Discussion of “A hierarchy of limitations in machine learning”

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Update: reproducibility in ML out!

SCIENCE ADVANCES | REVIEW

RESEARCH METHODS

REFORMS: Consensus-based Recommendations for Machine-learning-based Science

Sayash Kapoor[1,2]*, Emily M. Cantrell[3,4], Kenny Peng[5], Thanh Hien Pham[1,2], Christopher A. Bail[6,7,8], Odd Erik Gundersen[9,10], Jake M. Hofman[11], Jessica Hullman[12], Michael A. Lones[13], Momin M. Malik[14,15,16], Priyanka Nanayakkara[12,17], Russell A. Poldrack[18], Inioluwa Deborah Raji[19], Michael Roberts[20,21], Matthew J. Salganik[2,3,22], Marta Serra-Garcia[23], Brandon M. Stewart[2,3,22,24], Gilles Vandewiele[25], Arvind Narayanan[1,2]

Machine learning (ML) methods are proliferating in scientific research. However, the adoption of these methods has been accompanied by failures of validity, reproducibility, and generalizability. These failures can hinder scientific progress, lead to false consensus around invalid claims, and undermine the credibility of ML-based science. ML methods are often applied and fail in similar ways across disciplines. Motivated by this observation, our goal is to provide clear recommendations for conducting and reporting ML-based science. Drawing from an extensive review of past literature, we present the REFORMS checklist (recommendations for machine-learning-based science). It consists of 32 questions and a paired set of guidelines. REFORMS was developed on the basis of a consensus of 19 researchers across computer science, data science, mathematics, social sciences, and biomedical sciences. REFORMS can serve as a resource for researchers when designing and implementing a study, for referees when reviewing

The effect of dependencies in machine learning

Summary

- Machine learning generally ignores dependencies between observations (assumes iid)
- This is usually justified for model *fitting*; and the major impact of dependencies is on *inference*.
- The problem is in our ability to estimate model *performance*; we think we are doing better than we actually are

Without (conditionally) iid, nonparametric models are unidentifiable

"A number of problems, some quite fundamental, occur when nonparametric regression is attempted in the presence of correlated errors. Indeed, **in the most general setting where no parametric shape is assumed for the mean nor the correlation function, the model is essentially unidentifiable**, so that it is theoretically impossible to estimate either function separately." (Opsomer et al. 2001)

Estimator properties of estimates of model performance

- "Metaprediction—the prediction about predictions—is… an integral component of the predictive enterprise itself… Indeed, to characterize someone as a reliable predictor… is in effect to predict on one's own account that this agent's predictions will generally come true—and is thereby to make a metaprediction of sorts." (Rescher 1998)
- Metaprediction to at least third order is worthwhile
- First-order prediction: the prediction itself, $\hat{y}$
- Second-order prediction: $\mathbb{E}(\hat{y})$, estimate via CV
- Third-order prediction: $\mathbb{E}(\hat{\mathbb{E}}(\hat{y}))$, look at properties of CV

Inference (in statistics): If uncertainty of an estimator is less than the “signal”

Random variable, X

Mean, $\mathbb{E}(X) = \mu$

Standard deviation, $\sqrt{\mathbb{V}(X)} = \sigma$

Estimator, $\widehat{\mu}$

Estimator, $\widehat{\sigma}$

Expected value, $\mathbb{E}(\widehat{\mu})$

$\boxed{\text{Standard error, } \sqrt{\mathbb{V}(\widehat{\mu})}}$

Standard error, $\sqrt{\mathbb{V}(\widehat{\sigma})}$

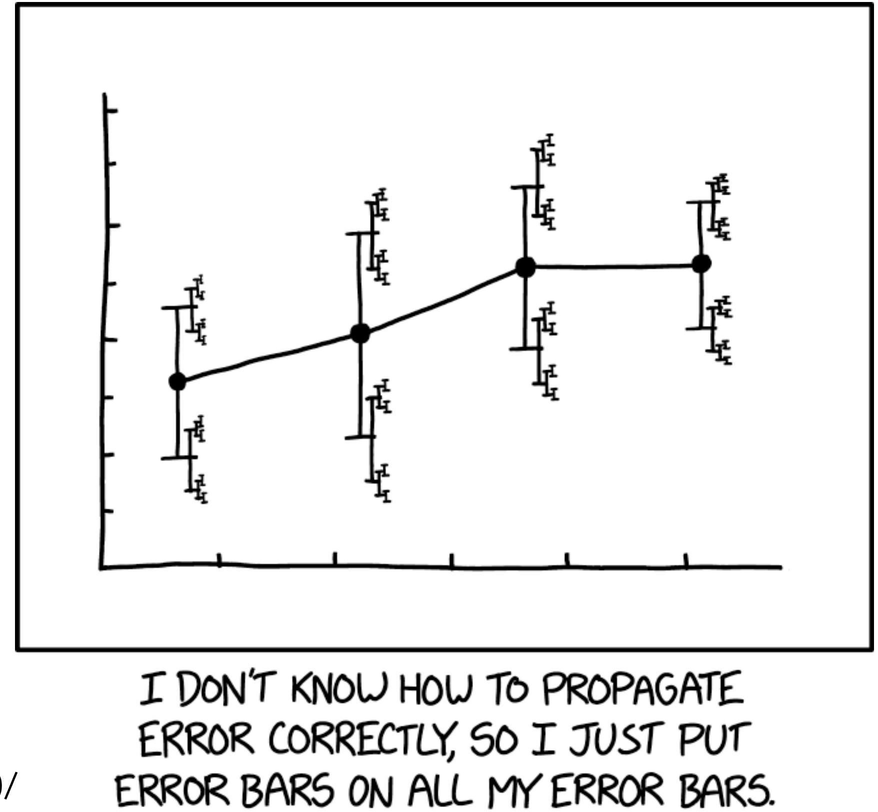
Expected value, $\mathbb{E}(\widehat{\sigma})$

The *variance* of the *estimator* of the *mean* gives us the uncertainty of the estimate, and is given the special name of the *standard error*. If the uncertainty is small enough, we say we have made an *inference* to the underlying data-generating process.

