

# Optimal data collection design in machine learning

# Introduction

A major current challenges in data science concerns:

1. Optimizing the acquisition costs (time and money) of big data to create novel opportunities for data analysts (Sivarajah et al., 2017).

Can we collect less data to reach the same desired statistical properties?

# Overview

**RQ:** is having "many but bad" examples always worse –in terms of minimization of the generalization error– than having "few but good" examples in a balanced fixed effects context with correlated errors?

## Main model

Fixed Effects GLS (FEGLS) output model taken from Wooldridge (2010) work 10:

$$y_{n,t} := \eta_n + \underline{\beta}' \underline{x}_{n,t}, \text{ for } n = 1, \dots, N, t = 1, \dots, T, \quad (1)$$

Outputs  $y_{n,t}$  are **unavailable** directly. Only noisy measurements  $z_{n,t}$  are available:

$$z_{n,t} := y_{n,t} + \varepsilon_{n,t}, \text{ for } n = 1, \dots, N, t = 1, \dots, T, \quad (2)$$

$\varepsilon_{n,t}$  identically distributed and  $\varepsilon_{n,t} \not\perp \varepsilon_{n,s}$ . We assume **strict exogeneity** of the explanatory variables conditional on  $\eta_n$  (Wooldridge, 2010). Notice that:

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{bmatrix}, \text{ where } X_n = \begin{bmatrix} \underline{x}'_{n,1} \\ \underline{x}'_{n,2} \\ \vdots \\ \underline{x}'_{n,T} \end{bmatrix} \text{ and } \underline{x}_{n,t} = ([x_{n,t,1} \cdots x_{n,t,p}])'$$

being  $\underline{x}_{n,t}$  the vector of features for unit  $n$  at time  $t$ .

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- ▶ An AR(1) model is assumed (Bhargava et al., 1982; Im et al., 1999):

$$\Lambda := \sigma^2 \Psi := \text{Var}(\underline{\varepsilon}_n) = \mathbb{E}\{\underline{\varepsilon}_n \underline{\varepsilon}_n'\} =$$

$$= \sigma^2 \begin{bmatrix} 1 & \rho & \rho^2 & \dots & \rho^{T-2} & \rho^{T-1} \\ \rho & 1 & \rho & \rho^2 & \dots & \rho^{T-2} \\ \rho^2 & \rho & 1 & \rho & \dots & \rho^{T-3} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \rho^{T-1} & \rho^{T-2} & \dots & \rho^2 & \rho & 1 \end{bmatrix} \in \mathbb{R}^{T \times T}, \quad (3)$$


$\Lambda$  matrix is

- **symmetric**
- positive semi-definite
- idempotent
- **positive-definite**
- eigenvalues multiplicity

After demeaning (Appendix) the resulting covariance matrix  $\mathbb{E}\{\underline{\tilde{\varepsilon}}_n \underline{\tilde{\varepsilon}}_n'\}$ —being  $\tilde{\varepsilon}$  the demeaned error term— has the expression

$$\begin{aligned}\Omega &:= \sigma^2 \Phi := \text{Var}(\underline{\tilde{\varepsilon}}_n) = \mathbb{E}\{\underline{\tilde{\varepsilon}}_n \underline{\tilde{\varepsilon}}_n'\} = Q_T \mathbb{E}\{\underline{\varepsilon}_n \underline{\varepsilon}_n'\} Q_T' = \\ &= Q_T \Lambda Q_T' = \sigma^2 Q_T \Psi Q_T',\end{aligned}\tag{4}$$

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- **symmetric**
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  - idempotent
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  - eigenvalues multiplicity

---

## PROBLEM:

Matrix (4) is rank deficient  
( $\text{rank}(\Omega) = T - 1 < T$ ).  
Cannot be inverted.

