Revisiting the Two Cultures in Statistical Modeling and Inference: the Statistics Wars and Their Potential Casualties

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1. Introduction

Paradigm shifts in statistics during the 20th century

- 2. Karl Pearson's descriptive statistics (1894-1920s)
 - The original curve-fitting
- 3. Fisher's model-based statistical induction (1922)

Securing statistical adequacy and the trustworthiness of evidence

- 4. *Graphical Causal modeling (1990s)
 - Curve-fitting substantive models
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1 Introduction

Breiman (2001): "There are two cultures in the use of statistical modeling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown."

During the 20th century **statistical modeling and inference** experienced several **paradigm shifts**, the most notable being:

Karl Pearson's descriptive statistics (-1920s), Fisher's model-based statistics (1920s), Nonparametric statistics (1970s), Graphical Causal modeling (1990s), and Data Science (Machine Learning, Statistical Learning Theory, etc.) (1990s).

Key points argued in the discussion that follows

- The discussions on **non-replication** overlook a <u>key contributor</u> to **un-trustworthy evidence**, **statistical misspecification**: <u>invalid probabilistic</u> assumptions imposed (explicitly or implicitly) on one's data $\mathbf{x}_0 := (x_1, ..., x_n)$.
- There is a direct connection between Karl Pearson's <u>descriptive statistics</u>, Nonparametric statistics and the Data Science curve-fitting.

- All three approaches rely on (i) curve-fitting, (ii) goodness-of-fit/prediction measures, and (iii) asymptotic inference results (as $n \to \infty$) based on non-testable probabilistic/mathematical assumptions.
- The Curve-Fitting Curse: when empirical modeling relies on curve-fitting of mathematical functions with a sufficiently large number of parameters to fine-tune (e.g. neural networks, orthogonal polynomials), one will always find a 'best' model on goodness-of-fit/prediction grounds, even if that model is totally false. Worse, one will be oblivious to the fact that such a 'best' model will commonly yield untrustworthy evidence!
- 'Best' goodness-of-fit/prediction, i.e. 'small' residuals/prediction errors relative to a particular loss function, is neither necessary nor sufficient for trustworthy evidence! What ensures the latter is the statistical adequacy (approximate validity) of the the invoked statistical model $\mathcal{M}_{\theta}(\mathbf{x})$ comprising the probabilistic assumptions imposed one one's data Spanos (2007).
- Trustworthy evidence stems from procedures whose <u>actual error probabilities</u> approximate 'closely' the <u>nominal ones</u> derived by presuming the validity of $\mathcal{M}_{\theta}(\mathbf{x})$. That is, the <u>trustworthiness of evidence</u> originates in the relevant error probabilities as they relate to the severity principle.

All approaches to statistics require three basic elements:

- (i) substantive questions of interest–however vague or highly specific,
- (ii) appropriate data \mathbf{x}_0 to shed light on these questions (learn from \mathbf{x}_0),
- (iii) **probabilistic assumptions** imposed (implicitly or explicitly) on the <u>observable</u> process $\{X_t, t \in \mathbb{N}\}$ underlying data \mathbf{x}_0 . These are the <u>assumptions</u> that **matter** for statistical inference purposes, and NOT those of any error terms.

Key differences of alternative approaches to statistics

- [a] **Inductive premises**: their framing of the <u>inductive premises</u> (probabilistic assumptions imposed on the data), and the interpretation of the selected model.
- [b] **Model choice**: the selection of the 'best' model for the particular data.
- [c] **Inductive inference**: the <u>underlying inductive reasoning</u> and the <u>nature</u> and interpretation of their <u>inferential claims</u>.
- [d] Substantive vs. statistical information/model: how they <u>conciliate</u> the <u>substantive</u> (theory-based) and <u>statistical</u> (data-based) information.

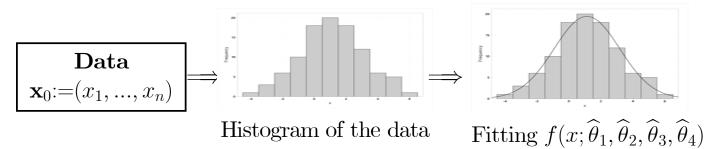


Diagram 1: Karl Pearson's approach to statistics

One begins with the raw data $\mathbf{x}_0 := (x_1, ..., x_n)$, whose initial 'rough summary' takes the form of a **histogram** with $m \geq 10$ bins. To provide a more succinct descriptive summary of the histogram Pearson would use the first four raw moments of \mathbf{x}_0 to select a frequency curve within a particular family known today as the Pearson family (\mathcal{F}_P) . Members of this family are generated by:

$$\mathcal{F}_P: \frac{d \ln f(x; \boldsymbol{\psi})}{dx} = \left[(x - \theta_1) / \left(\theta_2 + \theta_3 x + \theta_4 x^2 \right) \right], \ \boldsymbol{\theta} \in \Theta \subset \mathbb{R}^4, \ x \in \mathbb{R} := (-\infty, \infty), \quad (2.0.1)$$

that includes several well-known distributions. \mathcal{F}_P is characterized by the four unknown parameters $\theta := (\theta_1, \theta_2, \theta_3, \theta_4)$ that are estimated using $\widehat{\mu}_k(\mathbf{x}_0) = \frac{1}{n} \sum_{t=1}^n x_t^k$, k=1,2,3,4, yielding $\widehat{\boldsymbol{\theta}}(\mathbf{x}_0) := (\widehat{\theta}_1, \widehat{\theta}_2, \widehat{\theta}_3, \widehat{\theta}_4)$. $\widehat{\boldsymbol{\theta}}(\mathbf{x}_0)$ is used to select $f_0(x) \in \mathcal{F}_P$

based on the estimated curve $\widehat{f}(x; \widehat{\boldsymbol{\theta}}(\mathbf{x}_0))$ that 'best' fits the histogram using Pearson's (1900) goodness-of-fit test:

$$\eta(\mathbf{X}) = \sum_{i=1}^{m} [(\widehat{f_i} - f_i)^2 / f_i] \underset{n \to \infty}{\backsim} \chi^2(m).$$
(2.0.2)

