Data enrichment for linear regression models

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*The work reported here was done for Google, not Stanford.

Some big and small data

1) Small targeted data set S, e.g.,
   - matched to target population (e.g. NYC area shoppers)
   - panel selected by probability sample (e.g. geographic distribution)
   - high quality covariates (e.g., age, gender, education)
2) Bigger, less targeted data set B, e.g.,
   - related population (e.g. entire US), or
   - panel accepted all who opted in, or,
   - some covariates imputed from a model

Goal

Fit a model for population S

taking advantage (if possible) from data B

Data

Small sample (X_i, Y_i) $i \in S$ $|S| = n$ observations

Big sample (X_i, Y_i) $i \in B$ $|B| = N$ observations

Issues

- Focus is on S
- B might have a different X distn
- B might have a different $Y \mid X = x$ distn
- X might be measured differently in B

Main choices

1) Model for $i \in S$ only
2) Model with $i \in S \cup B$ (pooling)
3) Choose 1 or 2 based on hypothesis test
4) Shrinkage $\checkmark$

Regression setup

$$Y_i = \begin{cases} X_i\beta + \varepsilon_i & i \in S \\ X_i(\beta + \gamma) + \varepsilon_i & i \in B \end{cases}$$

$$\text{Bias}: \quad \gamma \in \mathbb{R}^d \qquad \text{Noise}: \quad \varepsilon_i \sim \mathcal{N}(0, \sigma_S^2), \quad \mathcal{N}(0, \sigma_B^2)$$

Vector version

$$Y_S = X_S\beta + \varepsilon_S \qquad \& \qquad Y_B = X_B(\beta + \gamma) + \varepsilon_B$$

NOTES

- Google problems usually have categorical responses
- Gaussian assumption allows non-asymptotic results

Related literatures

Area	Method	One starting point
Survey sampling	Small area estimation	Rao (2003)
Chemometrics	Transfer calibration	Feudale et al. (2002)
Machine learning	Transfer learning	Cortes & Mohri (2011)
Medicine/Education	Meta-analysis	Borenstein et al. (2009)
Marketing	Data fusion	D'Orazio et al. (2006)

There are Bayesian approaches too.

Our approach is Steinian.

Data enriched regression

Minimize over β, γ:

$$\sum_{i\in S}(Y_i - X_i\beta)^2 + \sum_{i\in B}(Y_i - X_i(\beta+\gamma))^2 + \lambda P(\gamma)$$

$$= \quad \|Y_S - X_S\beta\|^2 \quad + \|Y_B - X_B(\beta+\gamma)\|^2 \quad + \lambda P(\gamma)$$

for fixed $\lambda \in [0,\infty]$ and penalty $P(\cdot)$.

Extreme cases

As $\lambda \to \infty$ we get pooling

As $\lambda \to 0$ we ignore the B data

Example penalties

$$\|\gamma\|^2 \qquad \|X_S\gamma\|^2 \qquad \|\gamma\|_1 \qquad \|X_S\gamma\|_1$$

First two are $\|X_T\gamma\|^2$, $X_T = X_S$ or $X_S = I$

As in ridge, we don't have to penalize the intercept

For large d we could/should also penalize β

Main findings

For $X_T = X_S$ or $X_T = I_d$ let

$$\hat{\beta}, \hat{\gamma} = \arg\min_{\beta,\gamma} \|Y_S - X_S\beta\|^2 + \|Y_B - X_B(\beta+\gamma)\|^2 + \lambda\|X_T\gamma\|^2$$

Our findings

1) how to compute $\hat{\beta}$ and $\hat{\gamma}$
2) fractional degrees of freedom as a function of λ
3) several ways to choose λ:
   AIC, AICc, cross-validation, bootstrap, plug-in
4) Stein-type result: using S only is inadmissible when $d \geqslant 5$ and error df $\geqslant 10$
5) Simulations validating theory

Stein results

Problem	Critical dimension	
Shrinking means to 0	$p \geqslant 3$	Stein
Shrinking means to common mean	$p \geqslant 4$	Efron & Morris
Shrinking regression coefficients	$p \geqslant 4$	Stein, Copas
Pooling two regression vectors	$p \geqslant 5$	us

Shrinking to something common seems to add 1 to the critical dimension

Our setting is a bit different. We measure loss only on S not B.