Going on *ad infinitum*…

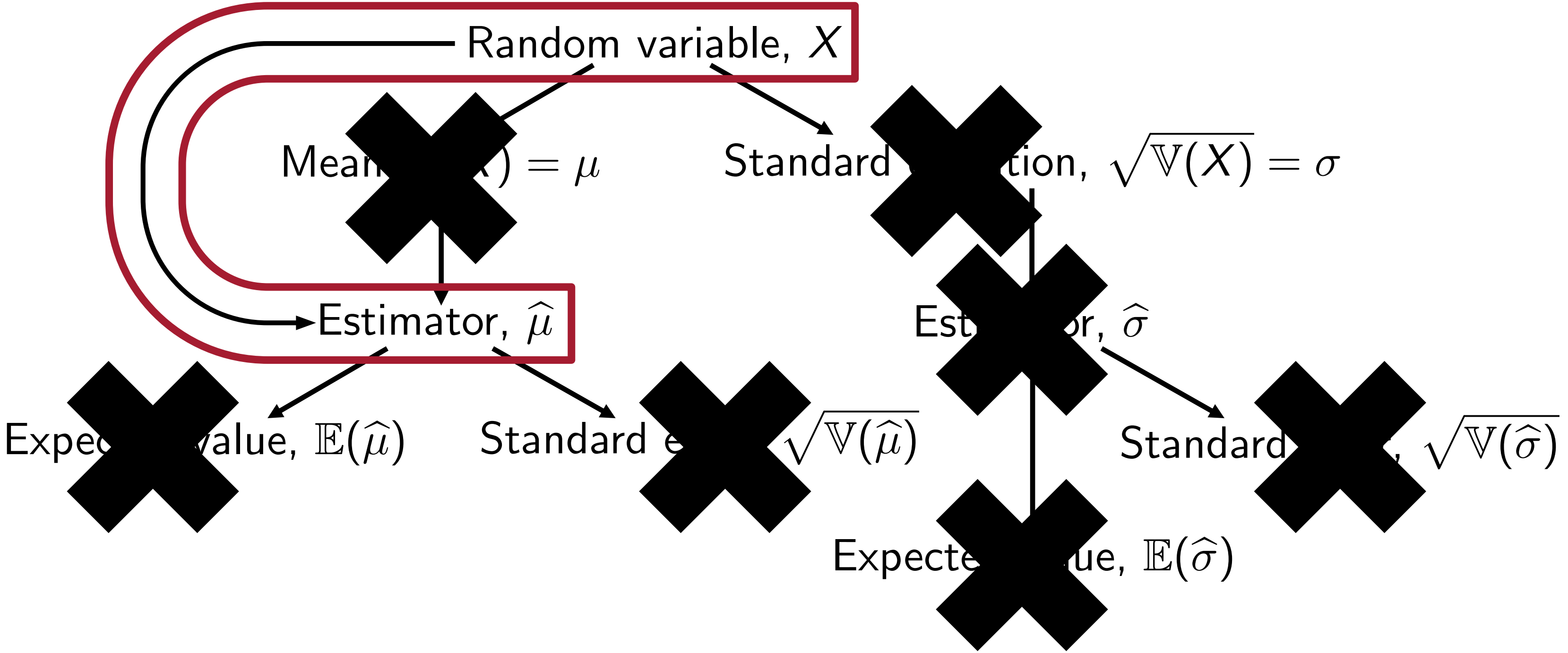
- Random variable, X
  - Mean, $\mathbb{E}(X) = \mu$
    - Estimator, $\widehat{\mu}$
      - Expected value, $\mathbb{E}(\widehat{\mu})$
      - Standard error, $\sqrt{\mathbb{V}(\widehat{\mu})}$
  - Standard deviation, $\sqrt{\mathbb{V}(X)} = \sigma$
    - Estimator, $\widehat{\sigma}$
      - Expected value, $\mathbb{E}(\widehat{\sigma})$
      - Standard error, $\sqrt{\mathbb{V}(\widehat{\sigma})}$

Going on *ad infinitum*…



https://xkcd.com/2110/

Machine learning: Instrumentalist



ML skips over the entire machinery of inference, creating estimators only to recover some aspect of held-out data. (*Statistical machine learning* brings theory back in, but for the purpose of seeing what best predicts, not what recovers information.) Part of what we argue in "REFORMS": must bring back in examination of properties of estimators of estimators (like held-out data)

Matrix bias-variance decomposition

$$
\begin{aligned}
\mathrm{err}(\hat{\mu}) &= \frac{1}{n}\mathbb{E}_f \| Y - \widehat{Y} \|_2^2 \\
&= \frac{1}{n}\left[\mathbb{E}_f \| Y \|_2^2 + \mathbb{E}_f \| \widehat{Y} \|_2^2 - 2\mathbb{E}_f (Y^T \widehat{Y})\right] \\
&= \frac{1}{n}\left[\mathbb{E}_f \| Y \|_2^2 + \mathbb{E}_f \| \widehat{Y} \|_2^2 - 2\,\mathrm{tr}\,\mathbb{E}_f (Y \widehat{Y}^T)\right] \\
&\quad + \frac{1}{n}\left[\ \mu^T\mu + \mathbb{E}_f(\widehat{Y})^T\mathbb{E}_f(\widehat{Y}) + 2\,\mathrm{tr}\,\mu\mathbb{E}_f(\widehat{Y})^T\right] \\
&\quad + \frac{1}{n}\left[-\mu^T\mu - \mathbb{E}_f(\widehat{Y})\mathbb{E}_f(\widehat{Y})^T - 2\mu^T\mathbb{E}_f(\widehat{Y})\right] \\
&= \frac{1}{n}\left[\underbrace{\mathrm{tr}\,\Sigma}_{\text{irreducible ("Bayes") error}} + \underbrace{\|\mu - \mathbb{E}(\widehat{Y})\|_2^2}_{\text{bias squared}} + \underbrace{\mathrm{tr}\,\mathrm{Var}_f(\widehat{Y})}_{\text{variance of the estimator}} - \underbrace{2\,\mathrm{tr}\,\mathrm{Cov}_f(Y, \widehat{Y})}_{\text{"optimism"}}\right]
\end{aligned}
$$

Classic argument for CV

Training:

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

Testing:

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

The difference is the *optimism* (Efron 2004; Rosset and Tibshirani 2020):

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

Apply this to non-iid data

- Imagine we have, for $\mathbf{\Sigma}_{ii} = \sigma^2$ and $\mathbf{\Sigma}_{ij} = \rho\sigma^2, \quad i \neq j$

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

- Then, optimism in the training set is:

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

- But test set also has nonzero optimism!

