Debugging the Machine Learning Pipeline

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joint work with Xuezhou Zhang, Stephen Wright

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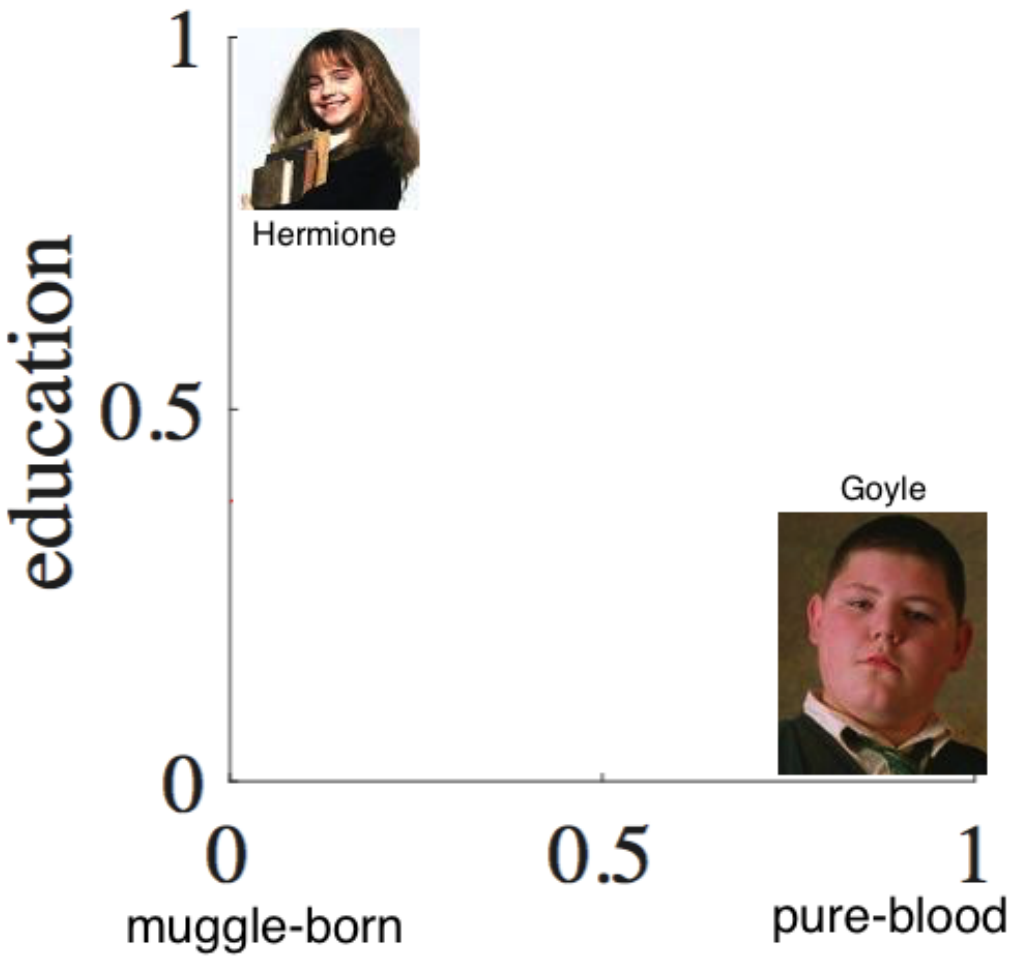
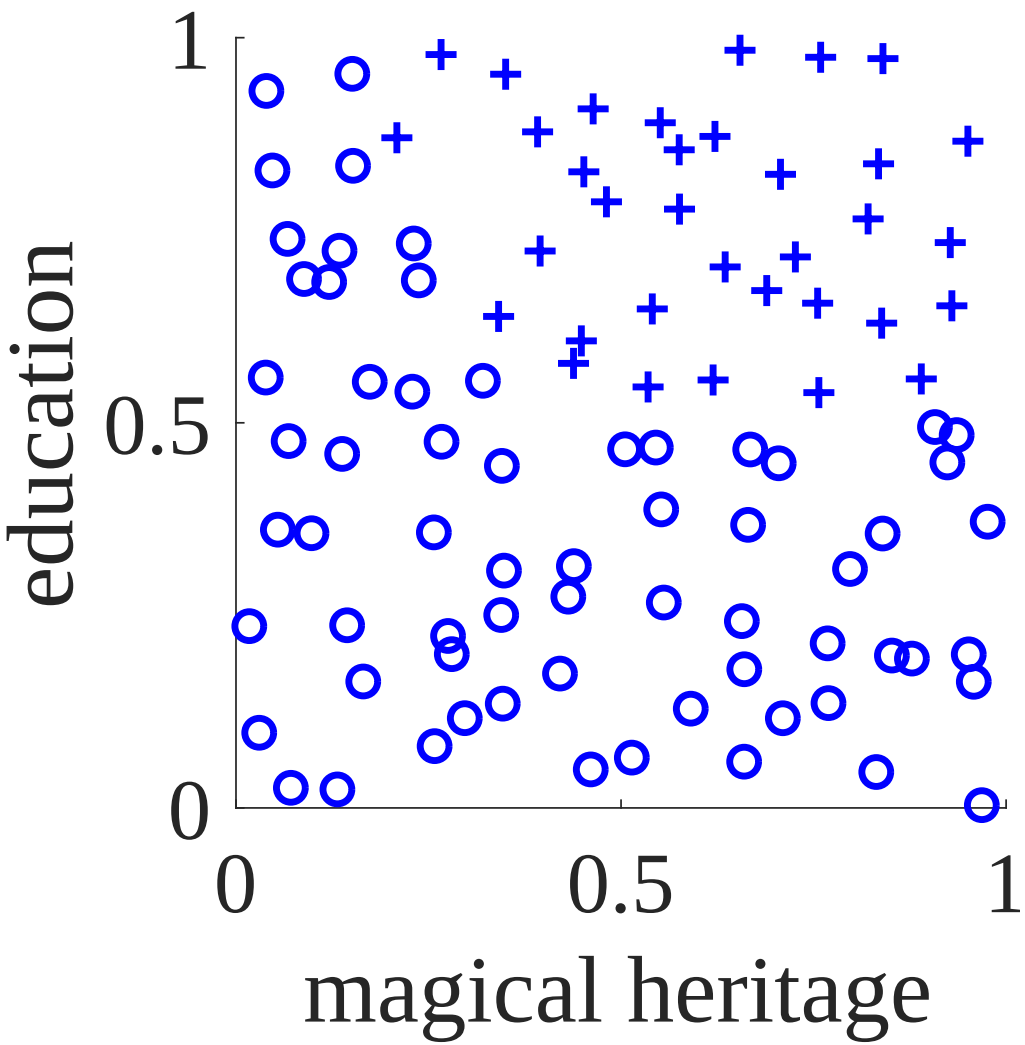
Debugging provides an opportunity for machine learning interpretability.