What Pearson and his contemporaries did not appreciate sufficiently is that, irrespective of whether one is <u>summarizing</u> the data for **descriptive** or **inferential purposes**, one <u>implicitly imposes</u> probabilistic assumptions on the data. For instance, the move from the raw data \mathbf{x}_0 to a histogram invokes a 'random' (IID) sample $\mathbf{X}:=(X_1,...,X_n)$ underlying data \mathbf{x}_0 , and so do the formulae:

$$\overline{x}_{n} = \frac{1}{n} \sum_{t=1}^{n} x_{t}, \ \widehat{\sigma}_{x}^{2} = \frac{1}{n} \sum_{t=1}^{n} (x_{t} - \overline{x}_{n})^{2}, \ \overline{y}_{n} = \frac{1}{n} \sum_{t=1}^{n} y_{t}, \ \widehat{\sigma}_{x}^{2} = \frac{1}{n} \sum_{t=1}^{n} (y_{t} - \overline{y}_{n})^{2},$$

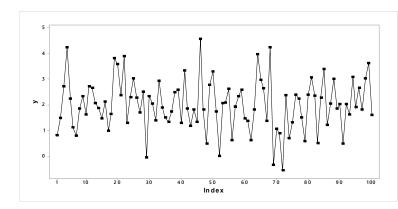
$$\widehat{\rho}_{xy} = \left[\left(\sum_{t=1}^{n} (x_{t} - \overline{x}_{n})(y_{t} - \overline{y}_{n}) \right) / \sqrt{\left[\sum_{t=1}^{n} (x_{t} - \overline{x}_{n})^{2} \right] \left[\sum_{t=1}^{n} (y_{t} - \overline{y}_{n})^{2} \right]} \right],$$

when estimating $E(X_t)$, $Var(X_t)$, $Corr(X_t, Y_t)$, etc.; see Yule (1926).

► Charging Karl Pearson with ignorance will be **anachronistic** since the theory of **stochastic processes** needed to understand the concept of **non-IID** samples was framed in the late 1920s early 1930s; Khitchin and Kolmogorov! What about the **current discussions on the replication crisis**?

Amrhein, Trafimow, Greenland (2019) "Inferential statistics as descriptive statistics: there is no replication crisis if we don't expect replication", is ill-conceived.

▶ The validity of the same probabilistic assumptions that **underwrite** the reliability of inferences also ensure the 'pertinence' of descriptive statistics.



Case 1: t-plot of IID data \mathbf{y}_0

Case 2 (ID false): t-plot of data \mathbf{x}_0

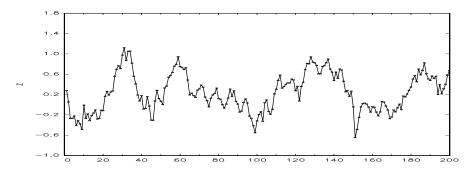
$$\overline{y} = \frac{1}{n} \sum_{t=1}^{n} y_{t} = 2.03 \ [E(Y_{t}) = 2], \qquad \overline{x} = \frac{1}{n} \sum_{t=1}^{n} x_{t} = 12.1 \ [E(X_{t}) = 2 - .2t]$$

$$s_{y}^{2} = \frac{1}{n} \sum_{t=1}^{n} (y_{t} - \overline{y})^{2} = 1.01 \ [Var(Y_{t}) = 1] \quad s_{x}^{2} = \frac{1}{n} \sum_{t=1}^{n} (x_{t} - \overline{x})^{2} = 34.21 \ [Var(X_{t}) = 1]$$

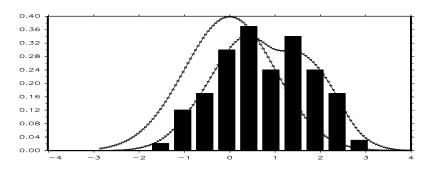
$$\overline{x} = \frac{1}{n} \sum_{t=1}^{n} x_t = 12.1 \ [E(X_t) = 2 - .2t]$$

$$s_x^2 = \frac{1}{n} \sum_{t=1}^{n} (x_t - \overline{x})^2 = 34.21 \ [Var(X_t) = 2 - .2t]$$

Consider case 3 where the Independence assumption is invalid.



Case 3 (I false): t-plot of data \mathbf{z}_0



Case 3: Histogram of data \mathbf{z}_0

▶ When the IID assumptions are invalid for \mathbf{x}_0 , not only the <u>descriptive statistics</u>, but also the estimated <u>frequency curve</u> chosen $f(x; \widehat{\boldsymbol{\theta}}(\mathbf{x}_0))$, <u>will be highly misleading</u>.

Fisher's Model-based frequentist approach

Fisher (1922) recast Pearson's curve-fitting into modern **model-based statistical induction** by viewing the data \mathbf{x}_0 as a 'typical realization' of a **parametric statistical model**, generically defined by:

$$\mathcal{M}_{\boldsymbol{\theta}}(\mathbf{x}) = \{ f(\mathbf{x}; \boldsymbol{\theta}), \ \boldsymbol{\theta} \in \Theta \}, \ \mathbf{x} \in \mathbb{R}^n_X, \text{ for } \Theta \subset \mathbb{R}^m, \ m < n.$$
 (3.0.3)

Example. The *simple Normal model* is specified by:

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$$X_t \sim \mathsf{NIID}(\mu, \sigma^2), \ \boldsymbol{\theta} := (\mu, \sigma^2) \in \Theta := (\mathbb{R} \times \mathbb{R}_+), \ x_t \in \mathbb{R}, \ t \in \mathbb{N} \},$$
 (3.0.4)

 $\mathcal{M}_{\theta}(\mathbf{x})$ is framed in terms of probabilistic assumptions from 3 broad categories:

(D) Distribution	(M) Dependence	(H) Heterogeneity
Normal	Independence	Identically Distributed
Beta	Correlation	Strict Stationarity
Gamma	Markov	Weak Stationarity
Bernoulli	Martingale	Separable heterogeneity
:	:	:

assigned to the stochastic process $\{X_t, t \in \mathbb{N}\}$ underlying data \mathbf{x}_0 .

These assumptions determine the joint distribution $f(\mathbf{x}; \boldsymbol{\theta})$, $\mathbf{x} \in \mathbb{R}_X^n$, of the sample $\mathbf{X} := (X_1, ..., X_n)$, including its parametrization $\boldsymbol{\theta} \in \Theta$, as well as the likelihood function $L(\boldsymbol{\theta}; \mathbf{x}_0) \propto f(\mathbf{x}_0; \boldsymbol{\theta})$, $\boldsymbol{\theta} \in \boldsymbol{\Theta}$; see Spanos (1986).