Estimation: just like ridge regression

$$\begin{pmatrix} \hat{\beta} \\ \hat{\gamma} \end{pmatrix} = (\mathcal{X}^\mathsf{T}\mathcal{X})^{-1}\mathcal{X}^\mathsf{T}\mathcal{Y}$$

$$\mathcal{X} = \begin{pmatrix} X_S & 0 \\ X_B & X_B \\ 0 & \lambda^{1/2} X_T \end{pmatrix} \qquad \mathcal{Y} = \begin{pmatrix} Y_S \\ Y_B \\ 0 \end{pmatrix}$$

E.g. $X_T = X_S$ or $X_T = I_d$

Degrees of freedom

For a matrix $W_\lambda \in \mathbb{R}^{d\times d}$ we get

$$\hat\beta = W_\lambda \hat\beta_S + (I - W_\lambda)\hat\beta_B$$
$$\hat\beta_S = (X_S^\mathsf{T} X_S)^{-1} X_S^\mathsf{T} Y_S$$
$$\hat\beta_B = (X_B^\mathsf{T} X_B)^{-1} X_B^\mathsf{T} Y_B$$

Ye & Efron df

$$\mathrm{df}(\lambda) \equiv \frac{1}{\sigma_S^2}\sum_{i\in S}\mathrm{Cov}(Y_i, \hat Y_i) = \mathrm{tr}(W_\lambda)$$

DF continued

Take special case penalty $P(\gamma) = \|X_S\gamma\|^2$ (i.e., $X_T = X_S$)

After some algebra

Let $\nu_1, \nu_2, \dots, \nu_d$ be eigenvalues of

$$(X_S^\mathsf{T} X_S)^{1/2}(X_B^\mathsf{T} X_B)^{-1}(X_S^\mathsf{T} X_S)^{1/2}$$

Then

$$\mathrm{df}(\lambda) = \sum_{j=1}^{d} \frac{1+\lambda\nu_j}{1+\lambda+\lambda\nu_j}$$

Upshot

- Easy to find λ for desired df
- df$(0) = d$
- df(∞) can be < 1

Picking λ

AIC: minimize $n\log\hat\sigma_S^2(\lambda)+n\Bigl(1+\frac{2\mathrm{df}(\lambda)}{n}\Bigr)$

AICc: minimize $n\log\hat\sigma_S^2(\lambda)+n\Bigl(\frac{1+\mathrm{df}(\lambda)/n}{1-(\mathrm{df}(\lambda)+2)/n}\Bigr)$ Hurvich & Tsai (1989)

Plug in

Derive optimal λ as if we knew γ, σ_S and σ_B

$$\lambda_{\mathrm{orcl}}(\gamma,\sigma_S,\sigma_B)$$

Plug in estimates

$$\hat\lambda=\lambda_{\mathrm{orcl}}(\hat\gamma,\hat\sigma_S,\hat\sigma_B)$$

Bias-corrected plug-in:

adjust for bias, eg $\mathbb{E}(\hat\gamma^{\mathsf{T}}\hat\gamma)\ne\gamma^{\mathsf{T}}\gamma$ for $\hat\gamma=\hat\beta_B-\hat\beta_S$

Sample reuse

Bootstrap: re-sample both S and B

Cross-validation: K-fold split of S, retain all of B

Special case: location

$$X_S = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^n \quad \text{and} \quad X_B = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^N$$

Rewrite model as

$$Y_i = \begin{cases} \mu + \varepsilon_i, & i \in S \\ \mu + \delta + \varepsilon_i, & i \in B \end{cases}$$

Minimize $\sum_{i \in S}(Y_i - \mu)^2 + \sum_{i \in B}(Y_i - \mu - \delta)^2 + \lambda\delta^2$

Get $\hat{\mu} = \omega \bar{Y}_S + (1 - \omega)\bar{Y}_B$

For $\omega = \frac{1+\lambda/N}{1+\lambda/N+\lambda/n}$

Location model

$$\hat{\mu} = \omega \bar{Y}_S + (1-\omega)\bar{Y}_B$$

We find

$$\omega_{\mathrm{orcl}} = \frac{\delta^2 + \sigma_B^2/N}{\delta^2 + \sigma_B^2/N + \sigma_S^2/n} \tag{1}$$

Judged by mean square error

Oracle's effective sample size is

$$n + \frac{\sigma_S^2}{\delta^2}$$

as $N \to \infty$ for fixed n.