Harry Potter toy example



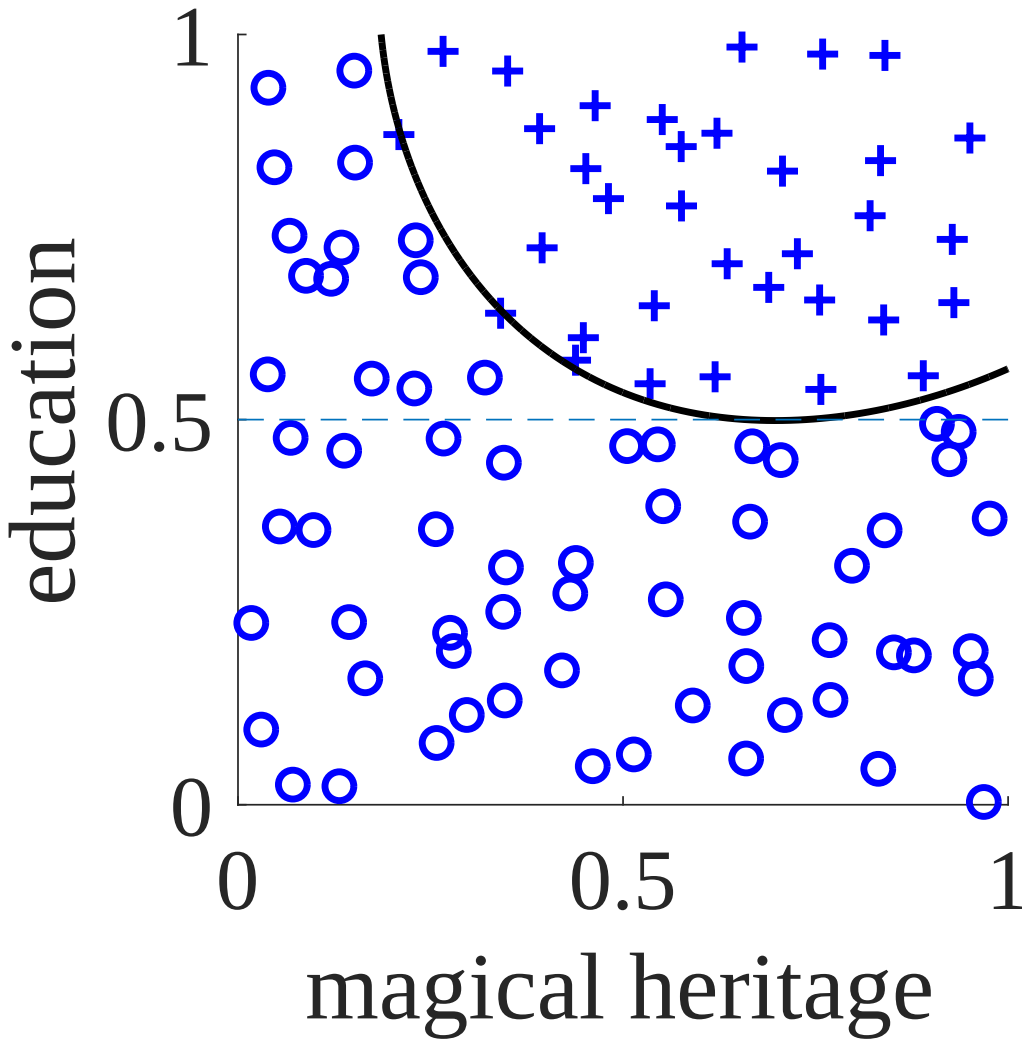
Hired by the Ministry of Magic?