These produce the same  
estimate of  $\underline{\beta}$

- (a) project Eq. (2) onto  $L$   
(set of vectors orthogonal to  $\underline{1}_T$ ) (b)  
apply ordinary GLS

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## SOLUTIONS:

1. drop one of the time periods from the analysis (see, e.g. Im et al., 1999, Theorem 4.3)

2. Use the Moore-Penrose pseudoinverse of  $\Omega$ , denoted as  $\Omega^+$  (a)



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## Definition 1

Generalization error or expected risk for the  $i^{\text{th}}$  unit ( $i = 1, \dots, N$ ), conditioned on the training input data,

$$R_i \left( \{\underline{x}_{n,t}\}_{n=1,\dots,N}^{t=1,\dots,T} \right) := \mathbb{E} \left\{ \left( \hat{\eta}_{i,FEGLS} + \hat{\underline{\beta}}'_{FEGLS} \underline{x}_i^{\text{test}} - \eta_i - \underline{\beta}' \underline{x}_i^{\text{test}} \right)^2 \mid \{\underline{x}_{n,t}\}_{n=1,\dots,N}^{t=1,\dots,T} \right\} \quad (5)$$

Notice that  $R_i$  is defined on test data being a performance index.

In the next slides we will rewrite  $R_i$  conveniently.

Details on computations leading to the following expression of  $R_i$  are reported in the paper. Here it is worth noticing that the generalization error can be split into 6 components, namely:

$$\begin{aligned}
 R_i \left( \left\{ \underline{x}_{n,t} \right\}_{n=1, \dots, N}^{t=1, \dots, T} \right) &= \\
 &= \frac{\sigma^2}{T^2} \mathbf{1}'_T \mathbf{X}_i \left( \sum_{n=1}^N \ddot{\mathbf{X}}'_n \Phi + \ddot{\mathbf{X}}_n \right)^{-1} \mathbf{X}'_i \mathbf{1}_T + \frac{\sigma^2}{T^2} \mathbf{1}'_T \Psi \mathbf{1}_T \\
 &- \frac{2\sigma^2}{T^2} \mathbf{1}'_T \mathbf{X}_i \left( \sum_{n=1}^N \ddot{\mathbf{X}}'_n \Phi + \ddot{\mathbf{X}}_n \right)^{-1} \ddot{\mathbf{X}}'_i \Phi + Q_T \Psi \mathbf{1}_T \\
 &+ \sigma^2 \mathbb{E} \left\{ \left( \underline{x}_i^{\text{test}} \right)' \left( \sum_{n=1}^N \ddot{\mathbf{X}}'_n \Phi + \ddot{\mathbf{X}}_n \right)^{-1} \underline{x}_i^{\text{test}} \left\{ \left\{ \underline{x}_{n,t} \right\}_{n=1, \dots, N}^{t=1, \dots, T} \right\} \right. \\
 &- \frac{2\sigma^2}{T} \mathbf{1}'_T \mathbf{X}_i \left( \sum_{n=1}^N \ddot{\mathbf{X}}'_n \Phi + \ddot{\mathbf{X}}_n \right)^{-1} \mathbb{E} \left\{ \underline{x}_i^{\text{test}} \right\} \\
 &+ \frac{2\sigma^2}{T} (Q_T \Psi \mathbf{1}_T)' \Phi + \ddot{\mathbf{X}}_i \left( \sum_{n=1}^N \ddot{\mathbf{X}}'_n \Phi + \ddot{\mathbf{X}}_n \right)^{-1} \mathbb{E} \left\{ \underline{x}_i^{\text{test}} \right\}, \tag{6}
 \end{aligned}$$

In the work we derived a large-sample approximation of (6) with respect to  $T$ , for fixed  $N$ , which has its major applications in macroeconometrics.

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$$\text{plim}_{T \rightarrow +\infty} \frac{1}{T} \mathbf{1}'_T \mathbf{X}_i = \left( \mathbb{E} \left\{ \underline{\mathbf{x}}_{i,1} \right\} \right)', \quad (7)$$

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▶ If  $\lim_{T \rightarrow \infty} \|\Phi^+ - \mathbf{Q}_T \Psi^{-1} \mathbf{Q}'_T\|_2 = 0$  holds, then

$$\text{plim}_{T \rightarrow +\infty} \frac{1}{T} \sum_{n=1}^N \ddot{\mathbf{X}}_n' \Phi^+ \ddot{\mathbf{X}}_n = \mathbf{A}_N, \quad (9)$$