Fisher proposed a complete reformulation of statistical induction by **modeling** the statistical Generating Mechanism (GM) $[\mathcal{M}_{\theta}(\mathbf{x})]$ framed in terms of the observable stochastic process $\{X_t, t \in \mathbb{N}\}$ underlying data \mathbf{x}_0 .

Fisher (1922) asserts that $\mathcal{M}_{\theta}(\mathbf{x})$ is chosen by responding to the question: "Of what population is this a random sample?" (p. 313), and adding that "and the adequacy of our choice may be tested posteriori." (314). The 'adequacy' can be evaluated using Mis-Specification (M-S) testing; see Spanos (2006).

That is, $\mathcal{M}_{\theta}(\mathbf{x})$ is selected to account for the chance regularities in data \mathbf{x}_0 , but its appropriateness is evaluated by M-S testing.

The **primary objective** of frequentist inference is to use the sample information, as summarized by $f(\mathbf{x}; \boldsymbol{\theta})$, $\mathbf{x} \in \mathbb{R}_X^n$, in conjunction with data \mathbf{x}_0 , to learn from data about $\boldsymbol{\theta}^*$ - true value of $\boldsymbol{\theta} \in \Theta$; shorthand for saying that $\mathcal{M}_{\boldsymbol{\theta}^*}(\mathbf{x}) = \{f(\mathbf{x}; \boldsymbol{\theta}^*)\}, \ \mathbf{x} \in \mathbb{R}_X^n$, could have generated data \mathbf{x}_0 .

Learning from \mathbf{x}_0 takes the form of 'statistical approximations' around $\boldsymbol{\theta}^*$, framed in terms of the sampling distribution, $f(y_n; \boldsymbol{\theta})$, $\forall y_n \in \mathbb{R}$, of a statistic (estimator,

test, predictor) $Y_n = g(X_1, ..., X_n)$, derived using two different forms of reasoning via:

$$F_n(y) = \mathbb{P}(Y_n \le y) = \underbrace{\int \int \cdots \int}_{\{\mathbf{x}: \ g(\mathbf{x}) \le y\}} f(\mathbf{x}; \boldsymbol{\theta}) d\mathbf{x}, \ \forall y \in \mathbb{R},$$
(3.0.5)

- (i) **Factual** (estimation and prediction): presuming that $\theta = \theta^* \in \Theta$, and
- (ii) **Hypothetical** (hypothesis testing): various hypothetical scenarios based on different prespecified values of $\boldsymbol{\theta}$, under H_0 : $\boldsymbol{\theta} \in \boldsymbol{\Theta}_0$ (presuming that $\boldsymbol{\theta} \in \boldsymbol{\Theta}_0$) and H_1 : $\boldsymbol{\theta} \in \boldsymbol{\Theta}_1$ (presuming that $\boldsymbol{\theta} \in \boldsymbol{\Theta}_1$), where $\boldsymbol{\Theta}_0$ and $\boldsymbol{\Theta}_1$ partition $\boldsymbol{\Theta}$.
- ▶ Crucially important: (i) the statistical adequacy of $\mathcal{M}_{\theta}(\mathbf{x})$ ensures that θ^* lies within $\mathcal{M}_{\theta}(\mathbf{x})$, and thus learning from data \mathbf{x}_0 is attainable.
- (ii) Neither form of frequentist reasoning (factual or hypothetical) involves conditioning on θ , an <u>unknown constant</u>.
- (iii) The <u>decision-theoretic reasoning</u>, for all values of θ in Θ ($\forall \theta \in \Theta$), <u>undermines</u> learning from data about θ^* , and gives rise to <u>Stein-type</u> paradoxes and <u>admissibility</u> fallacies; Spanos (2017).
- ▶ Misspecification. When $\mathcal{M}_{\theta}(\mathbf{x})$ is misspecified, $f(\mathbf{x}; \theta)$ is incorrect, and this distorts $f(y_n; \theta)$, and often induces inconsistency in estimators and size-

able discrepancies between the <u>actual</u> and <u>nominal error probabilities</u> in Confidence Intervals (CIs), testing and prediction. This is why **Akaike-type model** selection procedures often go astray, since all goodness-of-fit/prediction measures presume the validity of $\mathcal{M}_{\theta}(\mathbf{x})$; Spanos (2010).

How can one apply Fisher's **model-based statistics** when the empirical modeling begins with a **substantive model** $\mathcal{M}_{\varphi}(\mathbf{x})$?

[i] Bring out the statistical model $\mathcal{M}_{\theta}(\mathbf{x})$ implicit in $\mathcal{M}_{\varphi}(\mathbf{x})$; there is always one that comprises solely the probabilistic assumptions imposed on data \mathbf{x}_0 ! It is defined as an <u>unrestricted</u> parametrization that follows from the probabilistic assumptions imposed on the process $\{X_t, t \in \mathbb{N}\}$ underlying \mathbf{x}_0 which includes $\mathcal{M}_{\varphi}(\mathbf{x})$ as a special case.

[ii] Relate the substantive parameters φ to θ via restrictions, say $\mathbf{g}(\varphi, \theta) = \mathbf{0}$, ensuring that the restrictions $\mathbf{g}(\varphi, \theta) = \mathbf{0}$ define φ uniquely in terms of θ .

Example. For the substantive model known as the Capital Asset Pricing:

$$\mathcal{M}_{\varphi}(\mathbf{z}): \qquad (Y_t - x_{2t}) = \alpha_1(x_{1t} - x_{2t}) + \varepsilon_t, \ (\varepsilon_t | \mathbf{X}_t = \mathbf{x}_t) \backsim \mathsf{NIID}(0, \ \sigma_{\varepsilon}^2), \ t \in \mathbb{N},$$

$$\mathcal{M}_{\theta}(\mathbf{z}): \qquad Y_t = \beta_0 + \beta_1 x_{1t} + \beta_2 x_{2t} + u_t, \ (u_t | \mathbf{X}_t = \mathbf{x}_t) \backsim \mathsf{NIID}(0, \ \sigma_u^2), \ t \in \mathbb{N},$$

$$\mathbf{g}(\varphi, \theta) = \mathbf{0}: \quad \beta_0 = 0, \ \beta_1 + \beta_2 - 1 = 0, \text{ where } \varphi = (\alpha_1, \sigma_{\varepsilon}^2), \ \theta = (\beta_0, \beta_1, \beta_2, \sigma_u^2).$$

[iii] Test the validity of H_0 : $\mathbf{g}(\boldsymbol{\varphi}, \boldsymbol{\theta}) = \mathbf{0}$ vs. H_1 : $\mathbf{g}(\boldsymbol{\varphi}, \boldsymbol{\theta}) \neq \mathbf{0}$ to establish whether the substantive model $\mathcal{M}_{\boldsymbol{\varphi}}(\mathbf{z})$ belies data \mathbf{z}_0 .