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

One draw as an example

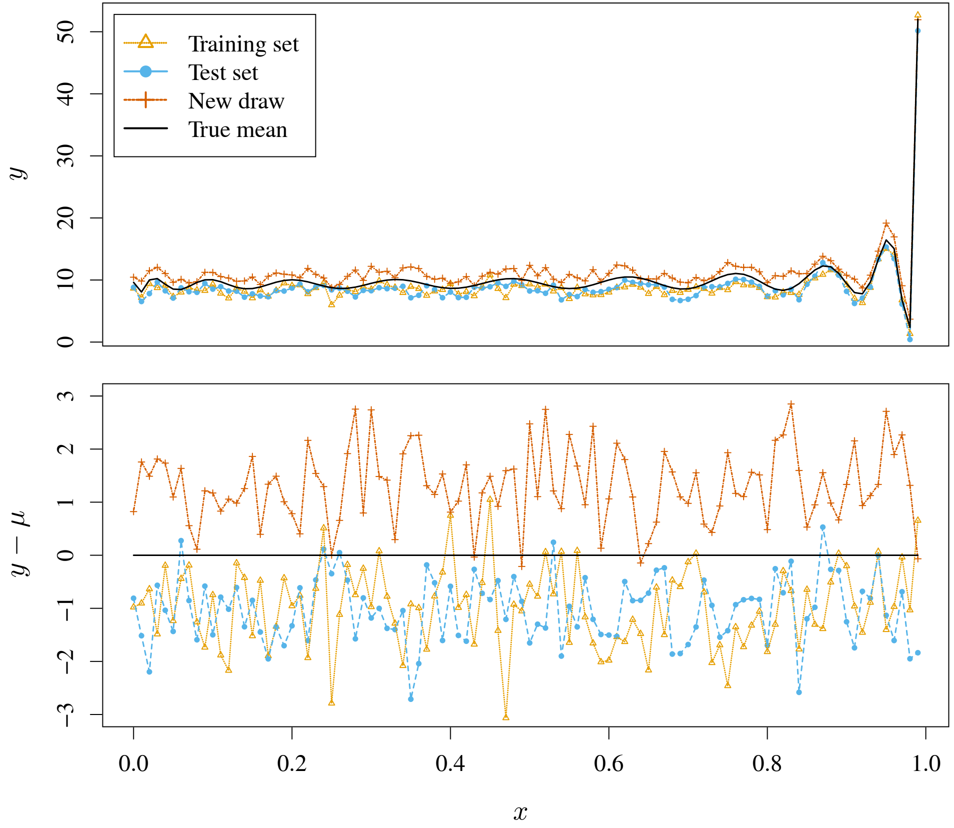
Paper out!

The effect of dependencies on machine learning

Other concerns

References

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



Simulated MSE

Paper out!