+ yes
o no



Data contain historical biases

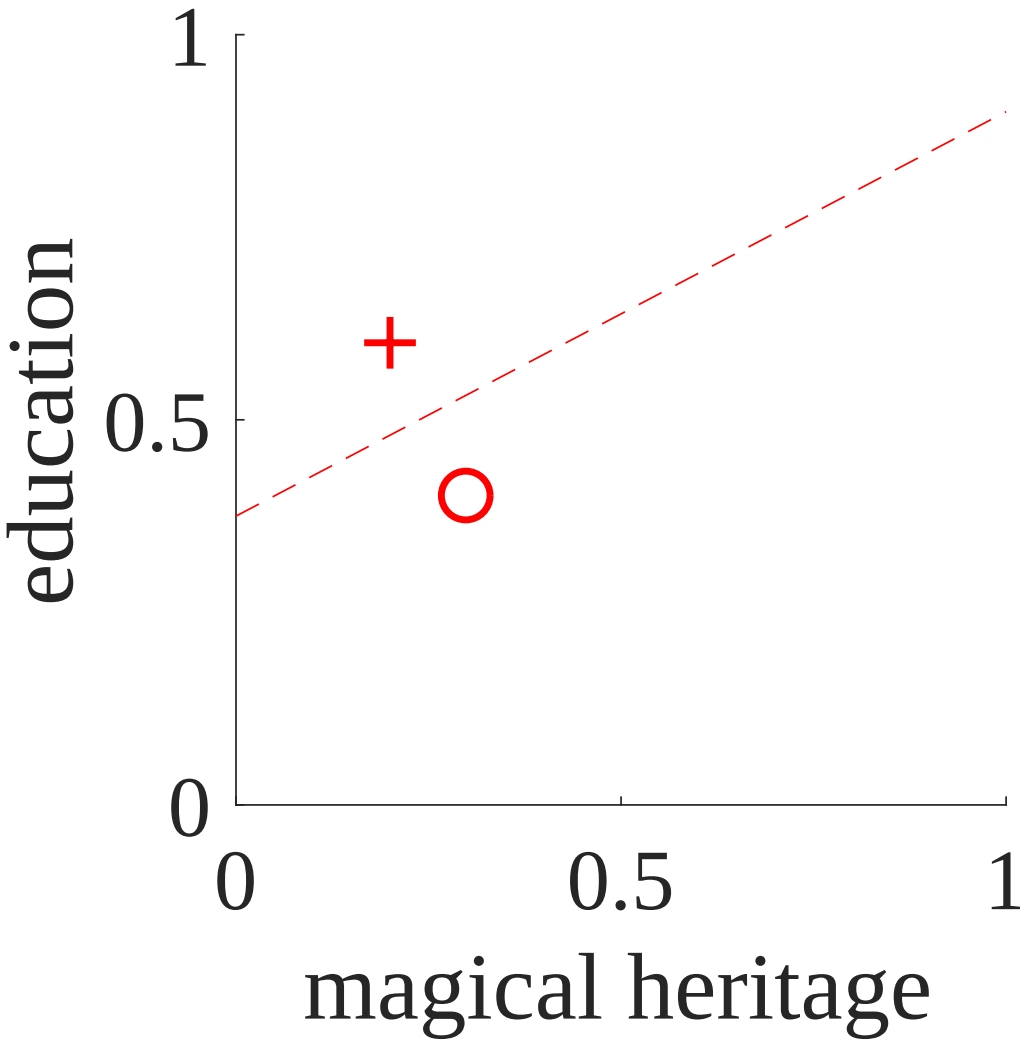
Learned vs. ideal decision boundary



(RBF kernel logistic regression)