When (7)-(8)-(9) hold, then we can write the large-sample approximation of the generalization error  $R_i \left( \{\underline{x}_{n,t}\}_{n=1,\dots,N}^{t=1,\dots,T} \right)$  w.r.t.  $T$  as:

$$\begin{aligned}
 (6) &\simeq \frac{\sigma^2}{T} \left( \mathbb{E} \{ \underline{x}_{i,1} \} \right)' A_N^{-1} \mathbb{E} \{ \underline{x}_{i,1} \} + \frac{\sigma^2}{T} \frac{1 + \rho}{1 - \rho} \\
 &\quad + \frac{\sigma^2}{T} \mathbb{E} \{ (\underline{x}_i^{\text{test}})' A_N^{-1} \underline{x}_i^{\text{test}} \} - 2 \frac{\sigma^2}{T} \left( \mathbb{E} \{ \underline{x}_{i,1} \} \right)' A_N^{-1} \mathbb{E} \{ \underline{x}_i^{\text{test}} \} \\
 &= \frac{\sigma^2}{T} \left( \frac{1 + \rho}{1 - \rho} + \mathbb{E} \left\{ \left\| A_N^{-\frac{1}{2}} \left( \mathbb{E} \{ \underline{x}_{i,1} \} - \underline{x}_i^{\text{test}} \right) \right\|_2^2 \right\} \right), \quad (10)
 \end{aligned}$$

**Blue** and **cyan** terms of (6) disappear due to (8).



## Time to optimize...

**Aim:** Optimize (10) when

$$\sigma^2 = kc^{-\alpha}$$

being  $c \in [c_{min}, c_{max}]$  the cost per example with upper bound  $C$  on total supervision cost  $NTc$ .  $T \in [\frac{C}{c_{max}}, \dots, \frac{C}{c_{min}}]$ .

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### Scenarios:

1. "decreasing returns to scale\*":  $0 < \alpha < 1$
2. "increasing returns to scale\*":  $\alpha > 1$
3. "constant returns to scale\*":  $\alpha = 1$

\* of the precision with respect to the cost per example

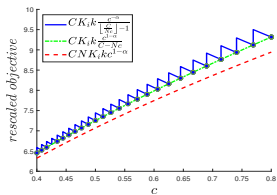
## Can we further simplify the analysis?

Actual optimization problem:

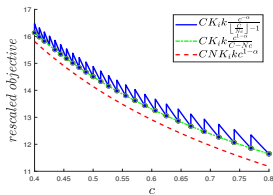
$$\underset{c \in [c_{\min}, c_{\max}]}{\text{minimize}} \quad K_i k \frac{c^{-\alpha}}{\left[ \frac{C}{Nc} \right]}. \quad (11)$$

**However...**

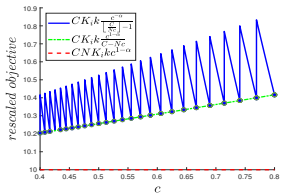
Following Gnecco and Nutarelli (2019<sup>[4]</sup>), the objective function of the optimization problem (11), rescaled by the multiplicative factor  $C$ , can be approximated, with a negligible error in the maximum norm on  $[c_{\min}, c_{\max}]$ , by  $NK_i kc^{1-\alpha}$ .



(a)  $\alpha = 0.5$



(b)  $\alpha = 1.5$



(c)  $\alpha = 1$

Figure 1: Plots of the rescaled objective functions  $CK_i k \frac{c^{-\alpha}}{\lfloor \frac{c}{Nc} \rfloor - 1}$ ,  $CNK_i k c^{1-\alpha}$ , and  $CNK_i k \frac{c^{1-\alpha}}{C - Nc}$

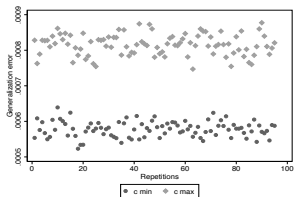
## Final optimization problem

$$\underset{c \in [c_{\min}, c_{\max}]}{\text{minimize}} \quad NK_j kc^{1-\alpha}, \quad (12)$$

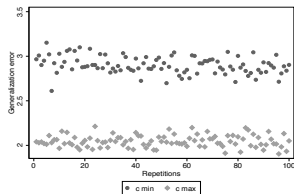
whose optimal solutions  $c^\circ$  have the following expressions:

1. if  $0 < \alpha < 1$  (“decreasing returns of scale”):  $c^\circ = c_{\min}$ ;
2. if  $\alpha > 1$  (“increasing returns of scale”):  $c^\circ = c_{\max}$ ;
3. if  $\alpha = 1$  (“constant returns of scale”):  $c^\circ =$  any cost  $c$  in the interval  $[c_{\min}, c_{\max}]$ .