Main features of the Fisher model-based approach

- [a] Inductive premises: $\mathcal{M}_{\theta}(\mathbf{x})$ comprises a set of complete, internally consistent, and testable probabilistic assumptions, relating to the **observable** process $\{X_t, t \in \mathbb{N}\}$ underlying data \mathbf{x}_0 , from the <u>Distribution</u>, <u>Dependence</u> and <u>Heterogeneity categories</u>. $\mathcal{M}_{\theta}(\mathbf{x})$ is viewed as a statistical <u>stochastic mechanism</u> aiming <u>to account</u> for all the **chance regularity patterns** in data \mathbf{x}_0 .
- [b] Model choice: the appropriate $\mathcal{M}_{\theta}(\mathbf{x})$ is chosen on statistical adequacy grounds using comprehensive Mis-Specification (M-S) testing to ensure that inferences are *reliable*: the actual \simeq nominal error probabilities.
- [c] Inductive inference: the interpretation of probability is frequentist and the underlying inductive reasoning is either factual (estimation, prediction) or hypothetical (testing) and relates to learning from data about θ^* . The effectiveness (optimality) of inference procedures is calibrated using error probabilities based on a statistically adequate $\mathcal{M}_{\theta}(\mathbf{x})$!

Regrettably, the replication crisis literature often **confuses** hypothetical reasoning with conditioning on H_0 !

Diaconis and Skyrms (2018) claim (tongue-in-cheek) that p-value testers conflate $P(H_0|\mathbf{x}_0)$ with $P(\mathbf{x}_0|H_0)$: "The <u>untutored</u> think they are getting the probability of effectiveness [of a drug] given the data, while they are being given conditional probabilities going in the opposite direction." (p. 67)

- ▶ The 'untutored' **know** from <u>basic</u> probability theory that <u>conditioning</u> on H_0 : $\theta = \theta_0$ is formally <u>illicit</u> since θ is <u>neither an event nor a random variable!</u>
- [d] Substantive vs. statistical: the substantive model, $\mathcal{M}_{\varphi}(\mathbf{x})$, is embedded into a statistically adequate $\mathcal{M}_{\theta}(\mathbf{x})$ via restrictions $\mathbf{g}(\theta, \varphi) = \mathbf{0}$, $\theta \in \Theta$, $\varphi \in \Phi$, whose rejection indicates that the substantive information in $\mathcal{M}_{\varphi}(\mathbf{x})$ belies \mathbf{x}_0 !
- The above modeling strategy [i]-[iv] can be used to provide sound statistical foundations for Graphical Causal Modeling that revolves around substantive causal models $[\mathcal{M}_{\varphi}(\mathbf{x})]$. It will enable a harmonious blending of the statistical with the substantive information without undermining the credibility of either and allow for probing the validity of causal information.

4 Graphical Causal (GC) Modeling

- Quantifying a Graphical Causal (GC) model based on directed acyclic graphs (DAG) (Pearl, 2009; Spirtes et. al 2000) constitutes another form of curve-fitting a priori postulated substantive model $\mathcal{M}_{\varphi}(\mathbf{z})$.
- An crucial weakness of the GC modeling is that the causal information (substantive) is usually treated as established knowledge instead of best-daresay conjectures whose soundness needs to be tested against data \mathbf{Z}_0 .
- ▶ Foisting a DAG substantive model, $\mathcal{M}_{\varphi}(\mathbf{z})$, on data \mathbf{Z}_0 , will usually yield a statistically and substantively misspecified model!
- This is because the **estimation** of $\mathcal{M}_{\varphi}(\mathbf{z})$ invokes a set of probabilistic assumptions relating to the observable process $\{\mathbf{Z}_t, t \in \mathbb{N}\}$ underlying data \mathbf{Z}_0 , the **implicit** statistical model $\mathcal{M}_{\theta}(\mathbf{z})$ whose **adequacy** is unknown!
- ► Can one guard against statistical and substantive misspecification?
- Embed the DAG model into the Fisher model-based framework
- Step 1. Unveil the statistical model $\mathcal{M}_{\theta}(\mathbf{z})$ implicit in the GC model.
- Step 2. Establish the statistical adequacy of $\mathcal{M}_{\theta}(\mathbf{z})$ using comprehensive M-S testing, and respecification when needed.

Substantive (GC) model [a] Z - **confounder**

$$\overline{Y_k = \beta_0 + \beta_1 X_k + \beta_2 Z_k + \varepsilon_{1k},}$$

$$X_k = \alpha_0 + \alpha_1 Z_k + \varepsilon_{2k}, \ k \in \mathbb{N}$$

Statistical model for [a]

$$Y_k = a_{01} + a_{11}Z_k + u_{1k},$$

$$X_k = a_{02} + a_{12}Z_k + u_{2k},$$

Substantive (GC) model

[b] Z - mediator

$$Y_k = \beta_0 + \beta_1 X_k + \beta_2 Z_k + \varepsilon_{1k},$$

$$Z_k = \gamma_0 + \gamma_1 X_k + \varepsilon_{3k}, \ k \in \mathbb{N},$$

Statistical model for [b]

$$Y_k = b_{01} + b_{11}X_k + u_{3k},$$

$$Z_k = b_{02} + b_{12}X_k + u_{4k},$$

Substantive (GC) model [c] Z - **collider**

$$\overline{Y_k = \delta_0 + \delta_1 X_k + \varepsilon_{4k}, \ k \in \mathbb{N},}$$

$$Z_k = c_0 + c_1 Y_k + c_2 X_k + \varepsilon_{5k},$$

Statistical model for [c]

$$Y_k = b_{01} + b_{11}X_k + u_{3k},$$

$$Z_k = b_{02} + b_{12}X_k + u_{4k},$$

Diagram 2: Functional Graphical Causal models

Step 3. Use a statistically adequate $\mathcal{M}_{\theta}(\mathbf{z})$ to address the identification and estimation of the structural parameters $\varphi \in \Phi$.