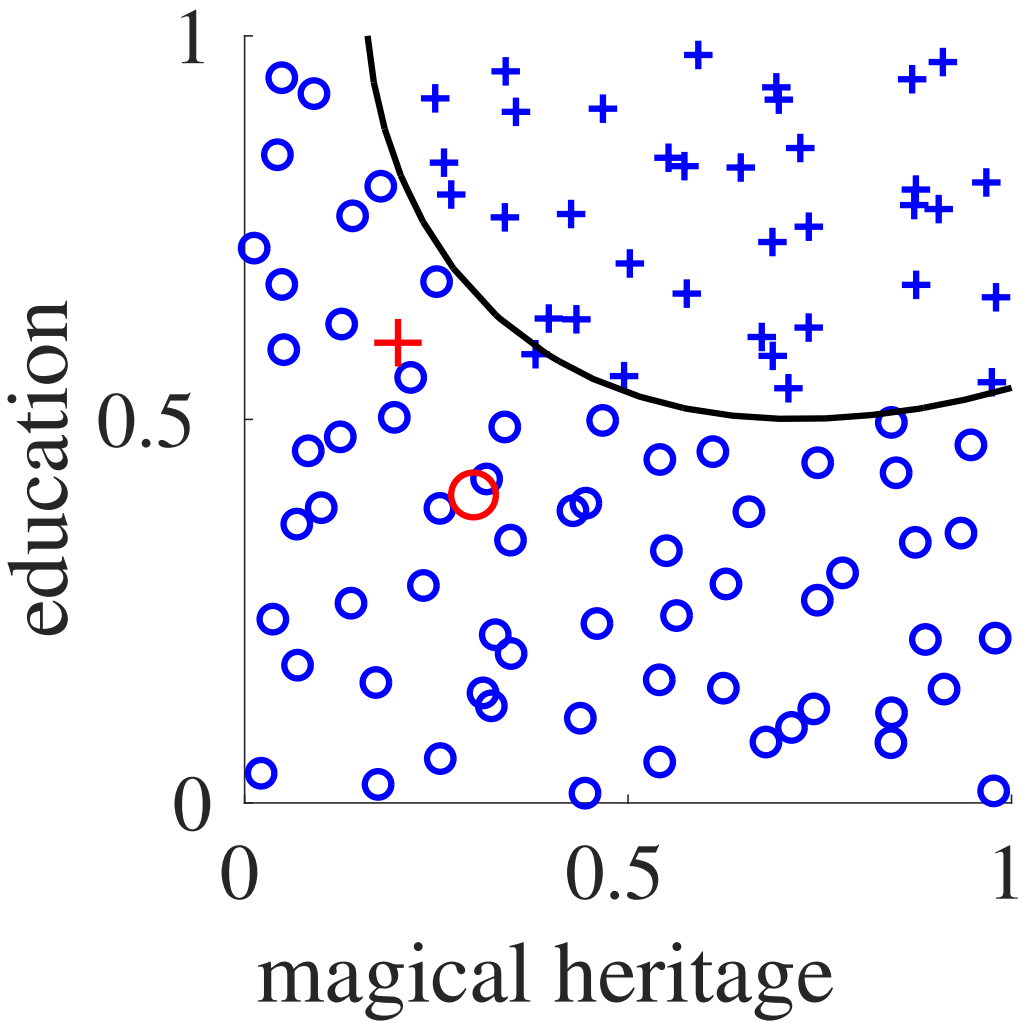
Trusted items

- obtained by expensive vetting
- insufficient to learn from



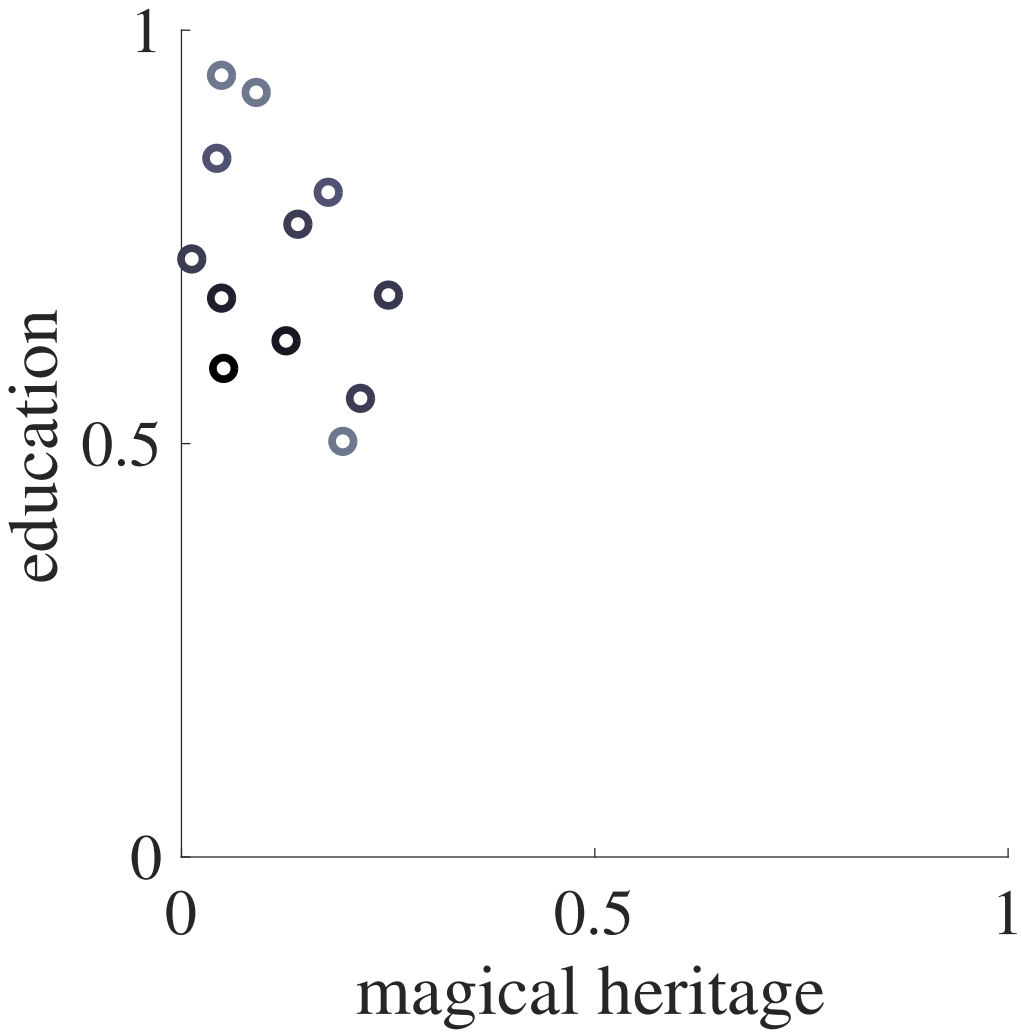
Debugging using trusted items

- propose training label bugs
- flipping them makes re-trained model agree with trusted items



Proposed bugs

- given to experts to interpret



The ML pipeline

$$\boxed{\text{data } (X, Y)} \rightarrow \boxed{\text{learner } \ell} \rightarrow \boxed{\text{parameters } \lambda} \rightarrow \boxed{\text{model } \hat{\theta}}$$

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmin}}\, \ell(X, Y, \theta) + \lambda \|\theta\|$$