Using the big sample adds information (does not multiply it).

Simulation (location)

$$X_i \sim \mathcal{N}(0,1), \qquad i \in S, \qquad n = 100$$

$$X_i \sim \mathcal{N}(\delta,1), \qquad i \in B, \qquad N = 1000$$

Relative bias

$$\delta_* = \frac{|\delta|}{\sigma_S/\sqrt{n}} = \sqrt{n}|\delta|$$

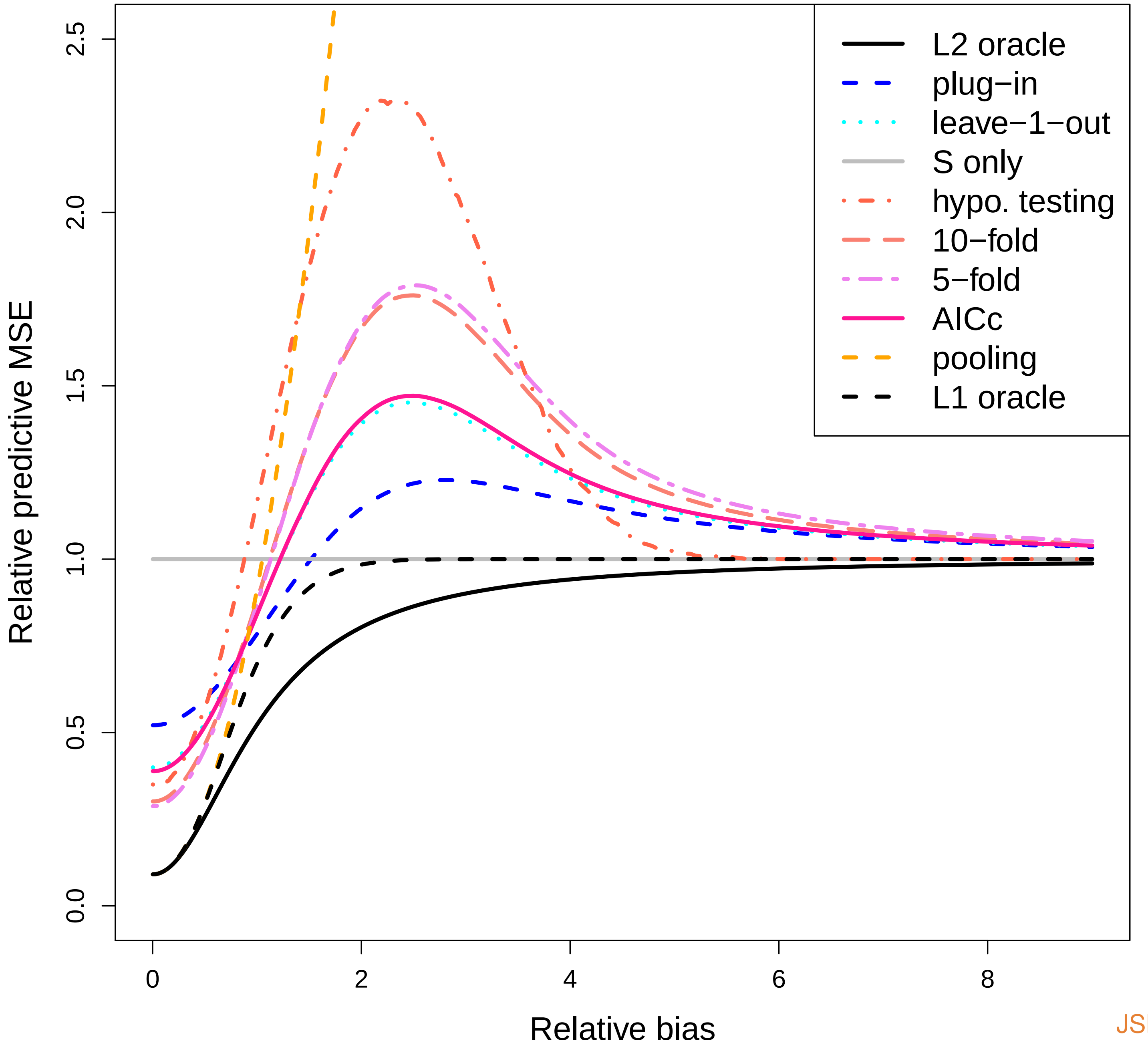
Relative MSE

$$\frac{(\hat{\mu}(\hat{\omega}) - \mu)^2}{\sigma_S^2/n}$$ equals 1 for $\bar{Y}_S$

repeat 10,000 times

NB: $\bar{Y}_S$ is admissible (Stein)

