

because this road is endless*.

machine learning

ALL MODELS ARE WRONG BUT SOME ARE USEFUL

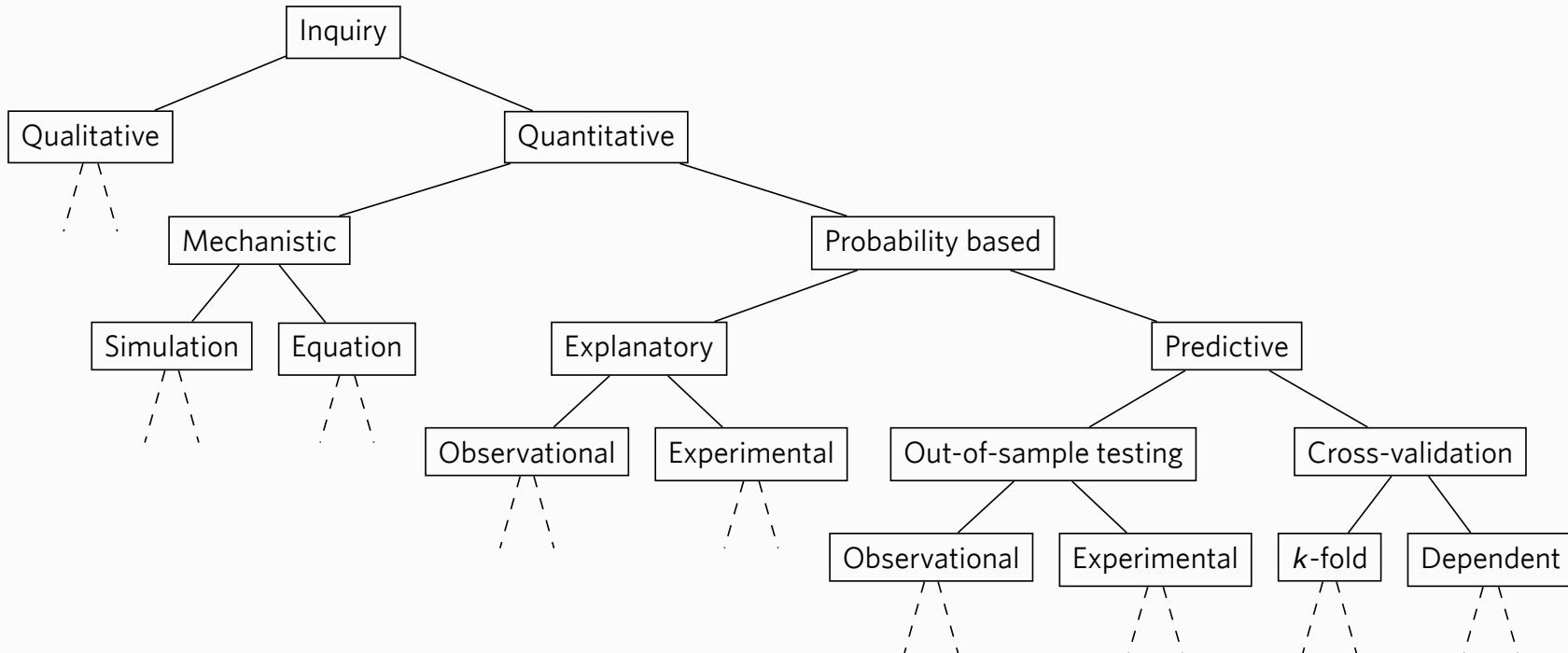


A Hierarchy of Limitations in Machine Learning

Momin M. Malik, Data Science Postdoctoral Fellow, Berkman Klein Center for Internet & Society at Harvard University (on leave)
NYU Center for Data Science, Math and Democracy Seminar, 05 Oct 2020

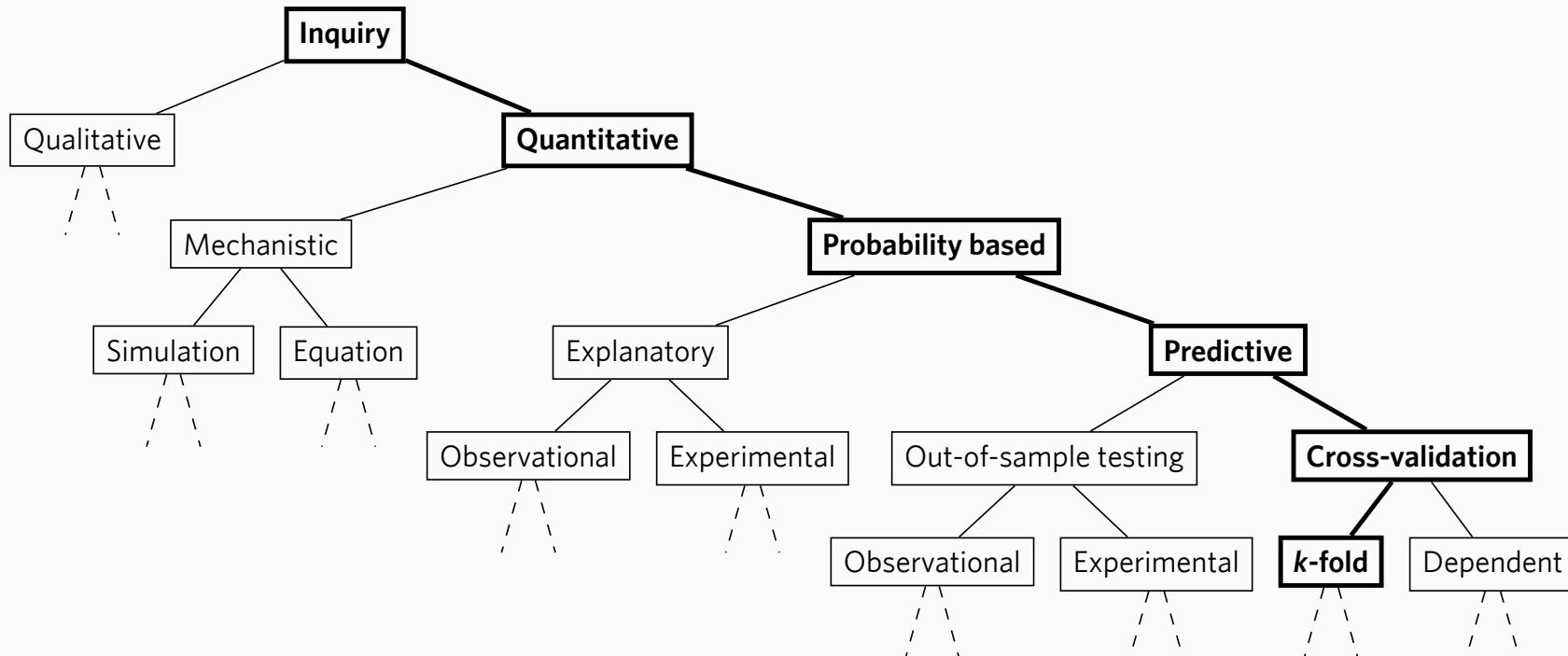
► The “hierarchy”

- Introduction
- Quantitative:
Meanings,
measurement,
and constructs
- Probability-
based: Central
tendency,
variability
- Predictive:
Correlation vs.
causation
- Cross-
validation:
Dependencies
and optimism
- Summary
- References



› Typical machine learning

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> Objectives

› Introduction

› Quantitative:
Meanings,
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and constructs

› Probability-based:
Central tendency,
variability

› Predictive:
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› Cross-validation:
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› References

- > What are the trade-offs associated with each branch?
- > When are we justified traveling down the machine learning (“predictive”) branch?
- > What are the consequences of using machine learning when it is *not* justified?

› Outline

1. Quantitative: Problems of meanings, measurement, and constructs
2. Probability-based: Problems of central tendencies, variability as nuisance
3. Predictive: Problems of correlation over causation
4. Cross-validation: Problems of dependencies and optimism

› Introduction

› Quantitative:
Meanings,
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and constructs

› Probability-
based: Central
tendency,
variability

› Predictive:
Correlation vs.
causation

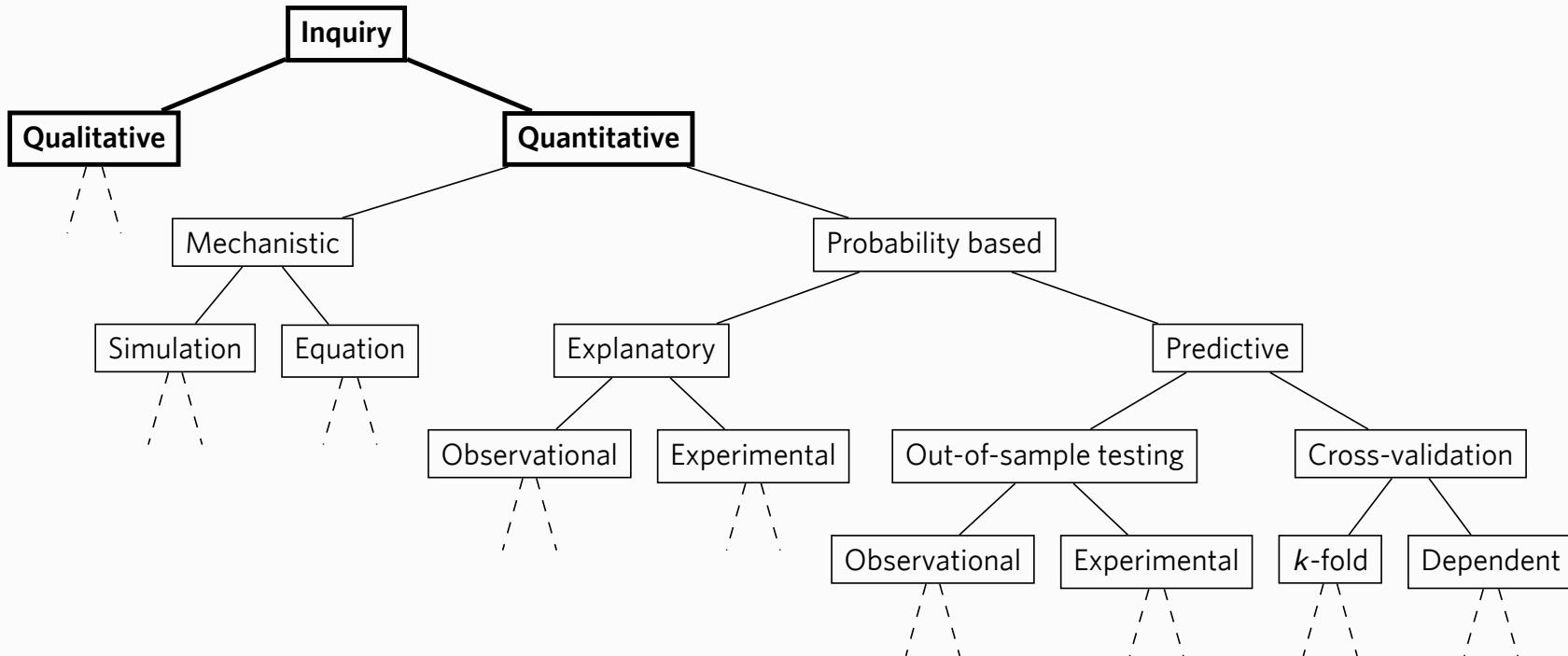
› Cross-
validation:
Dependencies
and optimism

› Summary

› References

1. Quantitative

- » Introduction
- » Quantitative: Meanings, measurement, and constructs
- » Probability-based: Central tendency, variability
- » Predictive: Correlation vs. causation
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> Meaning-making

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“During the writing of this book, my first grandchild was born. The hospital records document her weight, height, health[;] the mother’s condition, length of labor, time of birth, and hospital stay... These are physiological and institutional metrics. When aggregated across many babies and mothers, they provide trend data about the beginning of life—birthing.”