Postconditions

$$\Psi(\hat{\theta})$$

Examples:

- "the learned model must correctly predict an important item $(\tilde{x}, \tilde{y})$"

$$\hat{\theta}(\tilde{x}) = \tilde{y}$$

- "the learned model must satisfy individual fairness"

$$\forall x, x', |p(y = 1 \mid x, \hat{\theta}) - p(y = 1 \mid x', \hat{\theta})| \leq L\|x - x'\|$$

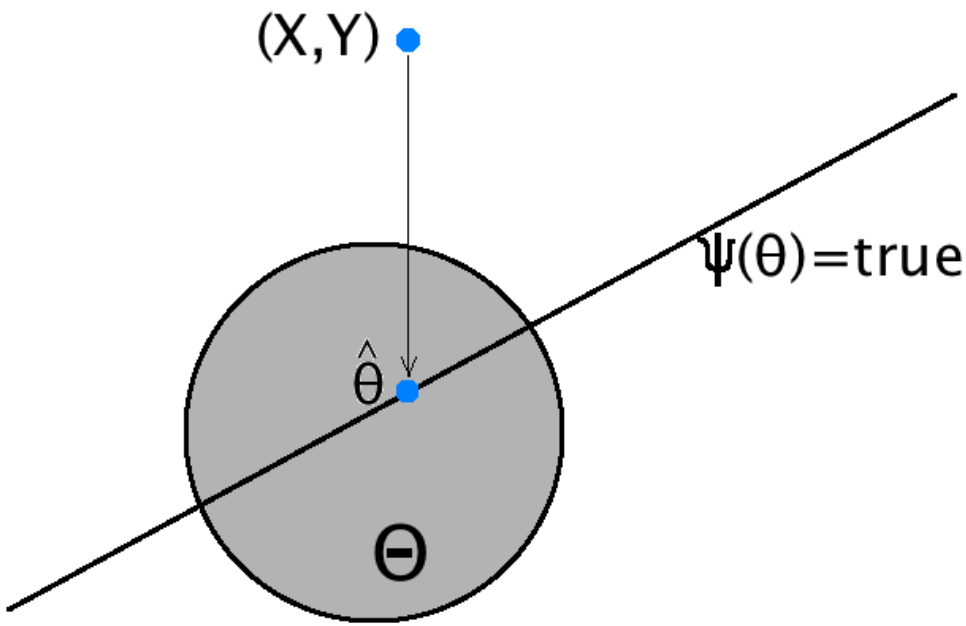
Bug Assumptions

- Ψ satisfied if we were to train through "clean pipeline"
- bugs are changes to the clean pipeline
- Ψ violated on the dirty pipeline