Simulation results



Simulation (regression)

Small sample, for $i \in S$

$$Y_i = X_i\beta + \varepsilon_i, \quad \text{(WLOG } \beta = 0\text{)}$$
$$X_i = (1, Z_i) \quad \text{(ie has intercept)}$$
$$Z_i \sim \mathcal{N}(0, C_S)$$
$$C_S \sim \text{Wishart}(I, d-1, d-1)$$

Big sample, for $i \in B$

$$Y_i = X_i\gamma + \varepsilon_i, \quad \gamma \text{ uniform on } d\text{-sphere}$$
$$X_i = (1, Z_i)$$
$$Z_i \sim \mathcal{N}(0, C_B)$$
$$C_B \sim \text{Wishart}(I, d-1, d-1)$$

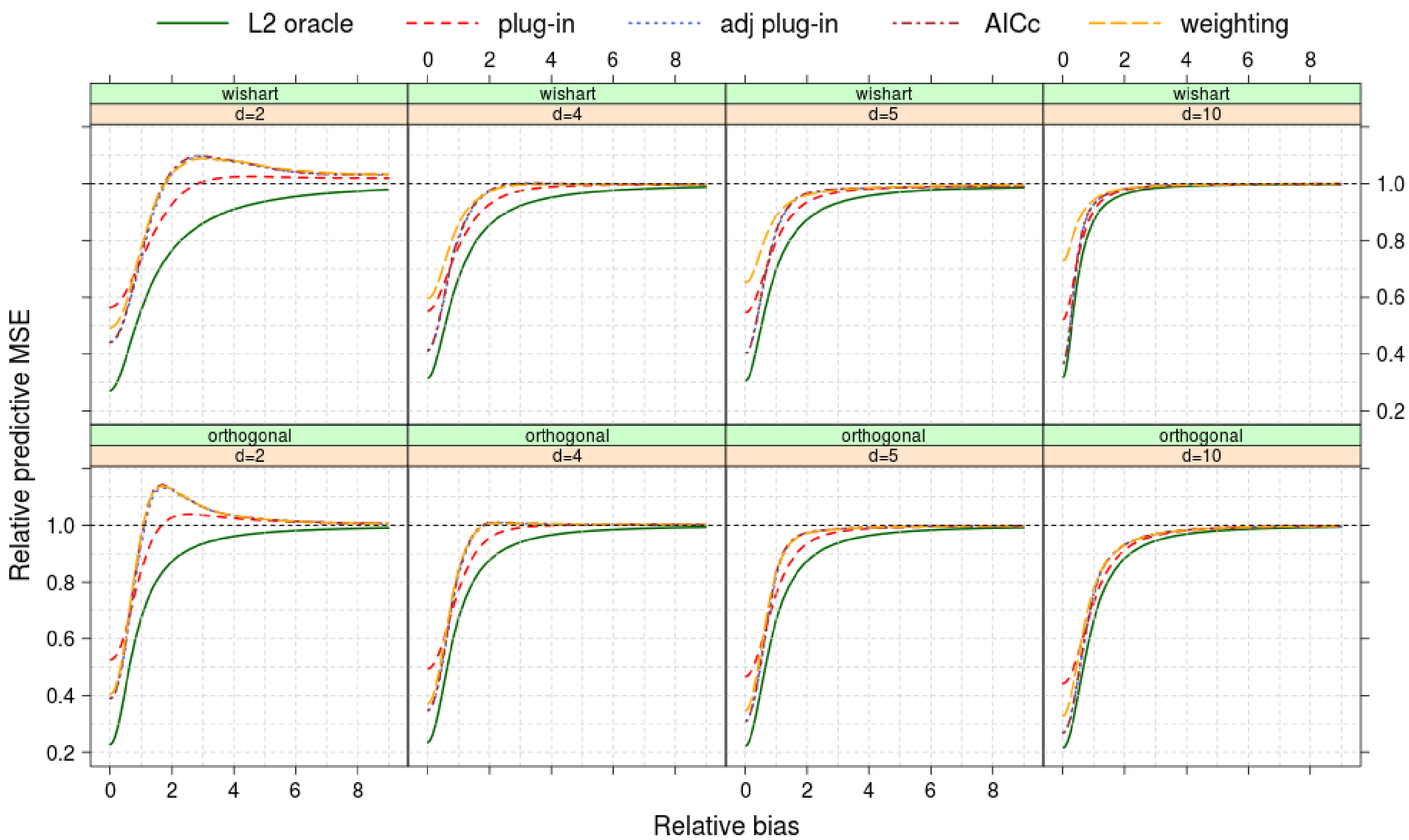
Second scenario

$$C_S = I + d u_S u_S^\mathsf{T} \qquad C_B = I + d u_B u_B^\mathsf{T} \qquad u_S, u_B \text{ uniform on } d-1\text{-sphere}$$

Sample sizes

$$n = 1000 \qquad N = 10{,}000$$

Regression results



Bias adjusted plug-in $\doteq$ AICc seem best overall (esp lower left & high dim)

Weighting is $\omega\hat\beta_S + (1-\omega)\hat\beta_B$ with plug-in ω

Inadmissibility of S only

1) Get the oracle's λ assuming $X_S^\mathsf{T} X_S = n\Sigma$ and $X_B^\mathsf{T} X_B = N\Sigma$
2) Plug-in estimates $\hat\gamma$, $\hat\sigma_S$, $\hat\sigma_B$ to pick λ
3) Resulting estimate makes $\hat\beta_S$ inadmissible
4) Even if assumption 1) is wrong

Inadmissibility ctd.

If $X_S^\mathsf{T} X_B = n\Sigma$ and $X_B^\mathsf{T} X_B = N\Sigma$, then

$$\hat\beta = \omega\hat\beta_S + (1-\omega)\hat\beta_B, \qquad 0 \leqslant \omega \leqslant 1$$