> Meaning-making

“But nowhere in the hospital records will you find anything about what the birth of Calla Quinn means. Her existence is documented but not what she means to our family, what decision-making process led up to her birth, the experience and meaning of the pregnancy, the family experience of the birth process, and the familial, social, cultural, political, and economic context...” (Patton, 2015)

▶ Introduction

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▶ Predictive:
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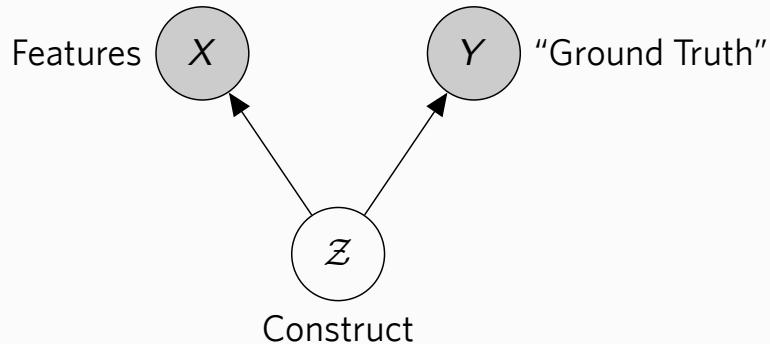
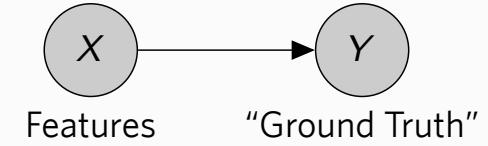
▶ Cross-
validation:
Dependencies
and optimism

▶ Summary

▶ References

> Measurement and constructs

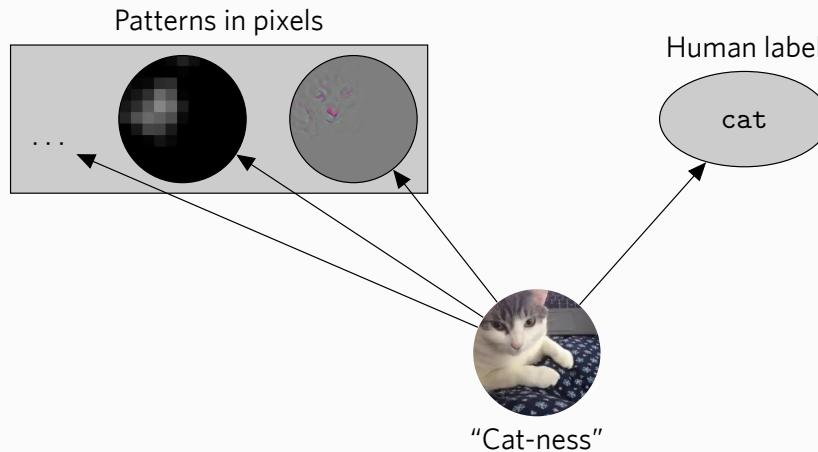
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- > Constructs: primitives of social science
 - What we care about
 - Often unobservable (and hypothetical/subjective, e.g. friendship)
 - Proxies always give errors (for binary-valued constructs: false negatives and false positives)

> Constructs: Subjective, multifaceted

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> Validating measurements

» Introduction

» Quantitative:
Meanings,
measurement,
and constructs

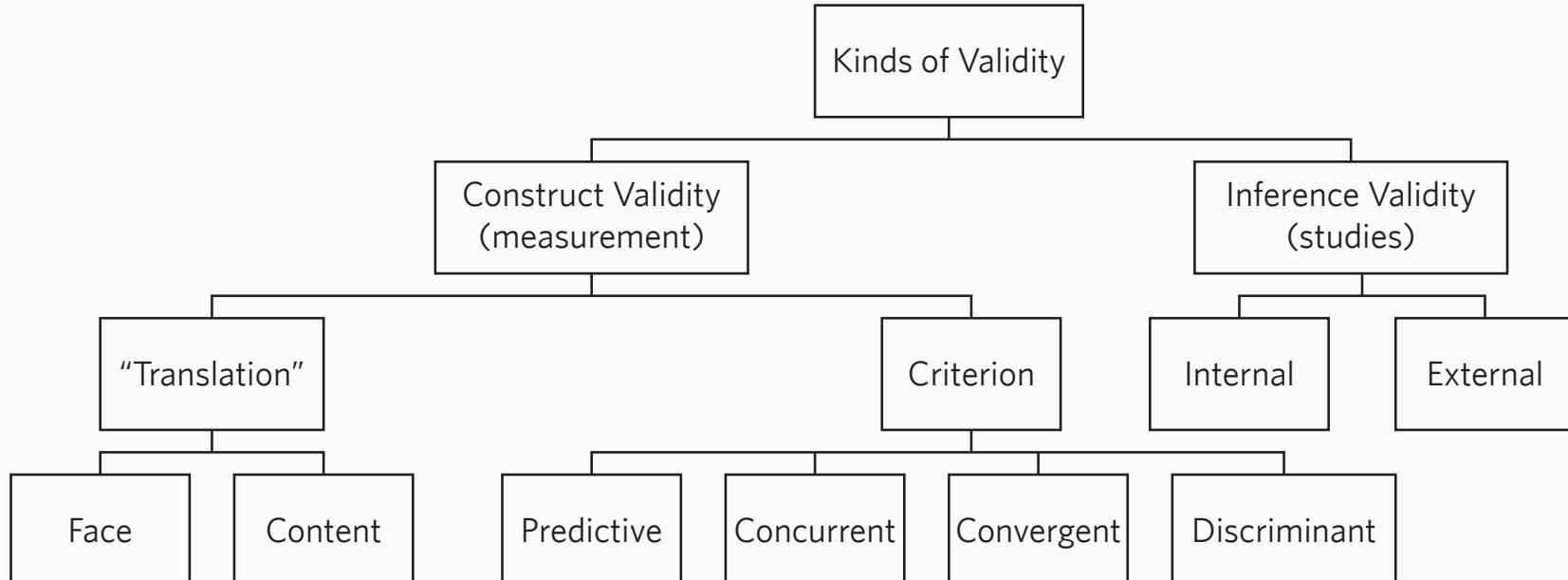
» Probability-
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causation

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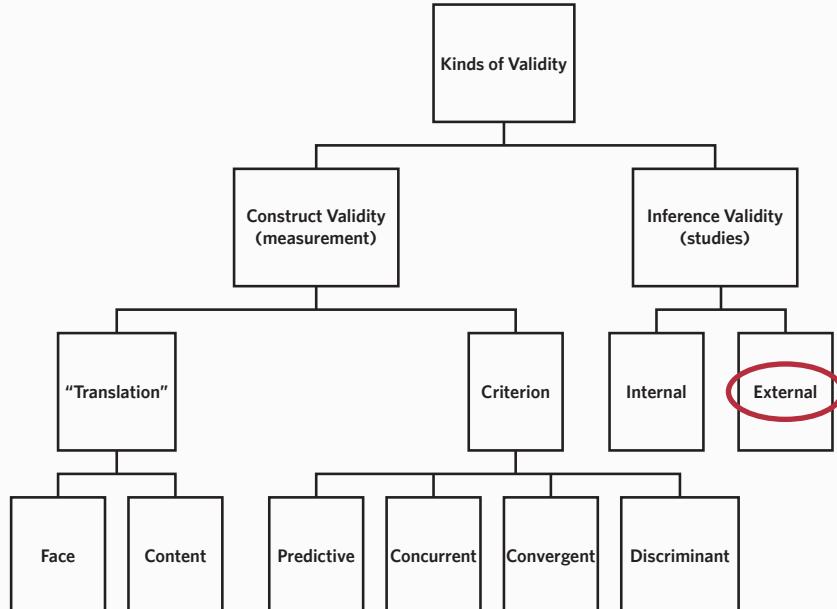
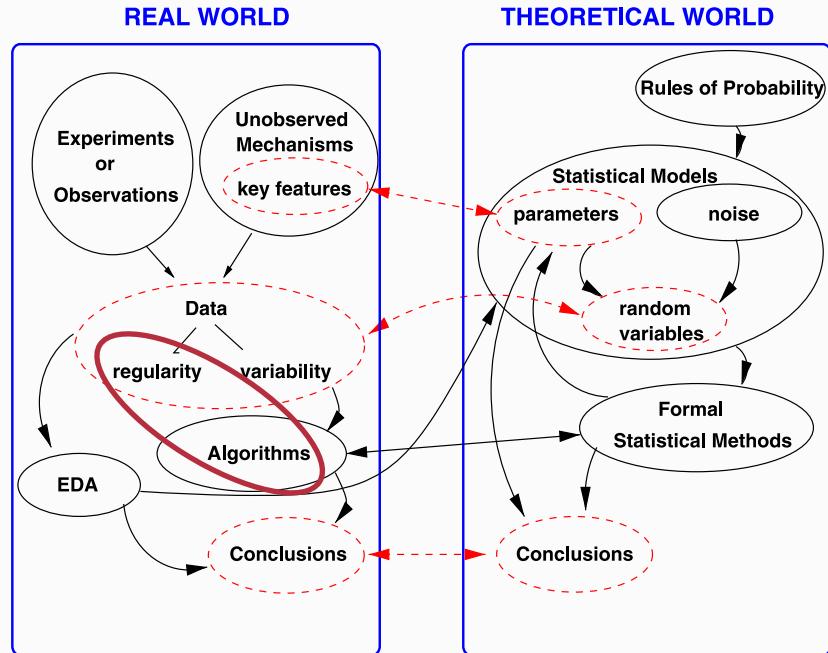


Adapted from Borgatti, 2012

A Hierarchy of Limitations of ML

> (ML: Only external validity)

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Kass, 2011, Stat. Sci.

A Hierarchy of Limitations of ML

Adapted from Borgatti, 2012

➤ “Thin description”

“what exactly is thin description? In a thin world, surfaces should be valid and deep meanings superfluous...

“The [quantitative social science] focus on behavior was a strategy to make social science into real science, something more like physics and less subject to values and prejudices because restricted to observable phenomena of the sort that could be registered by instruments. The **sacrifice of human meaning** seemed **not just a price worth paying for solid results, but the liberating essence of a proper objective methodology that now would rise above stubborn tradition and invisible culture.**” (Porter, 2012)

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➤ Consequences

- The world is, ultimately, “thick”: the same behavior can have infinitely many different meanings
- What is it we ultimately care about? Relating to human experience? Or “solid results”?
- Quantification requires choosing one set of meanings; nothing subsequent can “unpack” this (it has to be done again), and there is never one “best” meaning
- Quantification solidifies that meaning, which lets us build upwards
- Quantification can serve to de-legitimize other meanings

➤ Introduction
Quantitative:
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➤ Probability-
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tendency,
variability