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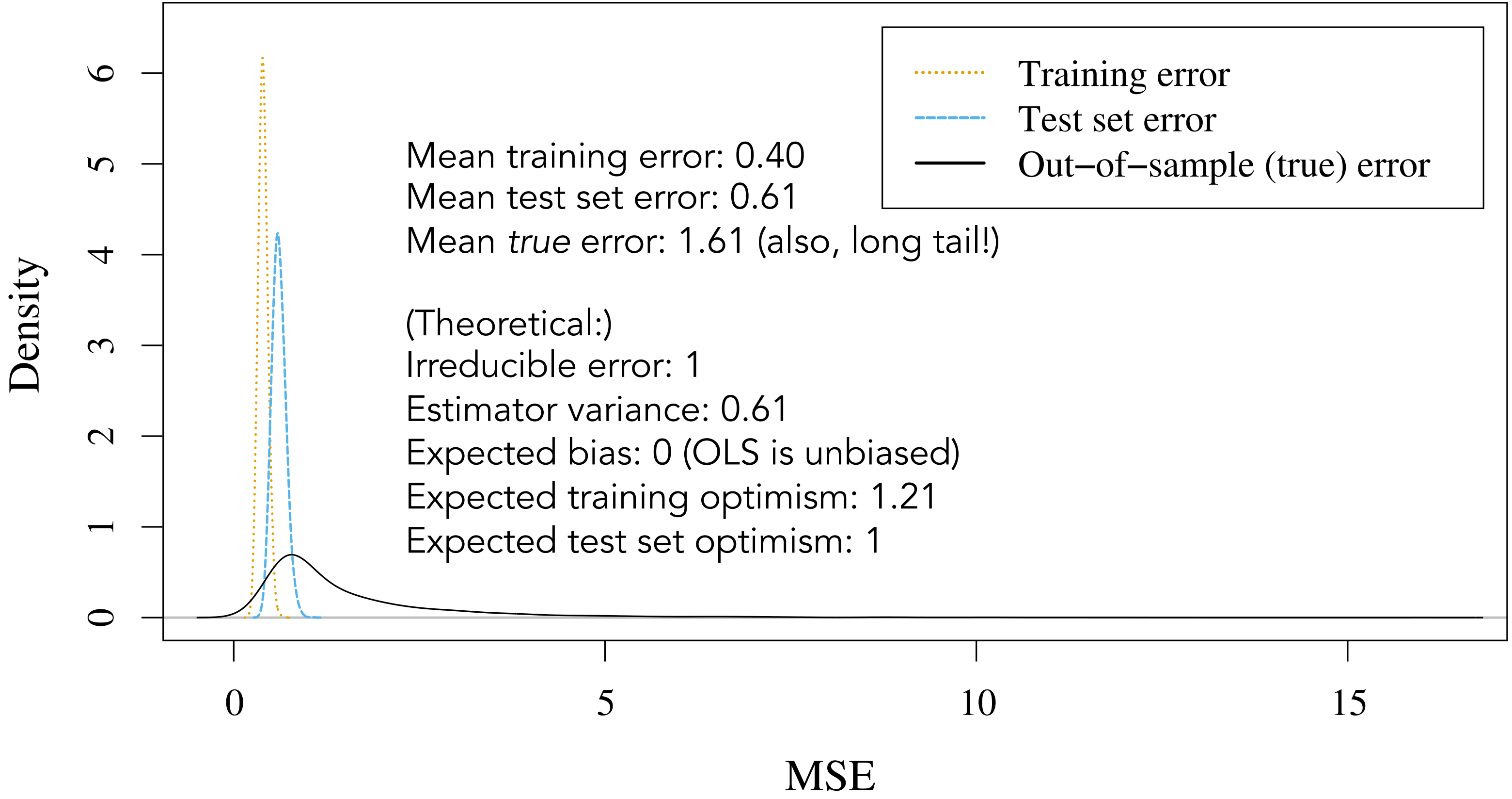
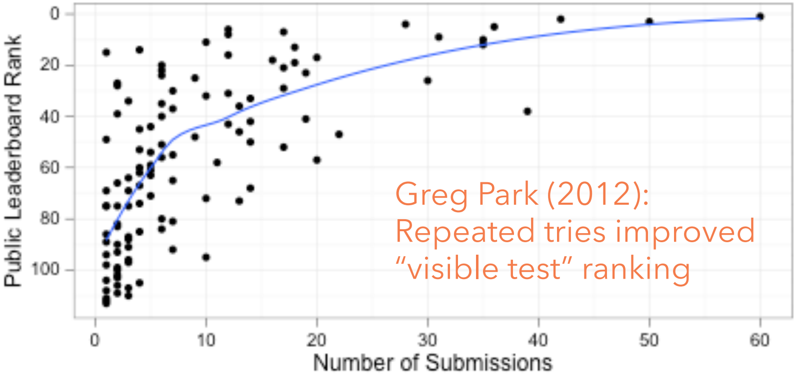
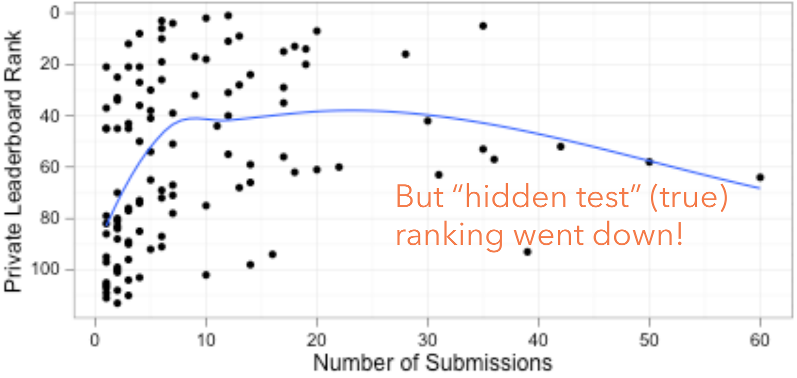


Dependencies and CV: examples

- Highly-cited "Twitter mood predicts the stock market" trains on future values, tests on past values: that is "time-traveling"! (see critique by Lachanski and Pav 2017)
- A colleague of mine trained a model to recognize birds on his windowsill in webcam images, splitting frames randomly…
- Park (2012) has a great example of overfitting to the test set in Kaggle. Having a "private leaderboard" helps catch overfitting in Kaggle (see also Dwork et al. 2015)
  - I agree with Wagstaff (2012) that in research, it's probably not worth having a test set we only use once (do we give up if performance is bad?). But we *should* temper our claims, and do out-of-sample testing





Applying to networks

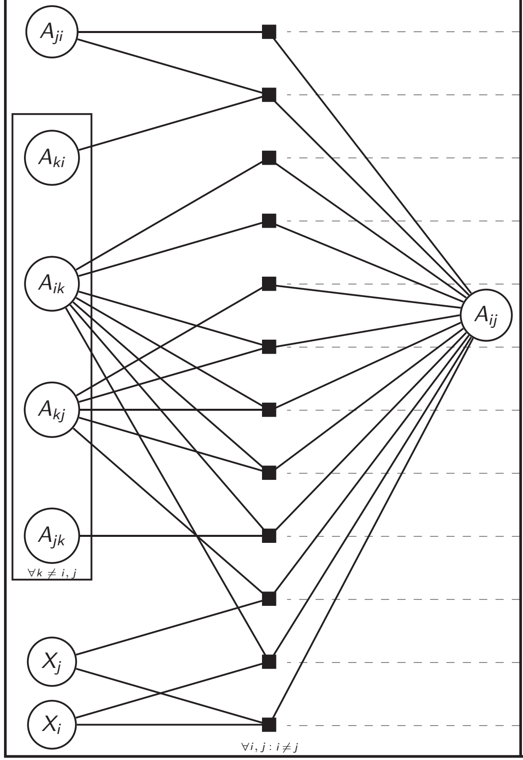
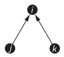
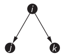
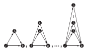
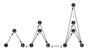
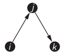
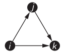
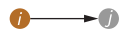
- This formulation would apply to a network autocorrelation model, where network is nuisance parameter
- But what if we are modeling the *edges*, which represent dependencies between observations?