This is not our goal

Just to learn a better model:

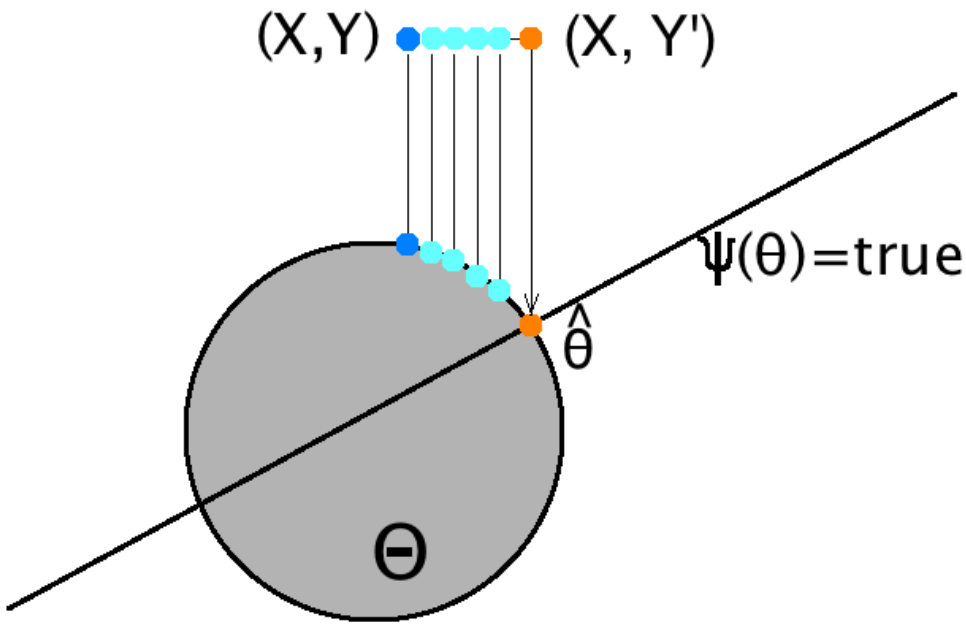
$$\begin{aligned} \min_{\theta \in \Theta} \quad & \ell(X, Y, \theta) + \lambda \|\theta\| \\ \text{s.t.} \quad & \Psi(\theta) = \text{true} \end{aligned}$$



This is our goal

To identify bugs and fix them (and learn a better model):

$$\begin{aligned} \min_{Y',\hat{\theta}} \quad & \|Y - Y'\| \\ \text{s.t.} \quad & \Psi(\hat{\theta}) = \text{true} \\ & \hat{\theta} = \operatorname*{argmin}_{\theta \in \Theta} \ell(X, Y', \theta) + \lambda \|\theta\| \end{aligned}$$



Special case: bugs in training labels

- Ψ satisfied if we were to train on "clean data" (X, Y')
- bugs are changes to clean labels

$$(X, Y) = (X, Y' + \Delta)$$

  - not just about outliers
  - may contain systematic biases

Input / output to our debugger

Input:

1. dirty training set (X, Y)
2. trusted items $(\tilde{X}, \tilde{Y})$
3. the learner

Output:

1. Y'
2. confidence

Formulation equivalent to machine teaching

$$\begin{aligned} \min_{Y'} \quad & \|Y' - Y\| \\ \text{s.t.} \quad & \hat{\theta}(\tilde{X}) = \tilde{Y} \\ & \hat{\theta} = \operatorname*{argmin}_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \ell(x_i, y_i', \theta) + \lambda \|\theta\|^2 \end{aligned}$$

Difficult!