➤ Predictive:
Correlation vs.
causation

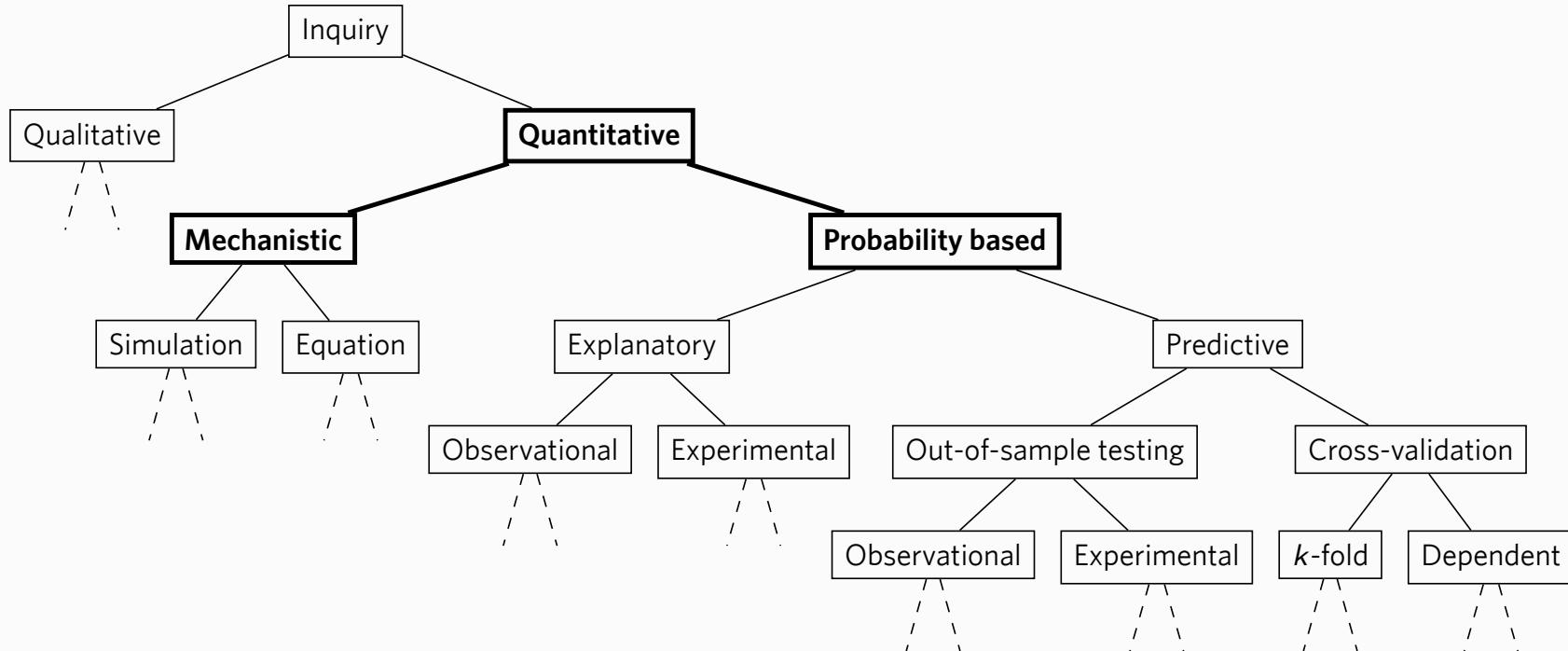
➤ Cross-
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➤ Summary

➤ References

2. Probability-based

- » Introduction
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➤ Probability: signal and noise

- “Probability is used in two distinct, although interrelated, ways in statistics, phenomenologically to describe haphazard variability arising in the real world and epistemologically to represent uncertainty of knowledge.” (Cox, 1990)
- Implies a philosophical commitment: the world is made up of entities that are interchangeable, where the important thing is *central tendency amidst variability*

► The world as a data matrix

► Introduction

► Quantitative:
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measurement,
and constructs

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variability

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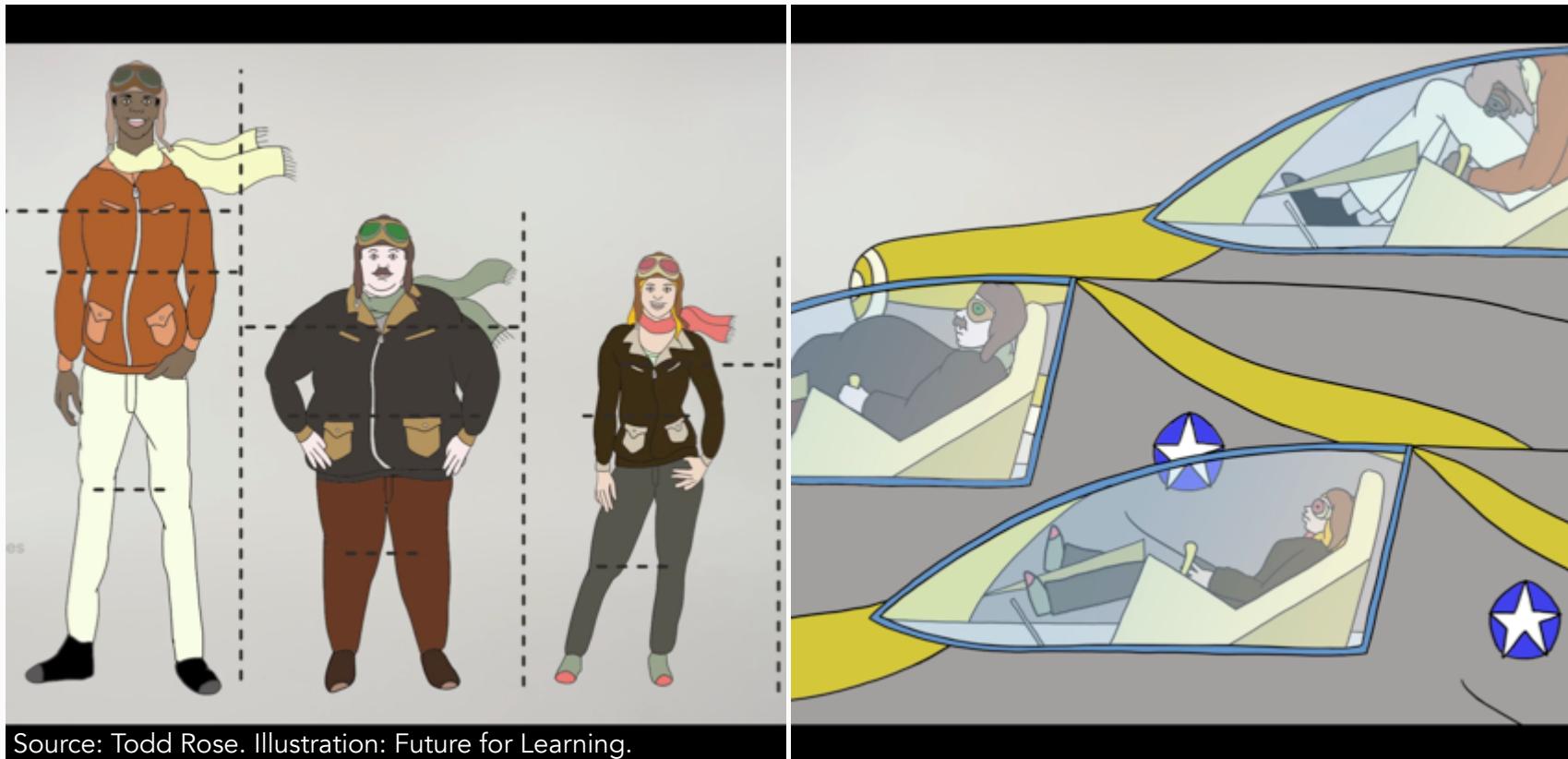
“it is striking how absolutely these assumptions contradict those of the major theoretical traditions of sociology.

Symbolic interactionism rejects the assumption of fixed entities and makes the meaning of a given occurrence depend on its location — within an interaction, within an actor's biography, within a sequence of events.

“Both the Marxian and Weberian traditions deny explicitly that a given property of a social actor has one and only one set of causal implications... Marx, Weber, and work deriving from them in historical sociology all approach social causality in terms of stories, rather than in terms of variable attributes.” (Abbott, 1988)

› Concretely: “Flaw of averages”

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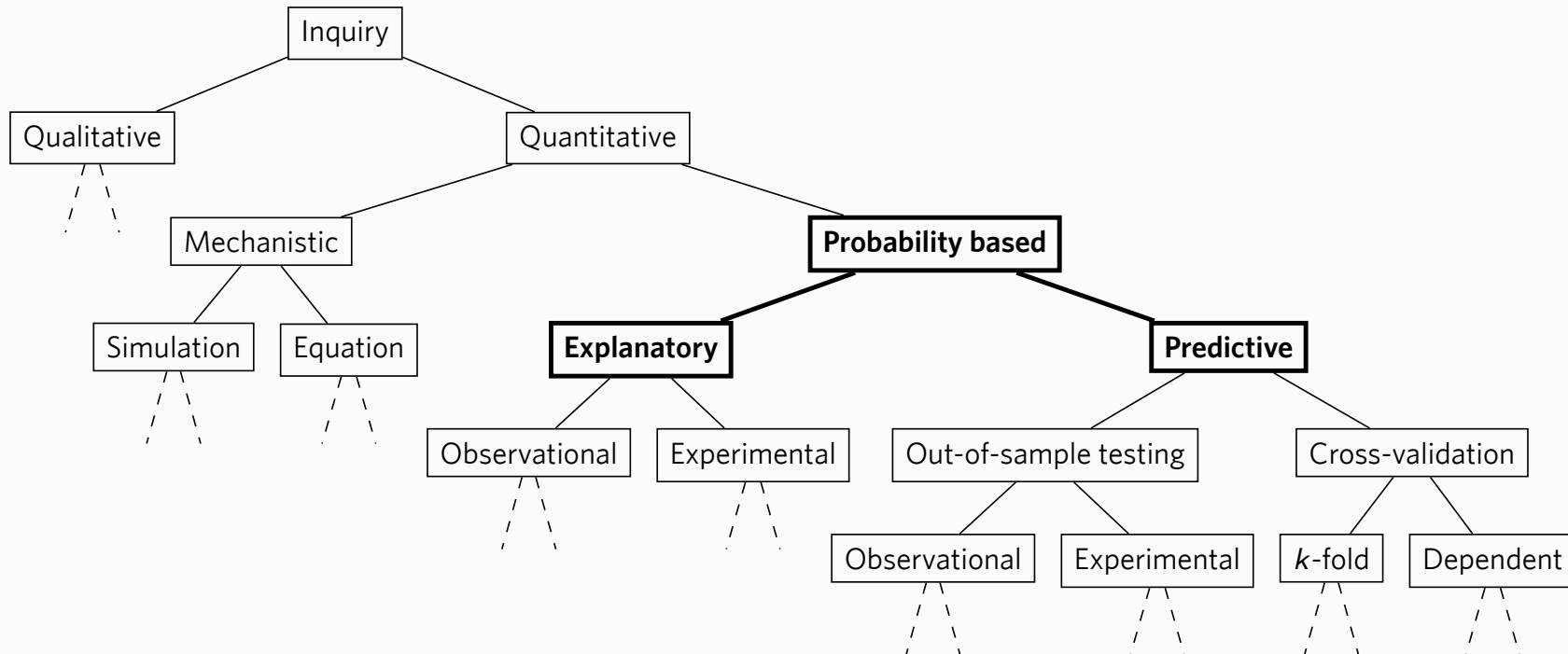
Source: Todd Rose. Illustration: Future for Learning.