Modeling the *edges*

	Y	X_1	X_2	$\cdots$	X_d
1	y_1	x_{11}	x_{12}	$\cdots$	x_{1d}
2	y_2	x_{21}	x_{22}	$\cdots$	x_{2d}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
n	y_n	x_{n1}	x_{n2}	$\cdots$	x_{nd}

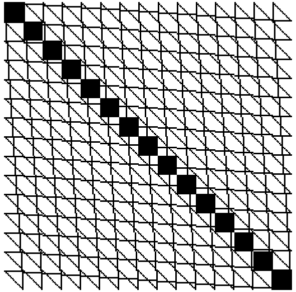
index	*from*	*to*	Y	W_1	W_2	W_3	$\cdots$
e_1	1	2	y_{12}	$\mathbf{1}(x_{11} = x_{21})$	$x_{12} - x_{22}$	x_{13}	$\cdots$
e_2	2	3	y_{23}	$\mathbf{1}(x_{11} = x_{31})$	$x_{12} - x_{32}$	x_{13}	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
e_{n+1}	2	1	y_{21}	$\mathbf{1}(x_{21} = x_{11})$	$x_{22} - x_{12}$	x_{23}	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$e_{2\binom{n}{2}}$	$n-1$	n	$y_{(n-1)n}$	$\mathbf{1}(x_{(n-1)1} = x_{n1})$	$x_{(n-1)2} - x_{n2}$	$x_{(n-1)3}$	$\cdots$

But dyads are dependent too!

Factor graph	Parameter name	Network Motif	Parameterization	Matrix notation
	mutual dyads		$\sum_{i<j} A_{ij} A_{ji}$	$\frac{1}{2}\,\mathrm{tr}\left(\mathbf{AA}^T\right)$
	in-two-stars		$\sum_{(i,j,k)} A_{ji} A_{ki}$	$\mathrm{sum}\left(\mathbf{AA}^T\right) - \mathrm{tr}\left(\mathbf{AA}^T\right)$
	out-two-stars		$\sum_{(i,j,k)} A_{ij} A_{ik}$	$\mathrm{sum}\left(\mathbf{A}^T\mathbf{A}\right) - \mathrm{tr}\left(\mathbf{A}^T\mathbf{A}\right)$
	geom. weighted out-degrees	—	$\sum_i \exp\left\{-\alpha \sum_k A_{ik}\right\}$	$\mathrm{sum}\left(\exp\{-\alpha\ \mathrm{rowsum}\left(\mathbf{A}\right)\}\right)$
	geom. weighted in-degrees	—	$\sum_j \exp\left\{-\alpha \sum_k A_{kj}\right\}$	$\mathrm{sum}\left(\exp\{-\alpha\ \mathrm{colsum}\left(\mathbf{A}\right)\}\right)$
	alternating transitive k-triplets		$\lambda \sum_{i,j} A_{ij} \left\{1-\left(1-\frac{1}{\lambda}\right)^{\sum_{k\neq i,j} A_{ik}A_{kj}}\right\}$	$\lambda\ \mathrm{sum}\left(\mathbf{A}\odot\left(1-\left(1-\frac{1}{\lambda}\right)^{\mathbf{AA}-\mathrm{diag}(\mathbf{AA})}\right)\right)$
	alternating indep. two-paths		$\lambda \sum_{i,j} \left\{1-\left(1-\frac{1}{\lambda}\right)^{\sum_{k\neq i,j} A_{ik}A_{kj}}\right\}$	$\lambda\ \mathrm{sum}\left(1-\left(1-\frac{1}{\lambda}\right)^{\mathbf{AA}-\mathrm{diag}(\mathbf{AA})}\right)$
	two-paths (mixed two-stars)		$\sum_{(i,k,j)} A_{ik} A_{kj}$	$\mathrm{sum}\left(\mathbf{AA}\right) - \mathrm{tr}\left(\mathbf{AA}\right)$
	transitive triads		$\sum_{(i,j,k)} A_{ij} A_{jk} A_{ik}$	$\mathrm{tr}\left(\mathbf{AAA}^T\right)$
	activity effect		$\sum_i X_i \sum_j A_{ij}$	$\mathrm{sum}\left(\mathbf{X}\odot\mathrm{rowsum}\left(\mathbf{A}\right)\right)$
	popularity effect		$\sum_j X_j \sum_i A_{ij}$	$\mathrm{sum}\left(\mathbf{X}\odot\mathrm{colsum}\left(\mathbf{A}\right)\right)$
	similarity effect		$\sum_{i,j} A_{ij}\left(1-\frac{\lvert X_i - X_j\rvert}{\max_{k,l}\lvert X_k - X_l\rvert}\right)$	$\mathrm{sum}\left(\mathbf{A}\odot\mathbf{S}\right)$

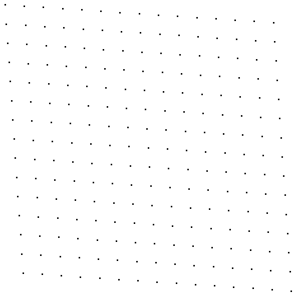
Graphical model and matrix notations for ERGM specification terms given in: Snijders et al. 2006. Joint work with Antonis Manousis and Naji Shajarisales, 2018.