Step 4. Test the validity of the **overidentifying restrictions** stemming from $\mathbf{g}(\boldsymbol{\theta}, \boldsymbol{\varphi}) = \mathbf{0}, \ \boldsymbol{\theta} \in \Theta, \ \boldsymbol{\varphi} \in \Phi.$

Excellent **goodness-of-fit/prediction** is relevant for **substantive adequacy**, which can only be probed <u>after</u>:

- (i) establishing the statistical adequacy of $\mathcal{M}_{\theta}(\mathbf{z})$, and
- (ii) evaluating the **validity** of the restrictions: H_0 : $\mathbf{g}(\boldsymbol{\theta}, \boldsymbol{\varphi}) = \mathbf{0}$ vs. H_1 : $\mathbf{g}(\boldsymbol{\theta}, \boldsymbol{\varphi}) \neq \mathbf{0}$.

Rejecting H_0 indicates that the <u>substantive information</u> in $\mathcal{M}_{\varphi}(\mathbf{x})$ <u>belies</u> \mathbf{x}_0 !

5 Nonparametric statistics & curve-fitting

Nonparametric statistics began in the 1970s extending Kolmogorov (1933a):

when the sample $\mathbf{X}:=(X_1,X_2,...,X_n)$ is IID, the empirical cdf $\widehat{F}_n(x)$ is a good estimator of the cdf F(x), for n large enough.

Attempts to find good estimators for the **density function** f(x), $x \in \mathbb{R}$, led to:

- (a) **kernel smoothing** and related techniques, including regression-type models,
- (b) series estimators of $\widehat{f}(x) = \sum_{i=0}^{m} \beta_i \phi_i(x_k)$, where $\{\phi_i(x_k), i=1, 2, ..., m\}$ are **polynomials**, usually **orthogonal**; see Wasserman (2006).

A nonparametric statistical model is specified in terms of a broader family \mathcal{F} of distributions (Wasserman, 2006):

$$\mathcal{M}_{\mathcal{F}}(\mathbf{x}) = \{ f(\mathbf{x}; \boldsymbol{\psi}_n), f \in \mathcal{F} \}, \boldsymbol{\psi}_n \in \boldsymbol{\Psi}, \mathbf{x} \in \mathbb{R}_X^n,$$

where \mathcal{F} is defined in terms of <u>indirect</u> & <u>non-testable</u> **Distribution** assumptions such as: (a) the **existence of moments** up to order $p \geq 1$, (see Bahadur and Savage, 1956, on such assumptions),

(b) **smoothness restrictions** on the **unknown** density function f(x), $x \in \mathbb{R}_X$ (symmetry, differentiability, unimodality of f(x), etc.).

Dickhaus (2018), p. 13: "Of course, the advantage of considering \mathcal{F} is that the issue of model misspecification, which is often problematic in parametric models, is avoided." Really?

Nonparametric models <u>always impose</u> **Dependence** and **Heterogeneity** assumptions (often Independent and Identically Distributed (IID))!

What are the consequences of replacing $f(\mathbf{x}; \boldsymbol{\theta})$ with $f(\mathbf{x}; \boldsymbol{\psi}_n)$, $f \in \mathcal{F}$?

The likelihood-based inference procedures are replaced by loss function-based procedures driven by mathematical approximations and goodness-of-fit measures, relying on asymptotic inference results at a high price in reliability and precision of inference since (i) the adequacy of $f(\mathbf{x}; \boldsymbol{\psi}_n)$, $f \in \mathcal{F}$ is impossible to establish, and (ii) the 'indirect' and non-testable distribution assumptions invariably contribute substantially to the imprecision/unreliability of inference.

► As argued by Le Cam (1986), p. xiv:

"... limit theorems "as n tends to infinity" are <u>logically devoid of content</u> about <u>what happens at any particular n</u>. All they can do is suggest certain approaches whose performance must then be checked on the case at hand. Unfortunately, the approximation bounds we could get are too often too crude and cumbersome to be of any practical use."

Data Science (Machine Learning and all that!)

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Big Data and Data Science includes Machine Learning (ML), Statistical Learning Theory (SLT), pattern recognition, data mining, etc.

As claimed by Vapnik (2000): "Between 1960 and 1980 a revolution in statistics occurred: Fisher's paradigm, ... was replaced by a new one. This paradigm reflects a new answer to the fundamental question: What must one know a priori about an unknown functional dependency in order to estimate it on the basis of observations? In Fisher's paradigm the answer was very restrictive – one must know almost everything. Namely, one must know the desired dependency up to the values of a finite number of parameters. ... In the new paradigm ... it is sufficient to know some general properties of the set of functions to which the unknown dependency belongs." (ix).

In **Fisher's model-based** approach one selects $\mathcal{M}_{\theta}(\mathbf{z})$ to account for the chance regularities in data \mathbf{Z}_0 , and evaluates its validity before any inferences are drawn, respecifying it when $\mathcal{M}_{\theta}(\mathbf{z})$ is misspecified. The form of dependence follows from the probabilistic assumptions of a statistically adequate $\mathcal{M}_{\theta}(\mathbf{z})$.

Example. Assuming that $\{Y_t, t \in \mathbb{N}\}$ is Normal, Markov and stationary, the dependence is an AR(1) model $Y_t = \alpha_0 + \alpha_1 Y_{t-1} + u_t$, $(u_t | \sigma(Y_{t-1})) \backsim \mathsf{NIID}(0, \sigma^2)$, $t \in \mathbb{N}$.

Machine Learning views statistical modeling as an optimization problem relating to how a machine can 'learn from data':

- (a) **learner's input**: a domain set \mathcal{X} , a label set \mathcal{Y} ,
- (b) training data $\mathcal{X} \times \mathcal{Y}$: $\mathbf{z}_i := (\mathbf{x}_i, y_i), i=1, 2, ..., n$,
- (c) with an **unknown distribution** $f^*(\mathbf{z})$, and
- (d) learner's output: $h(.): \mathcal{X} \to \mathcal{Y}$.

The learning algorithm is all about choosing h(.) to approximate 'closely' the true relationship $y_i=g(\mathbf{x}_i),\ i\in\mathbb{N}$, by minimizing the distance $||h(\mathbf{x})-g(\mathbf{x})||$.

Barriers to entry? The underlying probabilistic and mathematical framework comes in the form of functional analysis: the study of infinite-dimensional vector (linear) spaces endowed with a topology (metric, norm, inner product) and a probability measure.