➤ Consequences

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- These problems are not necessarily unique to probability-based modeling
 - SIR equations are “equilibrium” solution
 - Agent-based modeling often has interchangeable agents, and summarizes outcomes over multiple simulations with summary statistics
- Neither statistics nor machine learning can do anything with an n of 1: cannot account for individuality, nor do anything with it
- Planning to the central tendency punishes outliers (Keyes 2018)

3. Predictive

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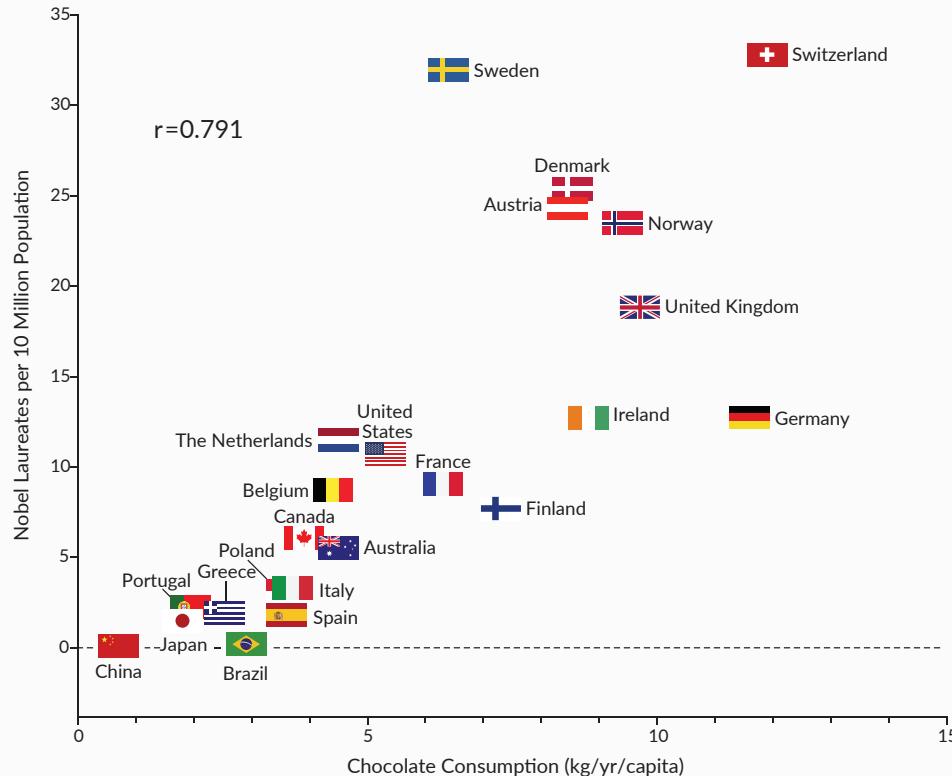


➤ “Prediction” is not prediction!

➤ “*It's not prediction at all! I have not found a single paper predicting a future result. All of them claim that a prediction could have been made; i.e. they are post-hoc analysis and, needless to say, negative results are rare to find.*” (Gayo-Avello, “I Wanted to Predict Elections with Twitter and all I got was this Lousy Paper”, 2012)

► “Predictions” are correlations

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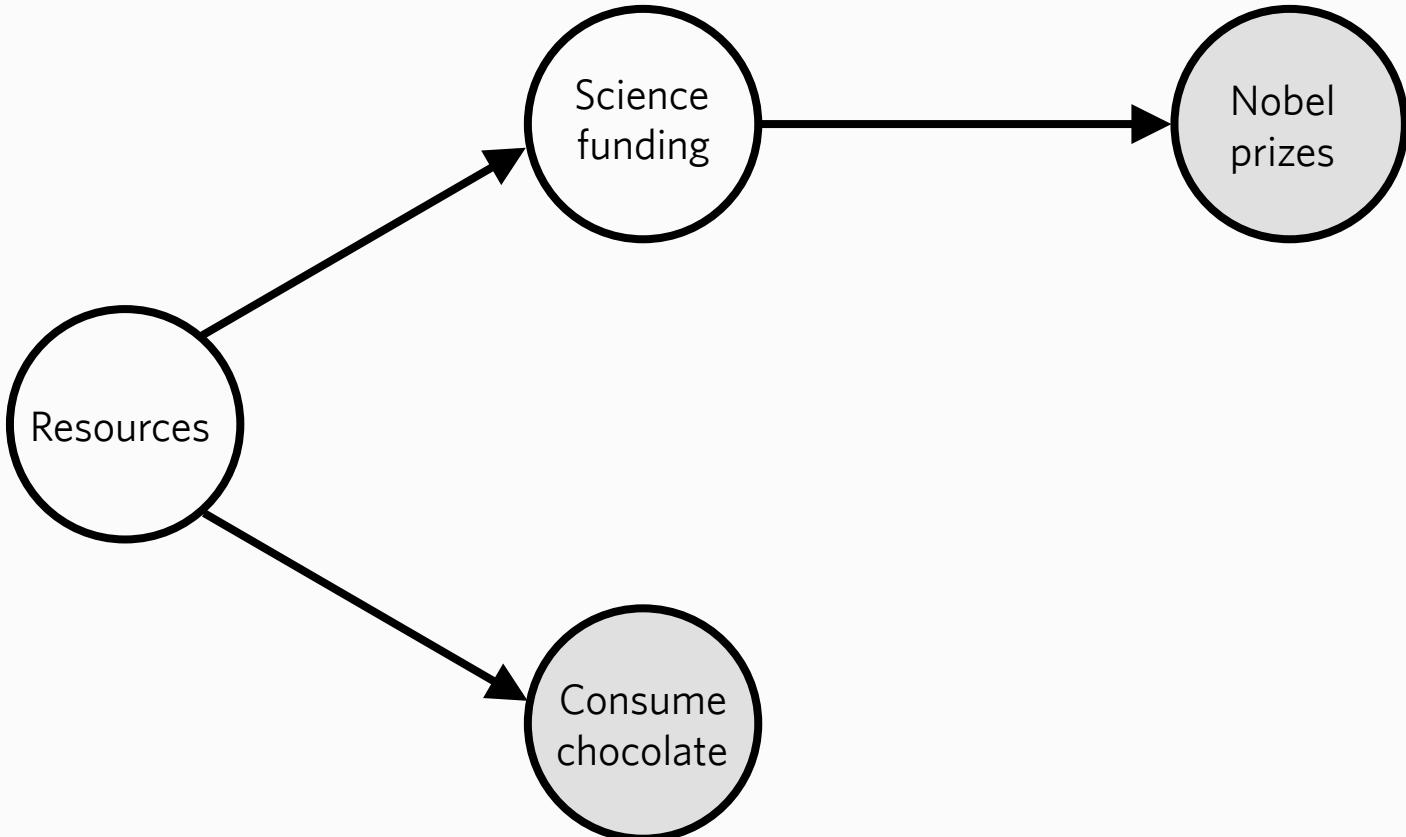


Messerli, 2012, NEJM

A Hierarchy of Limitations of ML

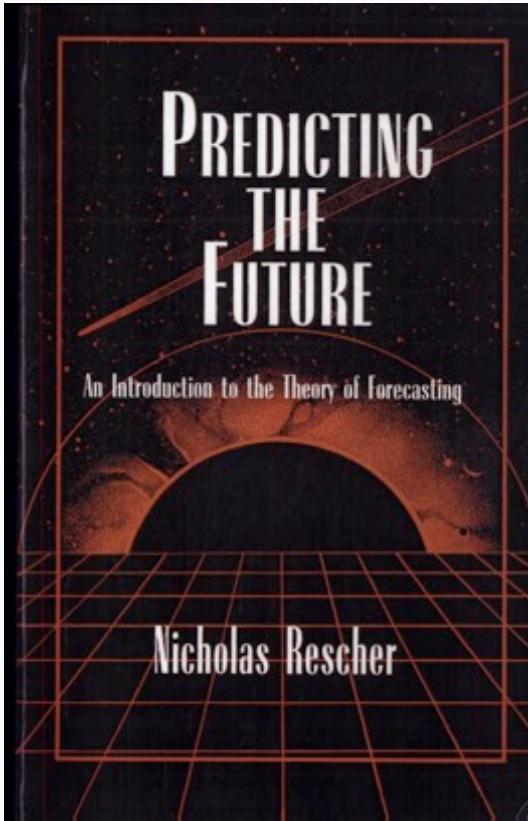
➤ Cause is resources

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Not an obvious usage of “predict”

- ▶ Introduction
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A Hierarchy of Limitations of ML

88 ■ PREDICTING THE FUTURE

TABLE 6.1: A SURVEY OF PREDICTIVE APPROACHES

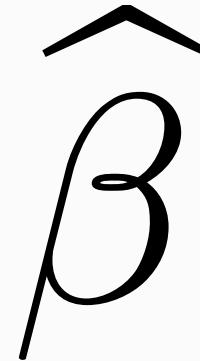
| Predictive Approaches | Linking Mechanism | Methodology Of Linkage |
|--|--|---|
| UNFORMALIZED/JUDGMENTAL | | |
| judgmental estimation | expert informants | informed judgment |
| FORMALIZED/INFERENTIAL | | |
| RUDIMENTARY (ELEMENTARY) | | |
| trend projection | prevailing trends | projection of prevailing trends |
| curve fitting | geometric patterns | subsumption under an established pattern |
| circumstantial analogy | comparability groupings | assimilation to an analogous situation |
| SCIENTIFIC (SOPHISTICATED) | | |
| indicator coordination | causal correlations | statistical subsumption into a correlation |
| law derivation (nomic) | accepted laws (deterministic or statistical) | inference from accepted laws |
| phenomenological modeling (analogical) | formal models (physical or mathematical) | analogizing of actual (“real-world”) processes with presumably isomorphic model process |

» Creates two types of modeling!



Correlations may “predict” well

- » Breiman, 2001: Prediction
- » Shmueli, 2010: Prediction
- » Kleinberg et al., 2015: Umbrella
- » Mullainathan & Spiess, 2017: \hat{y}

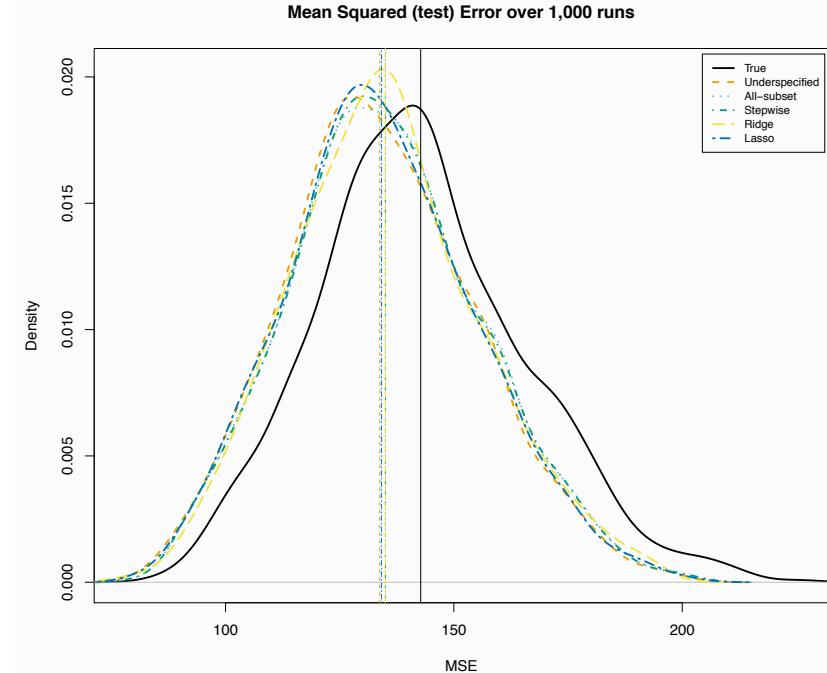
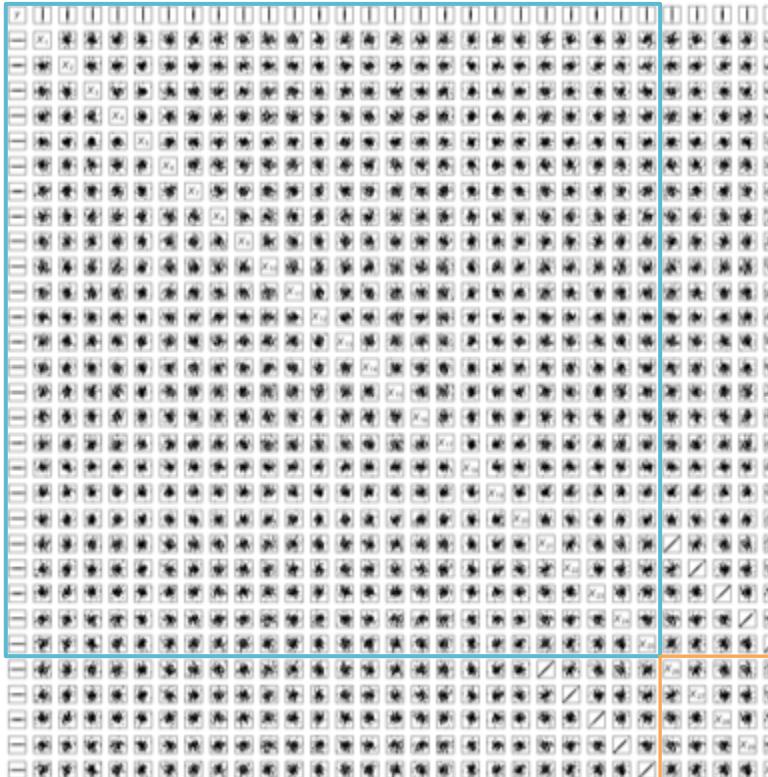


Informative models may not fit well

- » Breiman 2001: Information
- » Shmueli 2010: Explanation
- » Kleinberg et al 2015: Rain dance
- » Mullainathan & Spiess, 2017: $\hat{\beta}$

► “True” model can predict worse!