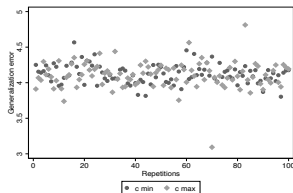
**Notice:** No assumptions of the probability distribution of the input examples is needed!



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(c)  $\alpha = 1$

Figure 2: Empirical approximations of the generalization error in the various scenarios  $\alpha = 0.5$ ,  $\alpha = 1.5$ ,  $\alpha = 1$

# Appendix



## Demearing step

Common practice in F.E.: eliminate unobserved individual heterogeneity ( $\eta_n$  in Eq. (1)). How?

**De-meaning** using  $Q_T \in \mathbb{R}^{T \times T}$

where

$$Q_T := I_T - \frac{1}{T} \mathbf{1}_T \mathbf{1}'_T$$

$Q_T$  matrix is

- **symmetric**
- **positive semi-definite**
- **idempotent**
- positive-definite
- **eigenvalues multiplicity**

## Proof of Eq.(7), sketch

$$\text{plim}_{T \rightarrow +\infty} \frac{1}{T} \mathbf{1}'_T \mathbf{X}_i = \left( \mathbb{E} \left\{ \underline{x}_{i,1} \right\} \right)',$$

### Proof.

- i) Replace the empirical average of  $\underline{x}'_{n,t}$  with the common expected value<sup>1</sup>
- ii) Apply Chebyshev's weak law of large numbers. □

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<sup>1</sup>since  $\mathbb{E} \left\{ \underline{x}_{i,t} \right\}$  is the same  $\forall t$  we arbitrarily chose  $t = 1$ .

## Proof of Eq.(8), sketch

$$\text{plim}_{T \rightarrow +\infty} \frac{1}{T} \ddot{X}'_i \Phi^+ Q_T \Psi \underline{1}_T = \underline{0}_p.$$

Proof.

- ▶ Step 1: define  $\underline{v}_T := Q' \Phi^+ Q \Psi \underline{1}_T = Q' \Phi^+ \underline{u}_T$
- ▶ Step 2: rewrite the argument of the *plim* using  $\underline{v}_T$ :

$$\frac{1}{T} \ddot{X}'_i \Phi^+ Q \Psi \underline{1}_T = \frac{1}{T} X'_i Q' \Phi^+ Q \Psi \underline{1}_T = \frac{1}{T} X'_i$$

- ▶ Step 3: Notice that in  $\frac{1}{T} X'_i$  is a weighted average with weights  $\underline{v}_T \rightarrow$  some law of large number must apply (Bai, Cheng, and Zhang (1997, Theorem 2.1));
- ▶ Step 4: check if  $\underline{v}_T$  and  $\frac{1}{T} X'_i$  satisfy the requirements of Bai, Cheng, and Zhang (1997, Theorem 2.1) (they do)

□

## Proof of Eq.(9), sketch

$$\text{plim}_{T \rightarrow +\infty} \frac{1}{T} \sum_{n=1}^N \ddot{X}'_n \Phi^+ \ddot{X}_n = A_N,$$

Proof.

- ▶ Step 1: prove that  $\ddot{X}'_n \Phi^+ \ddot{X}_n = X'_n Q' \Phi^+ Q X_n = X'_n \Phi^+ X_n = X'_n [\Phi^+ - Q\Psi^{-1}Q'] X_n + X'_n Q\Psi^{-1}Q' X_n$  .;
- ▶ Step 2: prove that  $\text{plim}_{T \rightarrow +\infty} \frac{1}{T} X'_n [\Phi^+ - Q\Psi^{-1}Q'] X_n = 0_{p \times p}$  .;
- ▶ Step 3: prove that  $\text{plim}_{T \rightarrow +\infty} \frac{1}{T} X'_n Q\Psi^{-1}Q' X_n = \frac{1+\rho^2}{1-\rho^2} \mathbb{E} \left\{ \left( \underline{x}_{n,1} - \mathbb{E} \left\{ \underline{x}_{n,1} \right\} \right) \left( \underline{x}_{n,1} - \mathbb{E} \left\{ \underline{x}_{n,1} \right\} \right)' \right\}$  .;
- ▶ Step 4: Combine Steps 1,2 and 3. Then sum over  $N$ .