Example. The normed linear space $(C[a, b], \| . \|_p)$ of all real-valued continuous functions g(x) defined on $[a, b] \subset \mathbb{R}$, with the *p*-norm (Murphy, 2022):

$$\|g\|_{p} = \left(\int_{a}^{b} |g(x)|^{p} dx\right)^{\frac{1}{p}}, \text{ or } \|g\|_{p} = \left(\sum_{i=0}^{n} |g(x_{i})|^{p}\right)^{\frac{1}{p}}, p=1, 2, \infty.$$
 (6.0.6)

The mathematical approximation problem is transformed into an <u>optimization</u> in the context of a **vector space** employing powerful theorems such as the open

mapping, the Banach-Steinhaus, the Hahn-Banach theorems; see Carlier (2022). To ensure the <u>existence</u> and <u>uniqueness</u> of the optimization solution, the <u>approximation problem</u> is often embedded in a <u>complete inner product vector (linear) space $(C[a, b], || . ||_2)$ of real or complex-valued functions $h(\mathbf{X})$, defined on $[a, b] \subset \mathbb{R}$, with the 2-norm, also known as a <u>Hilbert space</u> of <u>square-integrable functions</u> $(E(|\mathbf{X}_t|^2))$, where $\{\mathbf{X}_t, t \in \mathbb{N}\}$ is a stochastic process. A Hilbert space generalizes the n-dimensional Euclidean geometry to an infinite dimensional inner product <u>space</u> that allows <u>lengths</u> and <u>angles</u> to be defined to render optimization possible.</u>

Supervised learning (Regression). A typical example is a regression model:

$$y_t = g(\mathbf{x}_t; \boldsymbol{\psi}_n) + v_t,$$

where $g(\mathbf{x}_t; \boldsymbol{\psi}_n) \in \mathcal{G}$, where \mathcal{G} is a family of smooth enough mathematical functions, is approximated using data $\mathbf{Z}_0 := \{(\mathbf{x}_t, y_t), t=1, 2, ..., n\}$.

Risk functions. The problem is framed in terms of a loss function:

$$L(y, g(\mathbf{x}; \boldsymbol{\psi}_n)), \ \forall \boldsymbol{\psi}_n \in \boldsymbol{\Psi}, \ \forall \mathbf{z} \in \mathbb{R}_Z^{nm},$$

(a)
$$||g||_2$$
: $L(y, g(\mathbf{x}; \boldsymbol{\psi}_n)) = (y - g(\mathbf{x}; \boldsymbol{\psi}_n))^2$, (b) $||g||_1$: $L(y, g(\mathbf{x}; \boldsymbol{\psi}_n)) = |y - g(\mathbf{x}; \boldsymbol{\psi}_n)|$.

To render $L(y, g(\mathbf{x}; \boldsymbol{\psi}_n))$ only a function of $\forall \boldsymbol{\psi}_n \in \boldsymbol{\Psi}$, $\forall \mathbf{z} \in \mathbb{R}_Z^{nm}$ is eliminated by taking expectations wrt the distribution of the sample \mathbf{Z} , $f^*(\mathbf{z})$ -presumed **unknown**, to define a **risk function**:

$$R(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n)) = E_{\mathbf{z}}(L(y, g(\mathbf{x}; \boldsymbol{\psi}_n))) = \int_{\mathbf{z}} L(y, g(\mathbf{x}; \boldsymbol{\psi}_n)) f^*(\mathbf{z}) d\mathbf{z}, \ \forall \boldsymbol{\psi}_n \in \boldsymbol{\Psi}.$$

The <u>statistical model implicit</u> in **Data Science** is: $\mathcal{M}_{\mathcal{F}}(\mathbf{z}) = \{f^*(\mathbf{z}), f \in \mathcal{F}(\boldsymbol{\psi})\},$ $\boldsymbol{\psi}_n \in \boldsymbol{\Psi}, \mathbf{z} \in \mathbb{R}_Z^{mn}$, and the ensuing **inference** revolves around the <u>risk function</u> using the **decision theoretic reasoning** based on $\forall \boldsymbol{\psi}_n \in \boldsymbol{\Psi}$.

Hence, <u>Data Science</u> tosses away all forms of **frequentist inference** apart from the **point estimation**. Since f^* is <u>unobservable</u> $R(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n))$ is estimated using basic **descriptive statistics:** $\widehat{E}(X_i) = \frac{1}{n} \sum_{i=1}^n X_i!$

Assuming that $\{\mathbf{Z}_t, t \in \mathbb{N}\}$ is **IID** (often not stated explicitly!) one can use the arithmetic average

 $\widehat{R}(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n)) = \frac{1}{n} \sum_{i=1}^n L(y_i, g(\mathbf{x}_i; \boldsymbol{\psi}_n(\mathbf{x}_i)))$, and then minimize it to yield a **consistent** estimator of $g(\mathbf{x}; \boldsymbol{\psi}_n)$:

$$\widehat{g}_{m}(\mathbf{z};\widehat{\boldsymbol{\psi}}_{n}(\mathbf{x})) = \arg\min_{g \in \mathcal{G}} \left[\frac{1}{n} \sum_{i=1}^{n} L(y_{i}, g(\mathbf{x}_{i}; \boldsymbol{\psi}_{n}(\mathbf{x}_{i}))) \right], \tag{6.0.7}$$

where $\widehat{y}_i = \widehat{g}_m(\mathbf{z}_i; \widehat{\boldsymbol{\psi}}_n(\mathbf{x}_i))$ minimizing (6.0.7) is inherently overparametrized!

Regularization. Depending on the dimension (effective number of parameters) of the class of functions \mathcal{G} , (6.0.7) will usually give rise to serious **overfitting** – near-interpolation! To reduce the <u>inherent</u> overparametrization problem ML methods impose ad hoc <u>restrictions</u> on the parameters, <u>euphemistically</u> known as **regularization**, to derive to $\widehat{y}_i = \widehat{g}_m(\mathbf{z}_i; \widehat{\boldsymbol{\phi}}_n(\mathbf{x}_i))$ via minimizing:

$$R_r(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n)) = R(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n)) + \lambda C(g(\mathbf{z}; \boldsymbol{\psi}_n)), \tag{6.0.8}$$

where $C(g(\mathbf{z}; \boldsymbol{\psi}_n))$ is often related to the algorithmic complexity of the class \mathcal{G} . **Example**. For the LR model $Y_t = \boldsymbol{\beta}^{\top} \mathbf{x}_t + u_t$, $\boldsymbol{\beta}$ is estimated by minimizing:

least-squares
$$\sum_{t=1}^{n} (Y_t - \boldsymbol{\beta}^{\top} \mathbf{x}_t)^2 + \lambda_1 \sum_{i=1}^{p} |\beta_i| + \lambda_2 \sum_{i=1}^{p} \beta_i^2.$$

The idea is that regularization reduces the <u>variance</u> of $\widehat{\boldsymbol{\beta}}$ with only small increases in its <u>bias</u>, which improves prediction MSE $\sum_{t=n+1}^{n+N} (Y_t - \widehat{\boldsymbol{\beta}}^{\top} \mathbf{x}_t)^2$ (artificially!), at the expense of learning from data; Spanos (2017).