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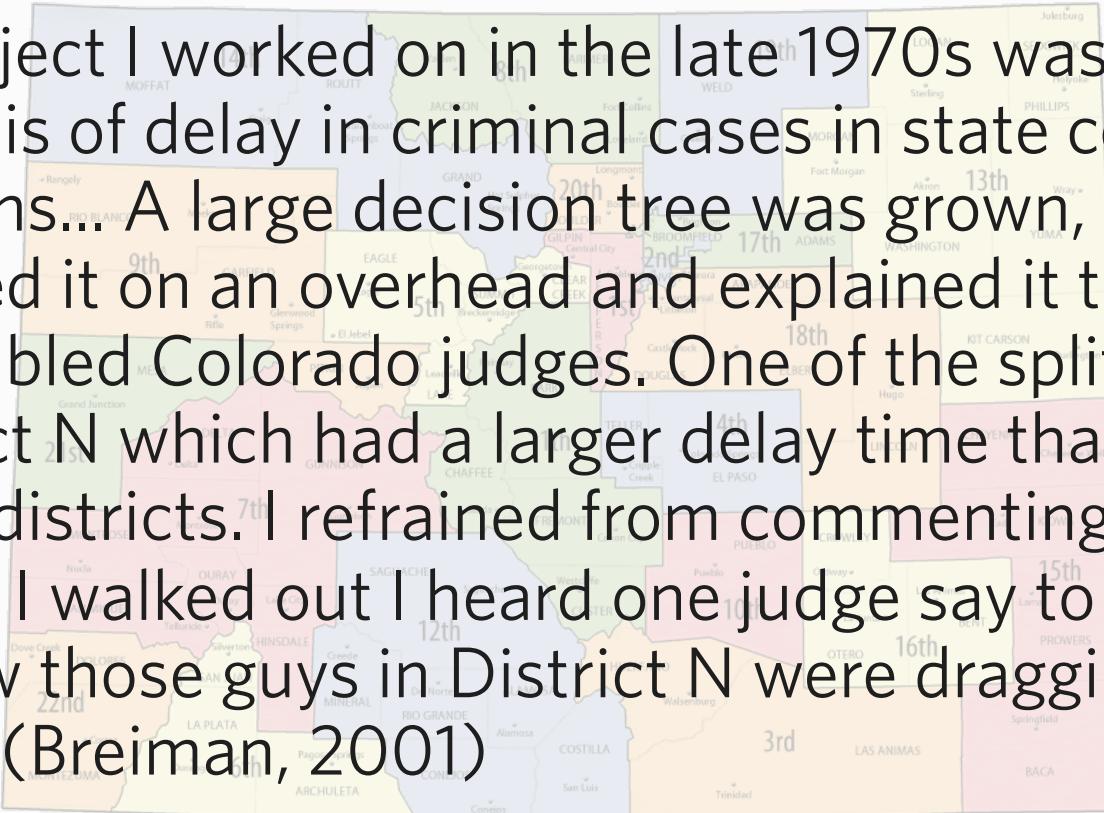


Simulation of Shmueli, 2010, *Stat. Sci.*

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› Sometimes, people want causality

- › “A project I worked on in the late 1970s was the analysis of delay in criminal cases in state court systems... A large decision tree was grown, and I showed it on an overhead and explained it to the assembled Colorado judges. One of the splits was on District N which had a larger delay time than the other districts. I refrained from commenting on this. But as I walked out I heard one judge say to another, ‘I knew those guys in District N were dragging their feet.’” (Breiman, 2001)



► Correlations and injustice

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Julius C. Chappelle proposed a bill in Massachusetts to ban charging Black people more for life insurance

A lawyer opposing the bill “cited statistics from around the nation showing shorter life spans for blacks, including 1870 census figures showing a 17.28 death rate for ‘colored people’ against 14.74 for whites. These numbers, Williams argued, and not any ‘discrimination on the ground of color’ motivated insurers’ rates. It was a ‘matter of business,’ and any interference, he warned ominously and presciently, ‘would probably cut off insurance entirely from the colored race.’”

► Correlations and injustice

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“Chappelle’s allies noted that Williams’s statistics, while bleak enough, answered the wrong question. The question was not whether blacks in slavery or adjusting to freedom were poor insurance risks, or even whether southern blacks were poor risks. The question was African Americans’ potential for equality and specifically the present and future state of Massachusetts’ African Americans—about whom no statistics had been offered by either side.” (Bouk, 2015)

► Sometimes, causality affects prediction

► Introduction

► Quantitative:
meanings,
measurement,
and constructs

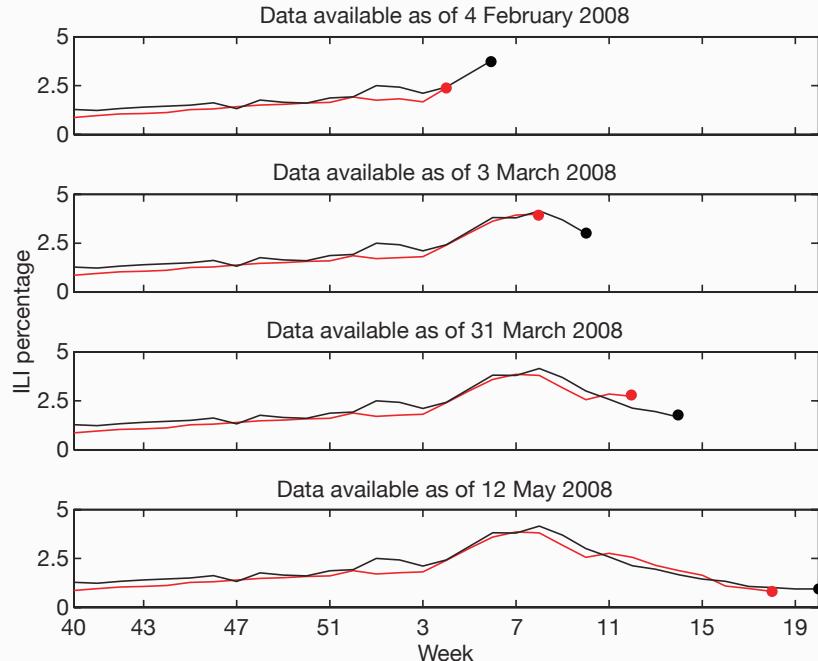
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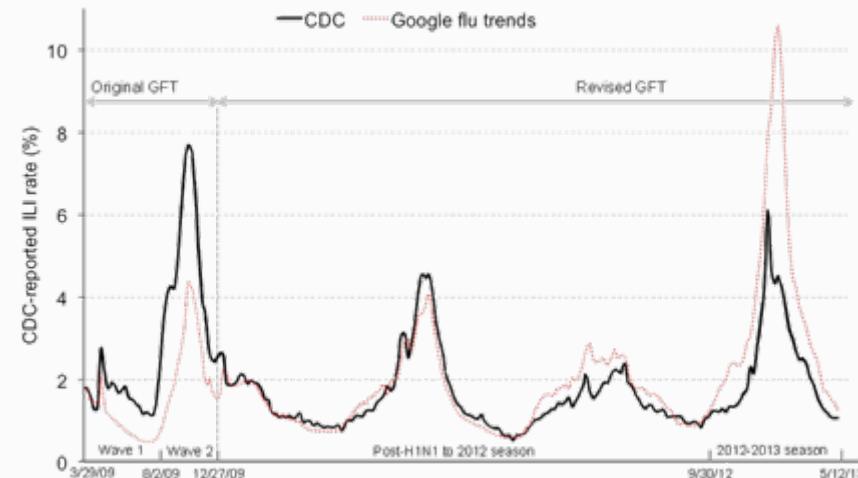
► Summary

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Ginsberg et al., 2012, *Nature*

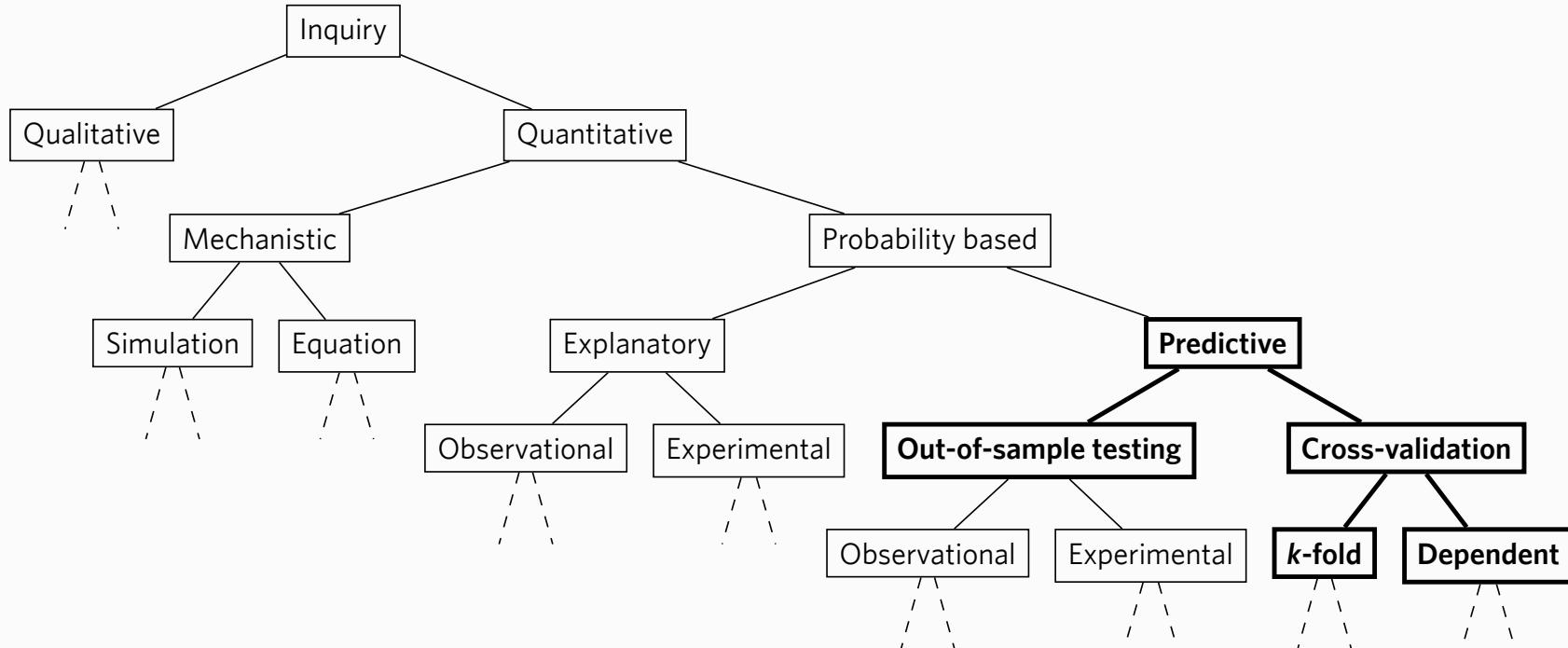
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Santillana et al., 2014, *Am. J. Prev. Med.*