Covariance structure of *edges* (*n* = 15)

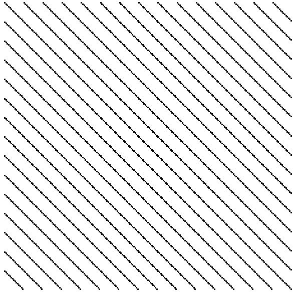


Total covariance between dyads

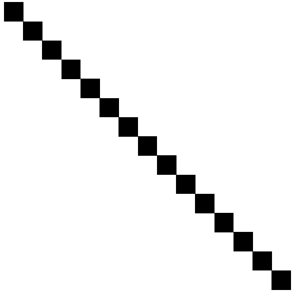
- The pairs of edges that are present together, or aren't present together
- Note: A theoretical construct, since we only see edges once (or once per time slice)



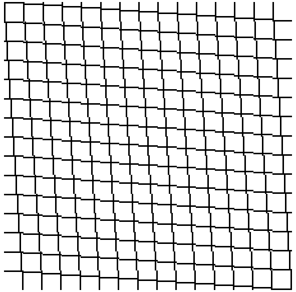
Mutual dyads



In-2-stars



Out-2-stars



2-paths

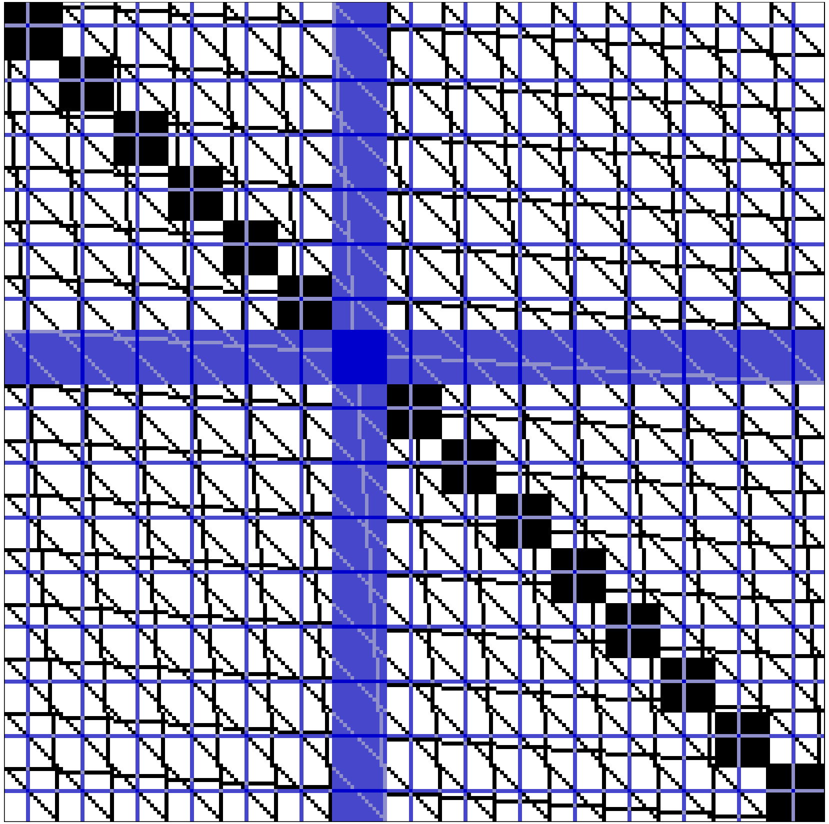
Paper out!

The effect of dependencies on machine learning

Other concerns

References

No data split would allow generalizable estimates



- Partition nodes into training and test sets?
  - Breaks up triads; omitted edges "share" information across training and test (diagram: blue are edges that include node 7)
- Partition dyads?
  - Breaks up nodes; even worse
- Can't *eliminate*, but can *minimize* optimism by careful data splitting

Other concerns

Quantification

Bias-variance tradeoff implies a “false” model can ‘predict’ better than the “true” model

Explanation (correlation) vs. prediction (causation)

Levels of prediction

“Prediction” and other language

Guarantees of what?

Quantification and “ways to understand a person” (see Kiviat 2023)

	As a case (quant)	In narrative (qual)
Context/circumstance	Stripped away	Key
Mental states	Absent (for the most part)	Crucial; constitutive
Relevant features	Determined in advance	Emergent
Orientation to time	Atemporal	Chronological
Ordering of features	Unimportant	Meaningful
Other actors	Invisible	Often present
Causal logic	Mathematical	Theoretical
Boost predictive validity	Add cases	Know person better

Slide from Barbara Kiviat, based on “Bowker and Star 2000; Bruner 1986; Desrosières 1998; Espeland 1998; Espeland and Stevens 1998, 2008; Fourcade and Healy 2017; Hacking 1990; Porter 1994, 1995; Ricouer 1998; White 1980, 1984”. I would add: Abbott 1988

Unbiased vs. minimizing loss: "True" model can "predict" worse!

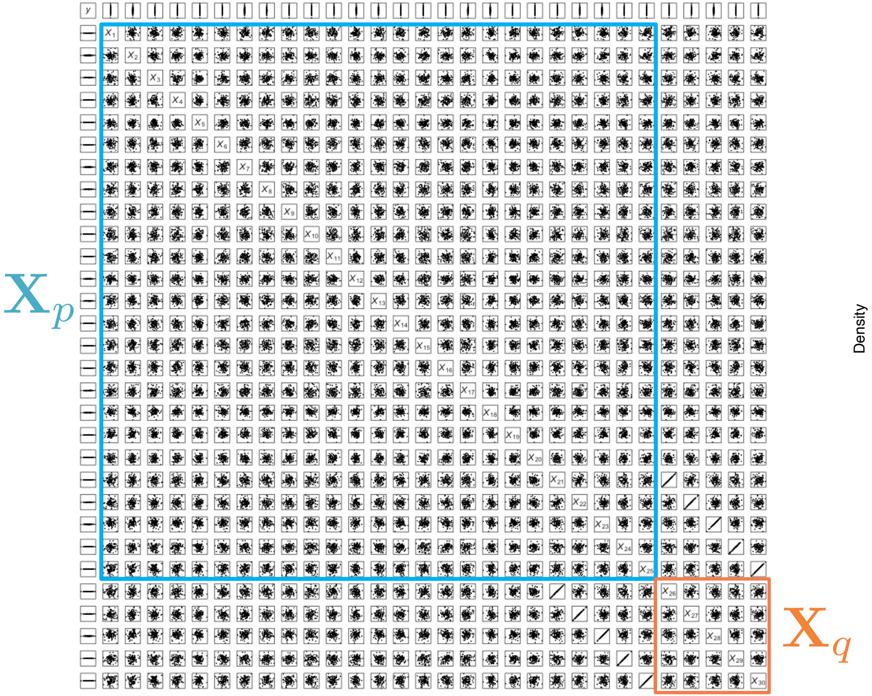
- A linear data-generating process.

