [1] M. Tsang, et al. Detecting statistical interactions from neural network weights. International Conference on Learning Representations, 2018.
- [2] S. Basu, et al. Iterative random forests to discover predictive and stable high-order interactions. Proceedings of the National Academy of Sciences, 2018.
- [3] C. S. Cox, et al. Plan and operation of the NHANES I Epidemiologic Follow up Study, 1992. 1997.