- combinatorial
- bilevel optimization (Stackelberg game)

[Dec. 9 Workshop on Teaching Machines, Robots, and Humans]

Combinatorial to continuous relaxation

step 1. label to probability simplex

$$y'_i \to \delta_i \in \Delta$$

step 2. counting to probability mass

$$\|Y' - Y\| \to \frac{1}{n} \sum_{i=1}^{n} (1 - \delta_{i,y_i})$$

step 3. soften postcondition

$$\hat{\theta}(\tilde{X}) = \tilde{Y} \to \frac{1}{m} \sum_{i=1}^{m} \ell(\tilde{x}_i, \tilde{y}_i, \theta)$$

Continuous now, but still bilevel

$$\begin{aligned} \underset{\delta \in \Delta^n, \hat{\theta}}{\operatorname{argmin}} \quad & \frac{1}{m} \sum_{i=1}^{m} \ell(\tilde{x}_i, \tilde{y}_i, \hat{\theta}) + \gamma \frac{1}{n} \sum_{i=1}^{n} (1 - \delta_{i,y_i}) \\ \text{s.t.} \quad & \hat{\theta} = \underset{\theta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} \delta_{ij} \ell(x_i, j, \theta) + \lambda \|\theta\|^2 \end{aligned}$$

Removing the lower level problem

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} \delta_{ij} \ell(x_i, j, \theta) + \lambda \|\theta\|^2$$

step 1. the KKT condition

$$\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} \delta_{ij} \nabla_\theta \ell(x_i, j, \theta) + 2\lambda\theta = 0$$

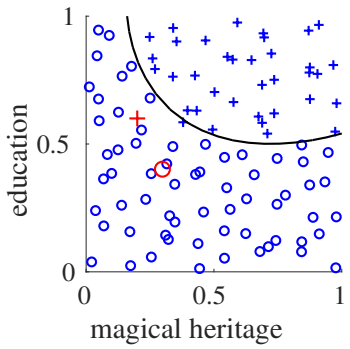
step 2. plug implicit function $\theta(\delta)$ into upper level problem

$$\underset{\delta}{\operatorname{argmin}} \quad \frac{1}{m} \sum_{i=1}^{m} \ell(\tilde{x}_i, \tilde{y}_i, \theta(\delta)) + \gamma \frac{1}{n} \sum_{i=1}^{n} (1 - \delta_{i,y_i})$$

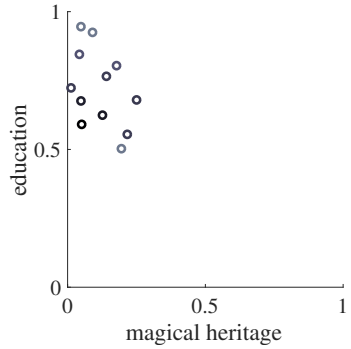
step 3. compute gradient ∇_δ with implicit function theorem

Software available.