□

## Set-up for simulations

For each  $c$ , an **empirical approximation** of the generalization error is computed:

$$\begin{aligned} & \sum_{i=1}^N \mathbb{E} \left\{ \left( \hat{\eta}_{i,FEGLS} + \hat{\underline{\beta}}'_{FEGLS} \underline{x}_i^{\text{test}} - \eta_i - \underline{\beta}' \underline{x}_i^{\text{test}} \right)^2 \mid \{ \underline{x}_{n,t} \}_{n=1, \dots, N}^{t=1, \dots, T} \right\} \\ \simeq & \frac{1}{N^{\text{test}}} \sum_{i=1}^N \sum_{h=1}^{N_i^{\text{test}}} \frac{1}{N^{\text{tr}}} \sum_{j=1}^{N^{\text{tr}}} \left( \hat{\eta}_{i,FEGLS}^j + \left( \hat{\underline{\beta}}_{FEGLS}^j \right)' \underline{x}_{i,h}^{\text{test}} - \eta_i - \underline{\beta}' \underline{x}_{i,h}^{\text{test}} \right)^2 \quad (13) \end{aligned}$$

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<sup>2</sup>Can provide further details at the end of the discussion

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(13) is based on  $N^{tr}$  training sets and  $N_i^{test}$  test examples for each unit  $i$  ( $i = 1, \dots, N$ ), hence on a total number  $N^{test} = \sum_{i=1}^N N_i^{test}$  of test examples.<sup>2</sup>

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## Details on simulations set-up

Fair comparison (since  $T$  depends on  $c$ ):

- ▶ The number of rows in each matrix  $X_n$  is increased when  $c$  is reduced from  $c_{\max}$  to  $c_{\min}$ , by increasing the number of observations  $T$ .
- ▶ For a fair comparison, when doing this, the rows already present in each matrix  $X_n$  **are kept fixed**.
- ▶ Finally, the **same** test examples (generated independently from the training sets) are used to assess the performance of the fixed effects generalized least squares estimates for different costs per example  $c$ .

We choose:

1.  $N = 20$ ,
2.  $p = 5$  (for the number of features),
3.  $c_{\min} = 2$ ,  $c_{\max} = 4$ ,
4.  $\mathcal{N}^{tr} = 100$  (for the number of training sets),
5.  $N_i^{test} = 50$  for the number of test examples per unit (hence the total number of test examples is  $N^{test} = 1000$ )

The number of training examples per unit is  $T = 50$  for  $c = c_{\min}$ , and  $T = 25$  for  $c = c_{\max}$ .<sup>3</sup> Without loss of generality, the constant  $k$  of the variance of the supervision cost is assumed to be equal to 1.

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<sup>3</sup>In this way, the (upper bound on the) total supervision cost is  $C = 2000$  for both cases.



The components of  $\underline{\beta}$  are generated randomly and independently according to a uniform distribution on  $[-1, 1]$ :



$$\underline{\beta} = [-0.8562, 0.6837, 0.2640, -0.0038, -0.0598]' . \quad (14)$$

The fixed effects  $\eta_n$  (for  $n = 1, \dots, N$ ) are generated similarly for each unit;




For both training and test sets, the input data associated with each unit are generated as realizations of a multivariate Gaussian distribution with mean  $\underline{0}$  and covariance matrix

$\text{Var}(\underline{x}_{n,t}) = \text{Var}(\underline{x}_i^{test}) = A_x A_x'$ , where the elements of  $A_x \in \mathbb{R}^{P \times P}$  have been randomly and independently generated according to a uniform probability density on the interval  $[0,1]$ .






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