Probably Approximately Correct (PAC) learnability refers to 'learning' (computationally) about $f^*(\mathbf{z})$ using a polynomial-time algorithm (N^k) to chose

 $g(\mathbf{z}; \boldsymbol{\psi}_n)$ in \mathcal{G} , in the form of an upper bound (Murphy, 2022):

$$\mathbb{P}(\max_{g \in \mathcal{G}} |\widehat{R}(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n)) - R(f^*, g(\mathbf{z}; \boldsymbol{\psi}_n))| > \epsilon) \leq 2\dim(\mathcal{G}) \exp(-2N\epsilon^2).$$

Statistical inference in <u>Data Science</u> is invariably based on <u>asymptotic results</u> ('as $n \to \infty$ ') invoking IID, such as the **Uniform** Law of Large Number (ULLN) for the whole family of functions \mathcal{G} , as well as more general asymptotic results derived by invoking **non-testable** mathematical and probabilistic assumptions ('as $n \to \infty$ '), such as <u>mixing conditions</u> (Dependence) and <u>asymptotic homogeneity</u> (Heterogeneity)!

Main features of the Data Science approach:

[a] Inductive premises: normed linear spaces $L_p(S, \mathfrak{F}, \mathbb{P}(.))$ endowed with a probability measure relating to the stochastic process $\{\mathbf{Z}_t, t \in \mathbb{N}\}$. The probabilistic assumptions underlying $\{\mathbf{Z}_t, t \in \mathbb{N}\}$ are often IID, with an indirect distribution assumption relating to a family of mathematical functions \mathcal{G} and chosen on mathematical approximation grounds.

[b] Model choice: the best fitted curve $\hat{\mathbf{y}}_i = \mathbf{G}_m(\mathbf{x}_i; \hat{\boldsymbol{\phi}}_n(\mathbf{x}_i))$ in \mathcal{G} is chosen on goodness-of-fit/prediction grounds or/and Akaike-type information criteria.

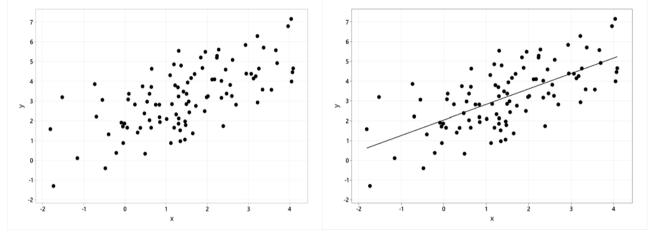
- [c] Inductive inference: the interpretation of probability can be both frequentist and Bayesian, but the <u>underlying reasoning</u> is decision theoretic $(\forall \psi_n \in \Psi)$ which is <u>at odds</u> with frequentist inference. The optimality of inference procedures is based on the the risk function and framed in terms of <u>asymptotic theorems</u> that invoke <u>non-testable mathematical</u> and <u>probabilistic assumptions</u>. The 'best' fitted-curve $\hat{\mathbf{y}}_i = \mathbf{G}_m(\mathbf{x}_i; \hat{\boldsymbol{\phi}}_n(\mathbf{x}_i))$ in \mathcal{G} is used for 'predictive learning'.
- [d] Substantive vs. statistical: the fitted curve $\hat{\mathbf{y}}_t = \mathbf{G}_m(\mathbf{x}_t; \hat{\boldsymbol{\phi}}_n)$ in \mathcal{G} is rendered a black box free of any statistical/substantive interpretation since the curve-fitting and regularization imposes arbitrary restrictions on $\boldsymbol{\psi}_n$ to fine-tune the prediction error. This obviates any possibility for interpreting $\hat{\boldsymbol{\phi}}_n(\mathbf{x}_i)$ or establishing any evidence for potential causal claims, etc.

Weaknesses of Data Science (ML, SLT, etc.) algorithmic methods

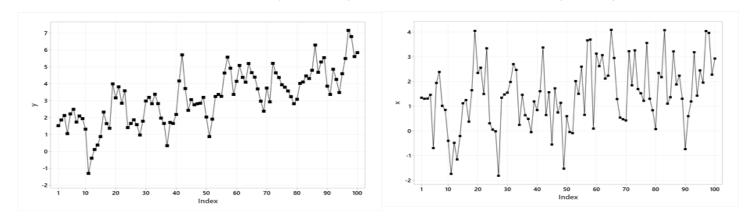
- 1. The Curve-Fitting Curse: viewing the modeling facet with data as an optimization problem in the context of a Hilbert space of overparametrized functions will always guarantee a unique solution on goodness-of-fit/prediction grounds, trustworthiness be damned.
- ▶ Minimizing $\sum_{i=n+1}^{N} (y_i \widehat{g}(\mathbf{x}_i; \boldsymbol{\psi}_n))^2$, using additional data in the **testing and**

- validation facets $\mathbf{z}_i := (\mathbf{x}_i, y_i)$ i = n+1, n+2, ..., N, has <u>no added value</u> in **learning from data** when training-based choice $\widehat{y}_t = \widehat{g}(\mathbf{x}_t; \boldsymbol{\psi}_n)$ is **statistically misspecified**. It just adds more scope for **tweaking**!
- 2. Is $L(\theta) = -\ln L(\theta; \mathbf{Z}_0)$, $\theta \in \Theta$, just another loss function (Cherkassky and Mulier, 2007, p. 31)? No! $\ln L(\theta; \mathbf{Z}_0)$ is based on **testable probabilistic** assumptions comprising $\mathcal{M}_{\theta}(\mathbf{z})$, as opposed to arbitrary loss functions based on information other than data \mathbf{Z}_0 (Spanos, 2017).
- 3. <u>Mathematical approximation error terms</u> are very different from white-noise statistical error terms. The former rely on <u>Jackson-type upper bounds</u> that are never <u>statistically non-systematic</u>. Hence, one can conflate the two errors at the <u>peril</u> of the <u>trusthworthiness</u> of evidence; Spanos (2010).
- 4. What patterns? Curve-fitting using mathematical approximation patterns is very different from recurring chance regularity patterns in data \mathbf{Z}_0 , that relate directly to probabilistic assumptions. Indeed, the former seek approximation patterns which often invoke the validity of certain probabilistic assumptions. For instance, supervised and unsupervised learning using scatterplots invokes IID for \mathbf{Z}_0 ; Wilmot (2019), p. 66.