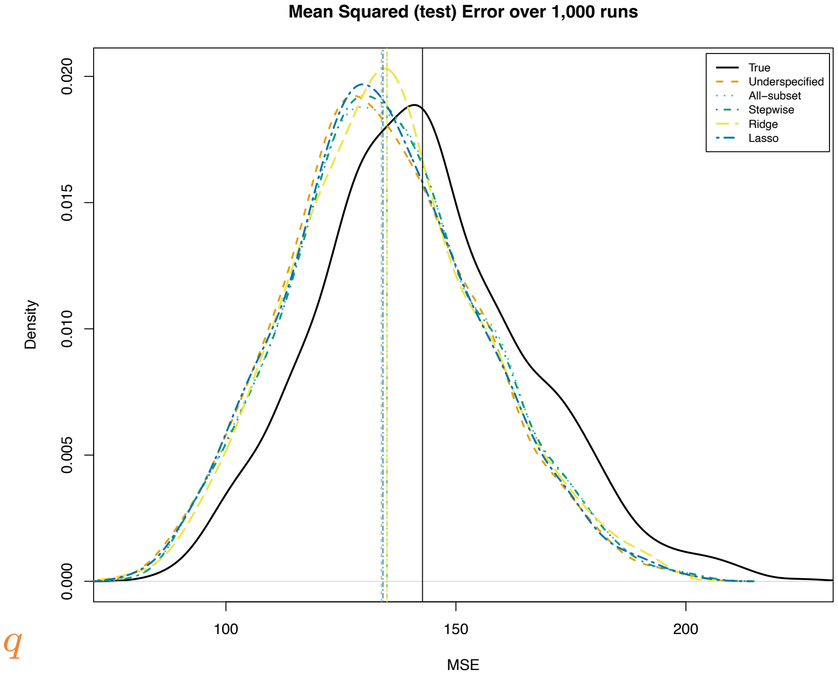
$$\mathbf{y} \sim \mathcal{N}\left(\beta_p \mathbf{X}_p + \beta_q \mathbf{X}_q, \sigma^2 \mathbf{I}\right)$$

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

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

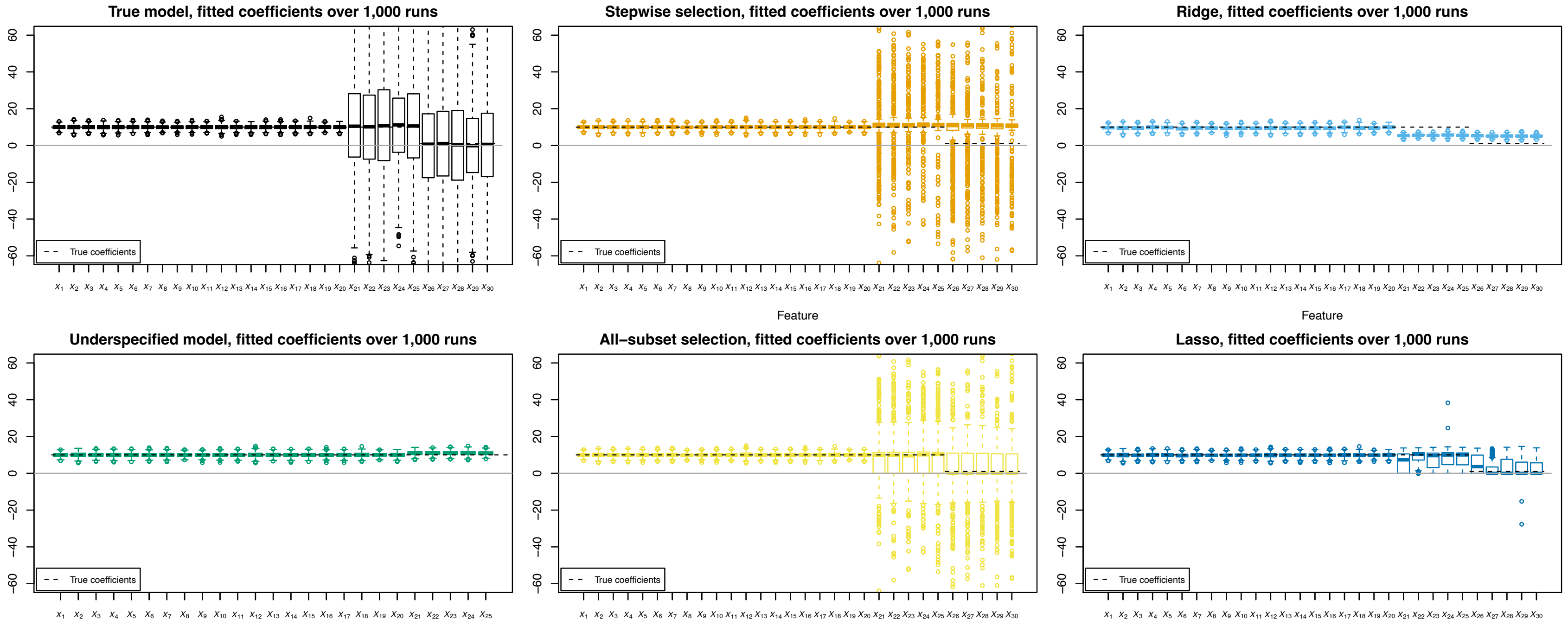
Simulation: 5 weak covariates, each highly correlated with a strong covariate