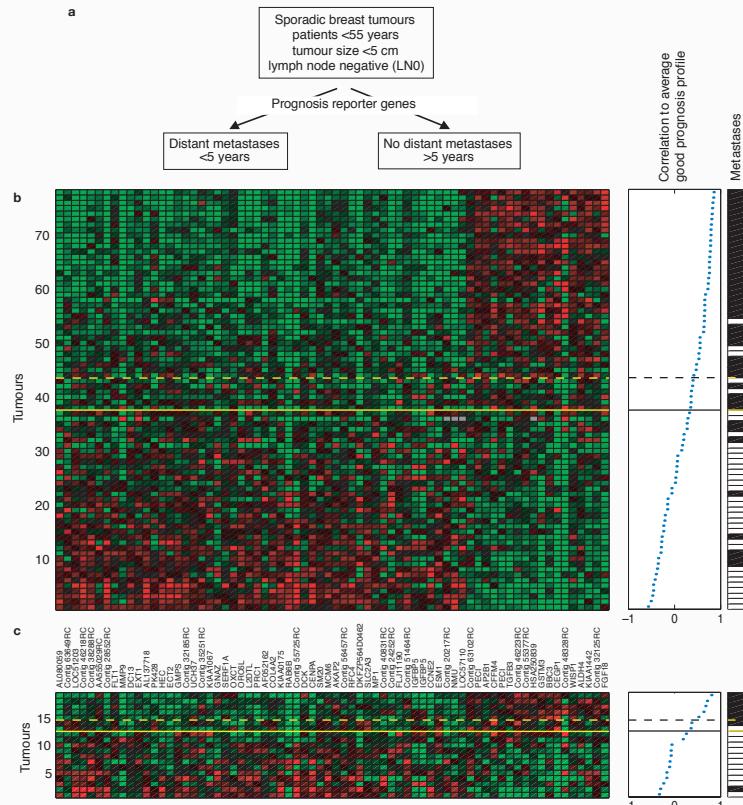
4. Cross-validation

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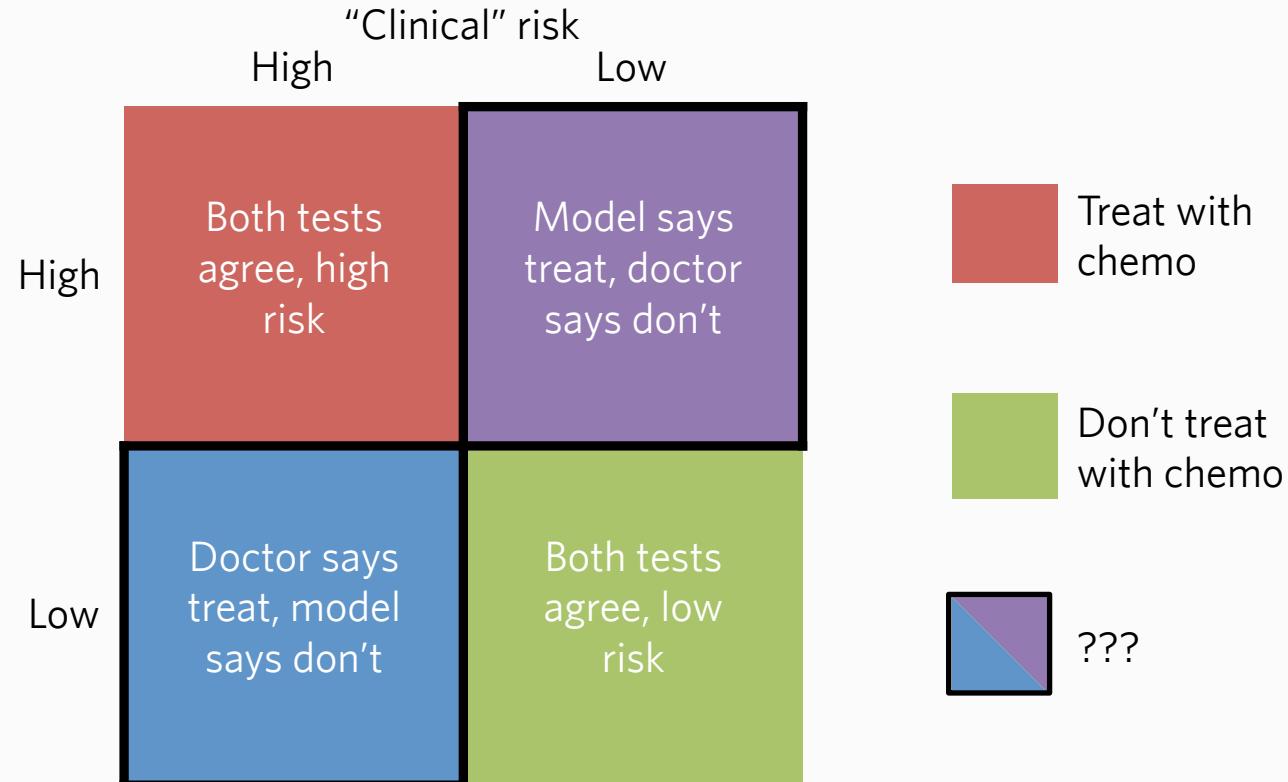
› Real-world testing of ML results



- › van't Veer et al. (2002) found 70 genes correlated with developing breast cancer
- › Of course the correlations were optimal, post-hoc. But did it generalize?

➤ Implementation testing

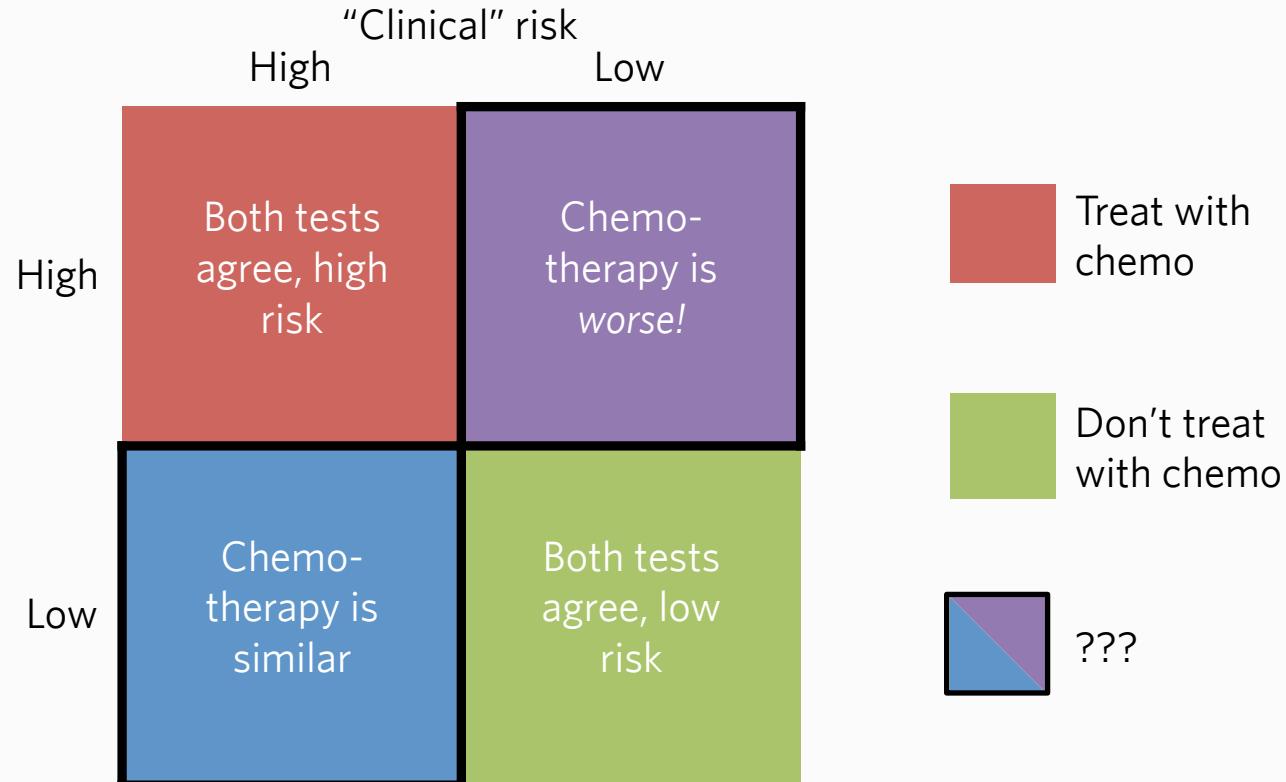
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Cardoso et al., 2016, NEJM

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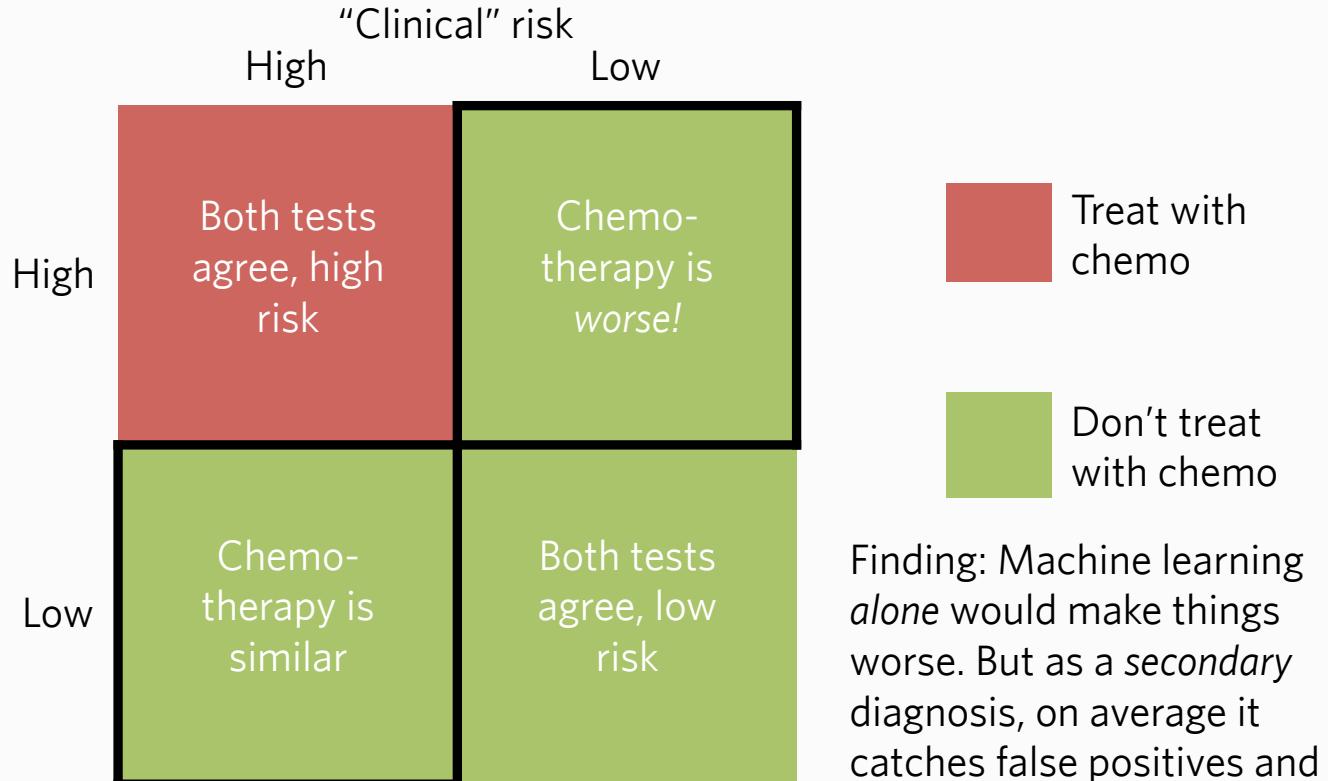