Example. For data $\mathbf{Z}_0 := \{(x_t, y_t), t=1, 2, ...n\}$ the scatterplot presupposes IID!



Unfortunately, the IID assumptions are **false** for both data series, shown below, that exhibit trending means (non-ID) and irregular cycles (non-I).



- 4. How reliable are Data Science inferences? The training/testing/validation split of the data can improve the selected models on prediction grounds, but will nothing not secure the reliability of inference.
- 5. It contrast to <u>PAC learnability</u> that takes the fitted $\widehat{\mathbf{y}}_i = \mathbf{G}_m(\mathbf{x}_i; \widehat{\boldsymbol{\phi}}_n(\mathbf{x}_i)) \in \mathcal{G}$ at face value <u>to learn about</u> $f^*(\mathbf{z})$, the <u>learning</u> in **Fisher's model-based statistics** stems from $f(\mathbf{z}; \boldsymbol{\theta})$, $\mathbf{z} \in \mathbb{R}^n_Z$, to $g(\mathbf{x}_t; \boldsymbol{\psi}(\boldsymbol{\theta})) = E(h(Y_t)|\mathbf{X}_t)$, where the probabilistic structure of $f(\mathbf{z}; \boldsymbol{\theta})$, determines $Y_i = g(\mathbf{x}_i; \boldsymbol{\psi}(\boldsymbol{\theta}))$ as well as $\boldsymbol{\psi}(\boldsymbol{\theta})$.
- 6. The impression in Data Science is that the combination of: (i) a very large sample size n for data \mathbb{Z}_0 , (ii) the training/testing/validation split, (iii) the asymptotic inference, renders the statistical adequacy problem irrelevant, is an illusion! Departures from IID will render both the reliability and precision worse & worse as n increases (Spanos & McGuirk, 2001). Moreover, invoking limit theorems 'as $n \to \infty$ ' based on non-testable Dependence and Heterogeneity is another head game.
- On a positive note, **ML can be useful** when: (i) the data \mathbf{Z}_0 is (luckily) IID, (ii) \mathbf{Z}_t includes a large number of variables, (iii) one has meager substantive information, and (iv) the sole objective is a short horizon 'makeshift' prediction.

7 Summary and conclusions

7.1 'Learning from data' about phenomena of interest

Breiman's (2001) claim that in Fisher's paradigm "One assumes that the data are generated by a given stochastic data model" refers to a common erroneous implementation of model-based statistics where $\mathcal{M}_{\theta}(\mathbf{z})$ is viewed as a priori postulated model – presumed to be valid no matter what; see Spanos (1986).

In fact, Fisher (1922), p. 314, emphasized the crucial importance of model validation: "For empirical as the specification of the hypothetical population $[\mathcal{M}_{\theta}(\mathbf{z})]$ may be, this empiricism is cleared of its dangers if we can apply a rigorous and objective test of the adequacy with which the proposed population $[\mathcal{M}_{\theta}(\mathbf{z})]$ represents the whole of the available facts." i.e. $\mathcal{M}_{\theta}(\mathbf{z})$ accounts for all the chance regularities in \mathbf{Z}_0 .

Fisher's parametric model-based $[\mathcal{M}_{\theta}(\mathbf{z})]$ statistics, relying on strong (not weak) probabilistic assumptions that are validated vis-a-vis data \mathbf{Z}_0 , provide the best way to learn from data using 'statistical approximations' around $\boldsymbol{\theta}^*$, framed in terms of sampling distributions of 'statistics' because they secure the effectiveness (reliability and precision) of inference and the trustworthiness of the ensuing evidence.

The <u>Data Science</u> algorithmic and the <u>Graphical Causal (GC) modeling</u> approaches share an <u>inbuilt proclivity</u> to <u>side-step</u> the **statistical misspecification** problem. The obvious way to <u>improve the trustworthiness of their evidence</u> is to **integrate** them within a broad **Fisher model-based statistical framework**. In turn, <u>sophisticated algorithms</u> can enhance the model-based approach in several ways, including more thorough M-S testing.

That, of course, would take a <u>generation</u> to be implemented mainly due to the pronounced <u>differences in culture</u> and terminology!

In the meantime the <u>trustworthiness of evidence</u> in <u>Data Science</u>, **can be ameliorated** using <u>simple M-S testing</u> to evaluate the <u>non-systematicity</u> of the **residuals** from the fitted curve $\hat{y}_t = g_m(\mathbf{x}_t; \hat{\boldsymbol{\psi}}_n)$, $\hat{\epsilon}_t = y_t - \hat{y}_t$, t = 1, 2, ..., n.

It is important to emphasize that **statistical 'excellent' prediction** is NOT just small prediction errors relative to a loss function, but non-systematic and 'small' prediction errors relative to <u>likelihood-based</u> goodness-of-prediction measures; see Spanos (2007).

"All models are wrong, but some are useful!" NO <u>statistically misspecified model</u> is useful for 'learning from data' about phenomena of interest!

7.2 Potential casualties of the STATISTICS WARS

- (1) Frequentist inference, in general, and hypothesis testing, in particular, as well as the frequentist underlying reasoning: factual and hypothetical.
- (2) Error probabilities and their key role in securing the trustworthiness of evidence by controlling & evaluating how severely tested claims are, including:
 - (a) Statistical adequacy: does $\mathcal{M}_{\theta}(\mathbf{z})$ account for the chance regularities in data \mathbf{Z}_0 ?
- (b) Substantive adequacy: does the model $\mathcal{M}_{\varphi}(\mathbf{z})$ shed adequate light on (describes, explains, predicts) the phenomenon of interest?
- (3) Mis-Specification (M-S) testing and respecification to account for the chance regularity patterns exhibited by data \mathbb{Z}_0 , and ensure that the substantive information does not belie the data.
- (4) Learning from data about phenomena of interest. Minimizing a risk function to reduce the <u>overall</u> Mean Square Prediction Error (MSPE) ' $\forall \psi_n \in \Psi$ ' <u>undermines</u> learning from \mathbf{Z}_0 about $\boldsymbol{\psi}^*$; Spanos (2017).

Thanks for listening!