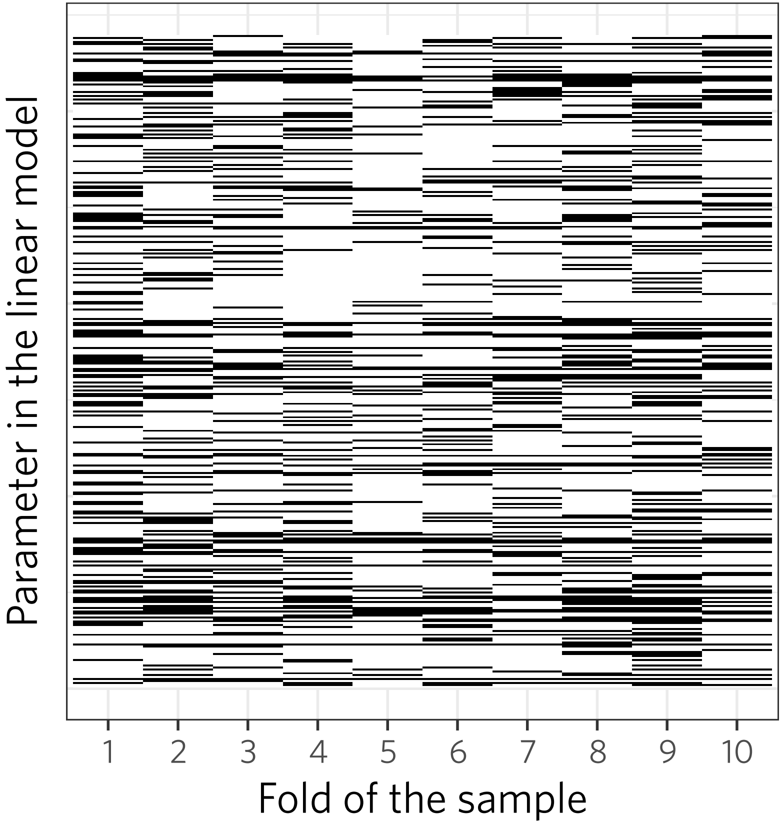


Simulation of Wu et al. (2007)

How the underspecified model, and regularized models, do better



Explanation (causation) vs. prediction (correlation)



- Very different sets of correlations can “predict” equally well (Mullainathan and Spiess 2017); Breiman (2001) called this the “Rashomon effect” and saw it as a point in favor of prediction over trying to get at causation
- But if we want to intervene, we need causation

Levels of prediction (Rescher 1998)

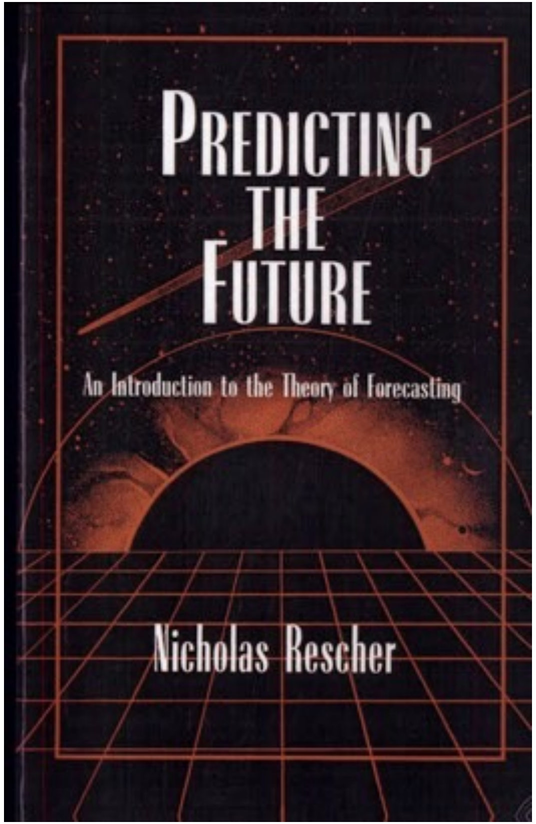


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TABLE 6.1: A SURVEY OF PREDICTIVE APPROACHES

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

“Prediction” and other language

- Communication: **stop saying “prediction” if it is really “correlation”**
  - **The use of ‘prediction’ leads to false, inflated expectations.** Instead of saying “prediction” for post-hoc demonstrations (Gayo-Avello 2012), use “retrodiction”: it is awkward, but that’s what we need. For time series: nowcasting, back-testing (although better language is not enough:
  - Partial correlation (i.e., for “ceteris paribus” interpretations) can be described with “association”
- “Prediction” is overused as it is
  - Statements like ”predict the probability of risk”, or “calculate the probability of a likelihood” exist and are redundant if not nonsensical (akin to, “a probability of a probability [of a probability]”).
    - Probabilities and risks are always latent (and indeed, are hypothetical and metaphysical), so how can we “predict” them? We should say that we *estimate* probabilities and risk (say *estimated probabilities*, etc.), and not overload on synonyms for probability
  - Use “detection” or “classification” if labels are manifest but unknown. E.g., we don’t “predict” race; “detecting” and “predicting” cancer imply two very different tasks; etc.
- **Models, not algorithms** (unless you really do mean an optimization algorithm). Why? Specificity: logistic regression is a *model*, IRLS is an algorithm. Random forests are a *model*, CART is an algorithm. And: we already know “all models are wrong” (Box 1979)

Guarantees of what?

- The Frequentist-Bayesian issues come back again
- To get information about the world, we want our models to give us $\mathbb{P}(H \mid \mathcal{D})$
- But we want to use methods with frequentist guarantees (e.g., a 95% credible interval, if repeated, will *not* necessarily contain the true value 95% of the time)
- There’s no way to get $\mathbb{P}(H \mid \mathcal{D})$ without a prior, and with priors, we don’t get frequency guarantees
- No frequency analysis is about the specific situation; it’s a property of the *procedure* (including what I did here)

Generalize to what?

- If by "generalizability," we mean that a fitted model will apply to very different contexts, probably very few ML models will generalize (at least for the social world)–or at least our theory gives us no guarantees that this will happen
- Our interest is in the quality of predictions that we can make *with a specific model*, but all our analysis refers to is if the ML *procedure* will generalize.
- Note that, despite many in ML claiming that it is Bayesian (e.g., Kevin Murphy's textbook), data splitting is a deeply frequentist procedure and so is mainstream ML overall

Paper out!

The effect of dependencies on machine learning

Other concerns

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