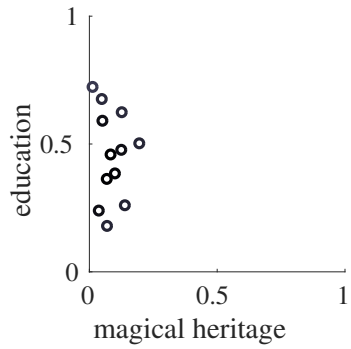
Harry Potter Toy Example



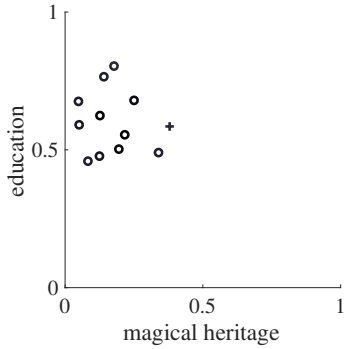
data



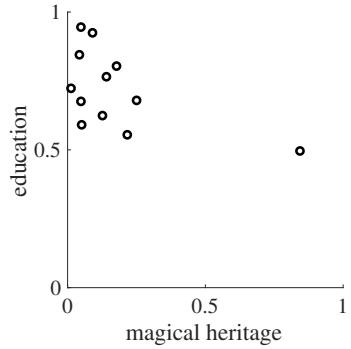
our debugger



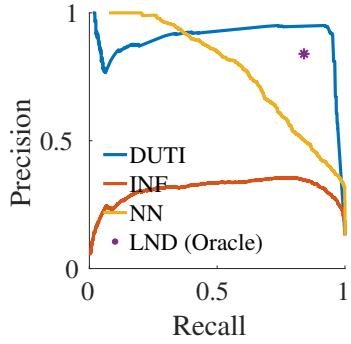
influence function



nearest neighbor

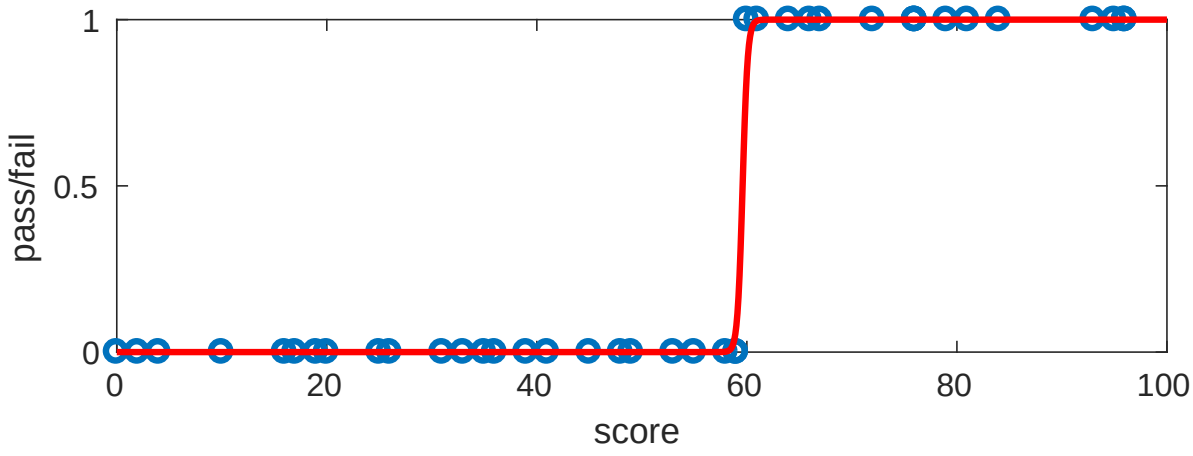


label noise detection



average PR

Another special case: bug in regularization weight



(logistic regression)

Postcondition violated

$\Psi(\hat{\theta})$: Individual fairness (Lipschitz condition)

$$\forall x, x', |p(y = 1 \mid x, \hat{\theta}) - p(y = 1 \mid x', \hat{\theta})| \leq L\|x - x'\|$$

Bug assumption

Learner's regularization weight $\lambda = 0.001$ was inappropriate

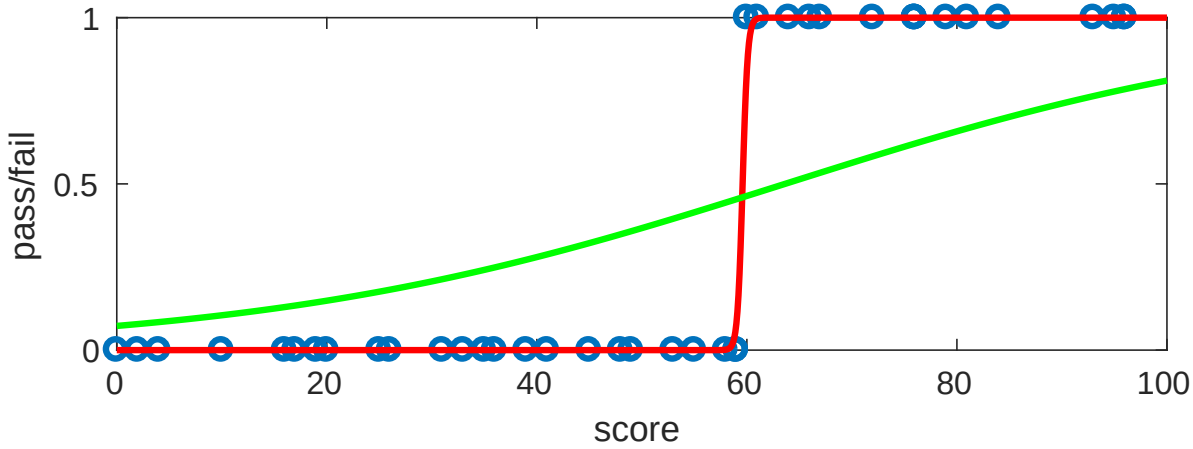
$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmin}}\, \ell(X, Y, \theta) + \lambda \|\theta\|^2$$

Debugging formulation

$$
\begin{aligned}
\min_{\lambda', \hat{\theta}} \quad & (\lambda' - \lambda)^2 \\
\text{s.t.} \quad & \Psi(\hat{\theta}) = \text{true} \\
& \hat{\theta} = \operatorname*{argmin}_{\theta \in \Theta} \ell(X, Y, \theta) + \lambda' \|\theta\|^2
\end{aligned}
$$

Suggested bug

$$\lambda = 0.001 \rightarrow \lambda' = 121$$



Call for ML bug repository

- like software bug repositories in software engineering
- need data provenance
  - which training items (or other things) were wrong
  - what they should be

References

- Xuezhou Zhang, Xiaojin Zhu, and Stephen Wright. Training set debugging using trusted items. AAAI 2018
- Gabriel Cadamuro, Ran Gilad-Bachrach, and Xiaojin Zhu. Debugging machine learning models. ICML Workshop on Reliable Machine Learning in the Wild, 2016.
- Shalini Ghosh, Patrick Lincoln, Ashish Tiwari, and Xiaojin Zhu. Trusted machine learning for probabilistic models. –
- `http://www.cs.wisc.edu/~jerryzhu/machineteaching/`