Cardoso et al., 2016, NEJM

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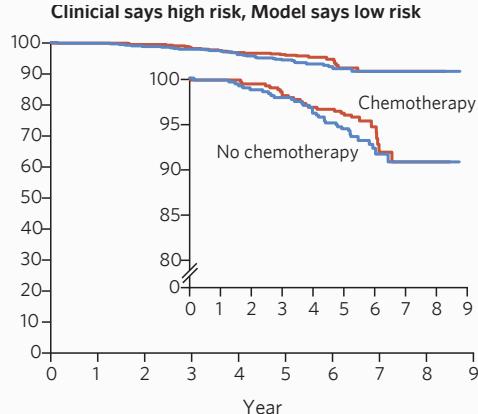
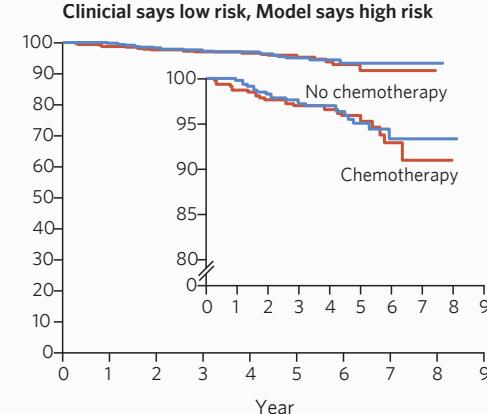
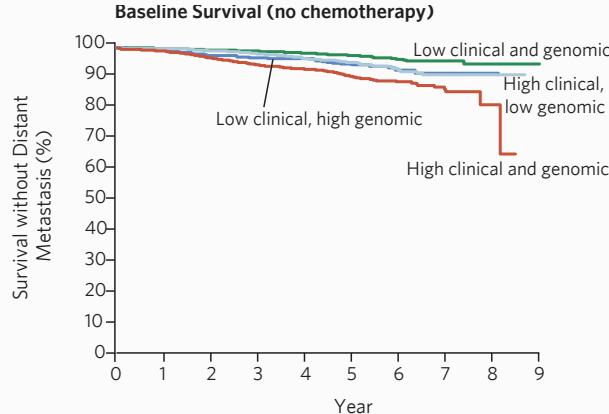
Risk via
correlations
with gene
expression



Cardoso et al., 2016, NEJM

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➤ Implementation testing: Details



➤ Before experiment (training data)

(Note: still limitations in how experimental subjects may be unrepresentative.)

➤ High model risk, low clinical risk: randomize.
Chemo worse!

➤ Low model risk, high clinical risk: chemo makes no difference

› Generalizability through CV

- › Non-experimentally, generalizability is shown *through cross validation*
- › CV can go wrong in known ways:
 - improper splitting
 - publication bias (Gayo-Avello, 2012)
 - overfitting to the test set (Dwork et al. 2015, Park 2012)
- › Not systematically acknowledged: *dependencies among observations*

► Classic argument for CV

Training:

$$\begin{aligned}\text{err}(\hat{\mu}) &= \frac{1}{n} \mathbb{E}_f \|Y - \hat{Y}\|_2^2 \\ &= \frac{1}{n} \left[\text{tr } \Sigma + \|\mu - \mathbb{E}(\hat{Y})\|_2^2 + \text{tr } \text{Var}_f(\hat{Y}) - 2 \text{tr } \text{Cov}_f(Y, \hat{Y}) \right]\end{aligned}$$

Testing:

$$\begin{aligned}\text{Err}(\hat{\mu}) &= \frac{1}{n} \mathbb{E}_f \|Y^* - \hat{Y}\|_2^2 \\ &= \frac{1}{n} \left[\text{tr } \Sigma + \|\mu - \mathbb{E}(\hat{Y})\|_2^2 + \text{tr } \text{Var}_f(\hat{Y}) - 2 \text{tr } \text{Cov}_f(Y^*, \hat{Y}) \right]\end{aligned}$$

The difference is the *optimism* (Efron, 2004; Rosset & Tibshirani, 2018):

$$\text{Opt}(\hat{\mu}) = \text{Err}(\hat{\mu}) - \text{err}(\hat{\mu}) = \frac{2}{n} \text{tr } \text{Cov}_f(Y, \hat{Y})$$

› Apply this to non-iid data

› Imagine we have, for $\Sigma_{ii} = \sigma^2$ and $\Sigma_{ij} = \rho\sigma^2$, $i \neq j$

$$\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{X} \\ \mathbf{X} \end{bmatrix} \beta, \begin{bmatrix} \Sigma & \rho\sigma^2 \mathbf{1} \mathbf{1}^T \\ \rho\sigma^2 \mathbf{1} \mathbf{1}^T & \Sigma \end{bmatrix} \right)$$

› Then, optimism in the training set is:

$$\frac{2}{n} \operatorname{tr} \operatorname{Cov}_f(Y_1, \hat{Y}_1) = \frac{2}{n} \operatorname{tr} \operatorname{Cov}_f(Y_1, \mathbf{H}Y_1) = \frac{2}{n} \operatorname{tr} \mathbf{H} \operatorname{Var}_f(Y_1) = \frac{2}{n} \operatorname{tr} \mathbf{H} \Sigma$$

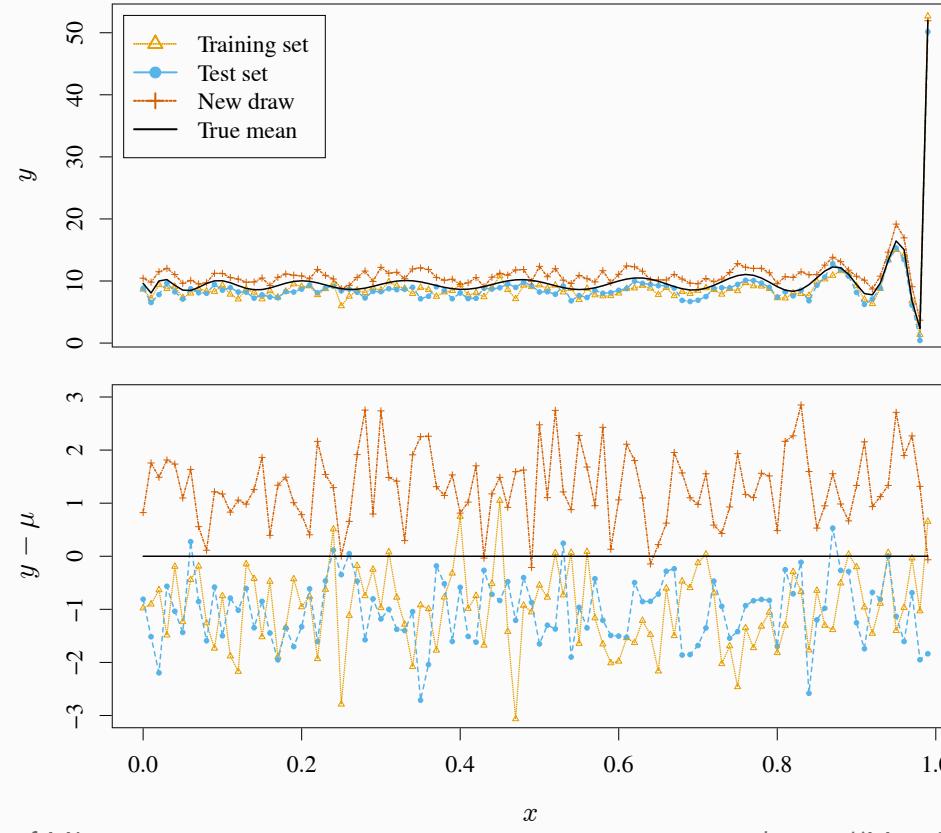
› But test set also has nonzero optimism!

$$\frac{2}{n} \operatorname{tr} \operatorname{Cov}_f(Y_2, \hat{Y}_1) = \frac{2}{n} \operatorname{tr} \operatorname{Cov}_f(Y_2, \mathbf{H}Y_1) = \frac{2\rho\sigma^2}{n} \operatorname{tr} \mathbf{H} \mathbf{1} \mathbf{1}^T = 2\rho\sigma^2$$

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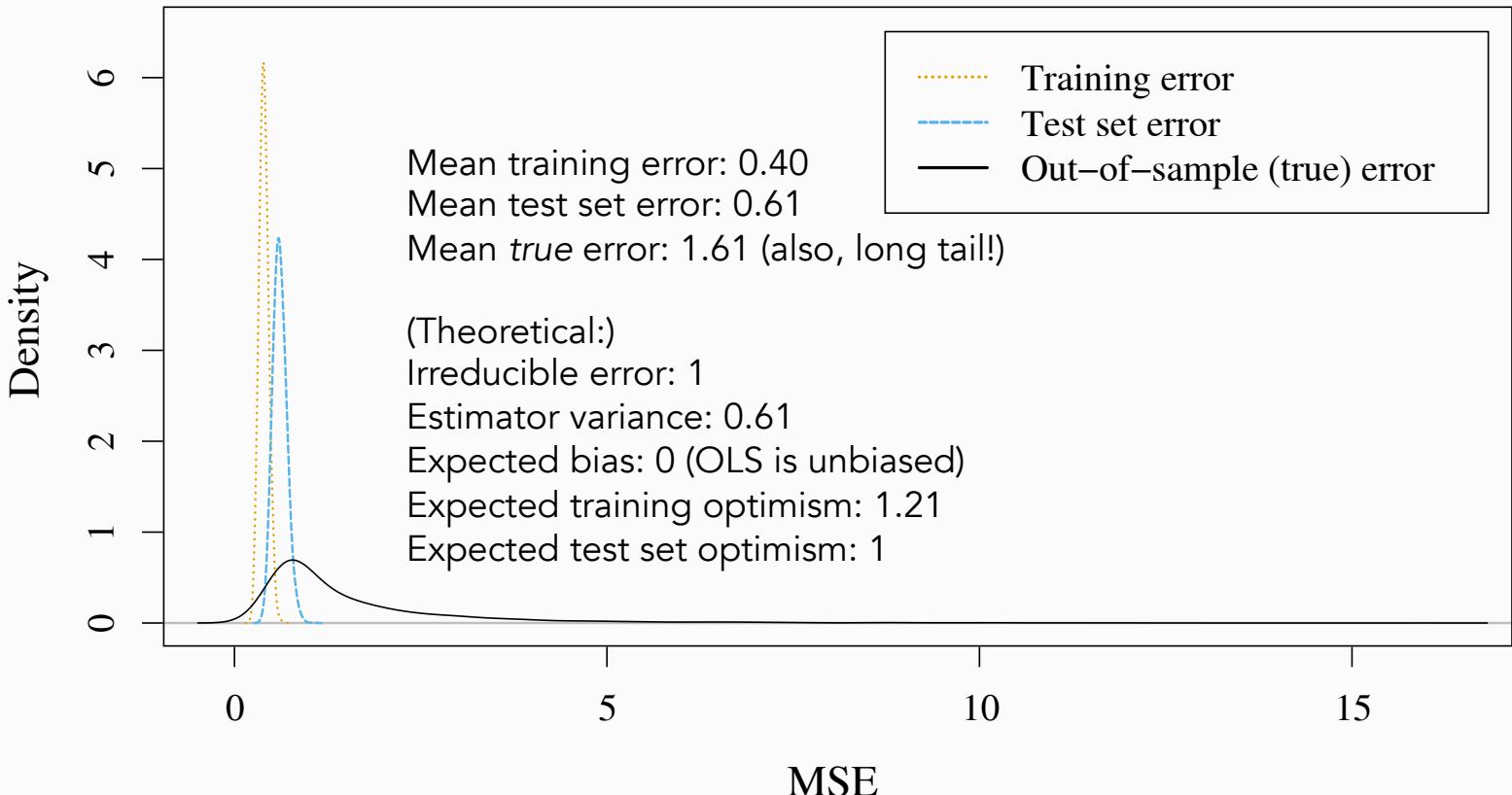
› One draw as an example

Correlation between observations can pull training and test observations close to one another, but potentially far from an independent draw



➤ Simulated MSE

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➤ Consequences

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- Non-experimental results are always preliminary
- Can try to split data around covariance (Bergmeir et al., 2018; Hammerla & Plötz, 2015)
 - But can't estimate both mean and the covariance structure, have to assume one (Opsomer et al., 2001)
 - For covariance, *no amount of data is ever enough!*

➤ Summary

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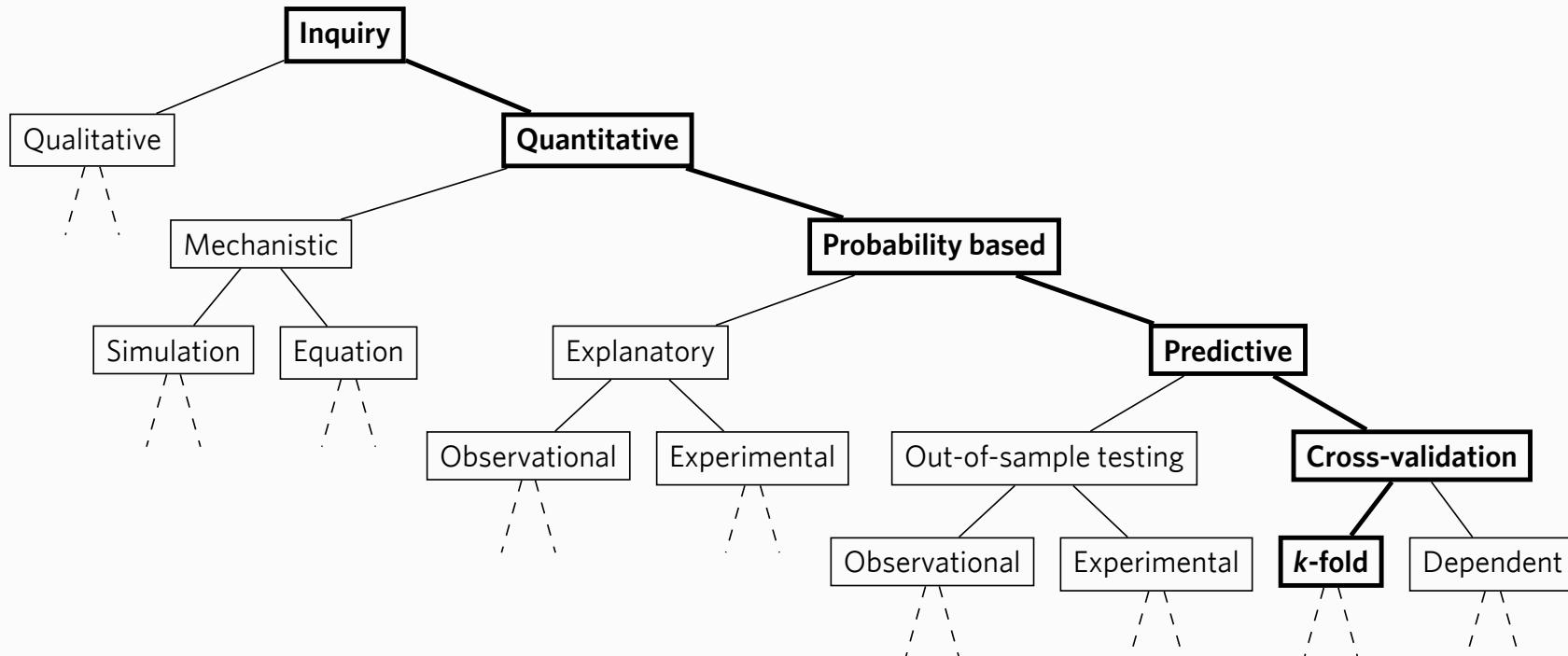
➤ References

- Quantification sacrifices multiplicity and depth of meaning, and is at the mercy of measurement processes that only imperfectly capture constructs
- Probability-based modeling requires multiple observations, and uses central tendencies which exclude outliers
- “Prediction” is based on correlation, which can sidestep responsibility, and are fragile to causation
- Cross-validation can fail if there are dependencies, or other problems

▶ Thank you!

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➤ Backup slides

➤ “True” models predict worse

- A linear data-generating process.

$$\mathbf{y} \sim \mathcal{N}(\beta_p \mathbf{X}_p + \beta_q \mathbf{X}_q, \sigma^2 \mathbf{I})$$

- Wu et al. (2007): Fitting only \mathbf{X}_p has lower expected MSE than fitting the model that generated the data when:

$$\beta_q^T \mathbf{X}_q^T (\mathbf{I}_n - \mathbf{H}_p) \mathbf{X}_q \beta_q < q\sigma^2$$

➤ Proposal: Precise language

- ~~Predict the likelihood~~: Calculate the likelihood
- ~~Predict the risk, predict the probability~~: Estimate the risk, estimate the probability
- ~~Prediction, predicted~~: Fitted value, fitted
- ~~We predict~~: We detect, we classify, we model
- ~~X predicts Y~~: X is correlated with Y
- ~~X predicts Y, ceteris paribus~~ (partial correlation): X is associated with Y

➤ Proposal: Alternative language

- Retrodiction
- Backtesting (retrodiction for testing)
- Hindcasting (backtesting for forecasting)
- In-sample vs. ➤ Out of-sample
- Interpolation vs. ➤ Extrapolation
- Diagnosis vs. ➤ Prognosis
- Retrospective vs. ➤ Prospective

➤ But language not enough

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Pseudo-Mathematics and Financial Charlatanism: The Effects of Backtest Overfitting on Out-of-Sample Performance

*David H. Bailey, Jonathan M. Borwein,
Marcos López de Prado, and Qiji Jim Zhu*

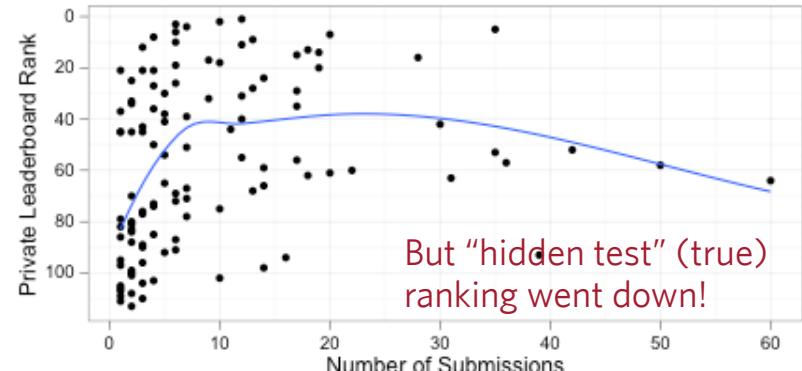
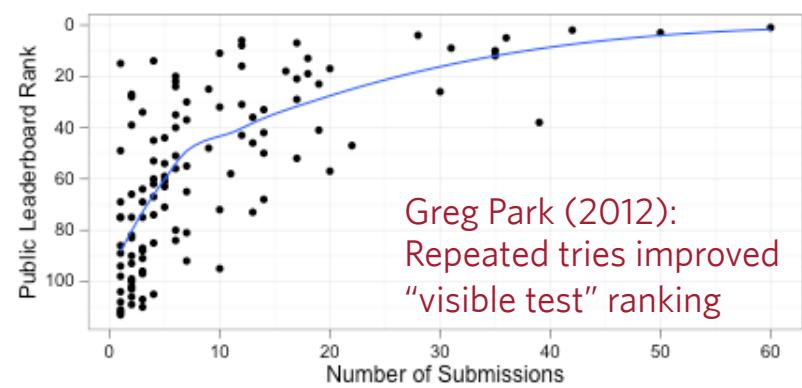
(I.e., using “backtest” in place of “predict” has not prevented financial analysts from unwitting overfitting)

Another thing I must point out is that you cannot prove a vague theory wrong. [...] Also, if the process of computing the consequences is indefinite, then with a little skill any experimental result can be made to look like the expected consequences

“training set” in the machine-learning literature). The OOS performance is simulated over a sample not used in the design of the strategy (a.k.a. “testing set”). A backtest is *realistic* when the IS performance

› Overfitting on the test set

- › Re-using a test set can overfit to the test set!
(Dwork et al., 2015)
- › Happens in Kaggle, which has public leaderboard (visible throughout) and private leaderboard (revealed only at end of competition)



> Matrix bias-variance decomposition

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$$\begin{aligned}
 \text{err}(\hat{\mu}) &= \frac{1}{n} \mathbb{E}_f \|Y - \hat{Y}\|_2^2 \\
 &= \frac{1}{n} \left[\mathbb{E}_f \|Y\|_2^2 + \mathbb{E}_f \|\hat{Y}\|_2^2 - 2 \mathbb{E}_f (Y^T \hat{Y}) \right] \\
 &= \frac{1}{n} \left[\mathbb{E}_f \|Y\|_2^2 + \mathbb{E}_f \|\hat{Y}\|_2^2 - 2 \text{tr} \mathbb{E}_f (Y \hat{Y}^T) \right] \\
 &\quad + \frac{1}{n} \left[\mu^T \mu + \mathbb{E}_f (\hat{Y})^T \mathbb{E}_f (\hat{Y}) + 2 \text{tr} \mu \mathbb{E}_f (\hat{Y})^T \right] \\
 &\quad + \frac{1}{n} \left[-\mu^T \mu - \mathbb{E}_f (\hat{Y}) \mathbb{E}_f (\hat{Y})^T - 2 \mu^T \mathbb{E}_f (\hat{Y}) \right] \\
 &= \frac{1}{n} \left[\text{tr} \Sigma + \|\mu - \mathbb{E}(\hat{Y})\|_2^2 + \text{tr} \text{Var}_f(\hat{Y}) \right] \quad \text{--- 2 tr Cov}_f(Y, \hat{Y})
 \end{aligned}$$

› Critical technical practice (1)

- › Agre (1997) describes “mov[ing] intellectually from AI to the social sciences — that is, to stop thinking the way that AI people think, and to start thinking the way that social scientists think...”
- › **“Criticisms of [AI], no matter how sophisticated and scholarly they might be, are certain to be met with the assertion that the author simply fails to understand a basic point... even though I was convinced that the field was misguided and stuck, it took tremendous effort and good fortune to understand how and why... I spent several years attempting to reform the field by providing it with the critical methods it needed — a critical technical practice.”**

› Critical technical practice (2)

- › “As an AI practitioner already well immersed in the literature, I had incorporated the field's taste for technical formalization so thoroughly into my own cognitive style that I literally could not read the literatures of nontechnical fields at anything beyond a popular level. The problem was not exactly that I could not understand the vocabulary, but that **I insisted on trying to read everything as a narration of the workings of a mechanism.**”
- › “At first I found [nontechnical] texts impenetrable, not only because of their irreducible difficulty but also because I was still tacitly attempting to read everything as a specification for a technical mechanism... My first intellectual breakthrough came when, for reasons I do not recall, **it finally occurred to me to stop translating these strange disciplinary languages into technical schemata, and instead simply to learn them on their own terms.**”

➤ Critical technical practice (3)

- “I still remember the **vertigo** I felt during this period; I was speaking these strange disciplinary languages, in a wobbly fashion at first, without knowing what they meant -- without knowing what sort of meaning they had.”
- “in retrospect this was the period during which **I began to ‘wake up’, breaking out of a technical cognitive style that I now regard as extremely constricting.”**

› Critical technical practice (4)

- › “Without the idea that ideologies and social structures can be reproduced through a myriad of unconscious mechanisms such as linguistic forms and bodily habits, all critical analysis may seem like accusations of conscious malfeasance. **Even sociological descriptions that seem perfectly neutral to their authors can seem like personal insults to their subjects if they presuppose forms of social order that exist below the level of conscious strategy and choice.”**