$$\omega_{\mathrm{orcl}} = \frac{\gamma^\mathsf{T}\Sigma\gamma + d\sigma_B^2/N}{\gamma^\mathsf{T}\Sigma\gamma + d\sigma_B^2/N + d\sigma_S^2/n}$$

Plug-in estimates

$$\hat\gamma = \hat\beta_B - \hat\beta_S, \quad \text{etc.}$$

$$\hat\omega_{\mathrm{plug}} = \frac{\hat\gamma^\mathsf{T}\Sigma\hat\gamma + d\hat\sigma_B^2/N}{\hat\gamma^\mathsf{T}\Sigma\hat\gamma + d\hat\sigma_B^2/N + d\hat\sigma_S^2/n}$$

$$\hat\omega_{\mathrm{plug},h} = \frac{\hat\gamma^\mathsf{T}\Sigma\hat\gamma + h(\hat\sigma_B^2)}{\hat\gamma^\mathsf{T}\Sigma\hat\gamma + h(\hat\sigma_B^2) + d\hat\sigma_S^2/n}$$

EG $h = 0$ or any $h \geqslant 0$ with $\mathbb{E}(h) < \infty$

Theorem

$X_S \in \mathbb{R}^{n\times d}, \qquad X_B \in \mathbb{R}^{N\times d}$ fixed full rank $\qquad X_S^\mathsf{T} X_S = n\Sigma$

$Y_S \sim \mathcal{N}(X_S\beta, \sigma_S^2 I_n) \qquad Y_B \sim \mathcal{N}(X_B(\beta+\gamma), \sigma_B^2 I_N)$ indep

If $d \geqslant 5$ and $n - d \geqslant 10$ then

$$\mathbb{E}\bigl(\|X_T(\hat\beta(\hat\omega) - \beta)\|^2\bigr) \; < \; \mathbb{E}\bigl(\|X_T(\hat\beta_S - \beta)\|^2\bigr)$$

For any $X_T^\mathsf{T} X_T = \Sigma$ and any $\hat\omega = \hat\omega_{\mathrm{plug},h}$

Chen, O, Shi (2012) on arXiv and

`http://research.google.com/pubs/pub41010.html`

Conclusions

There is something to gain by using data from a closely related sample

For $d \geqslant 5$ and $n - d \geqslant 10$ (and Gaussian data) ignoring the related sample is inadmissible

A key step is Stein's lemma which requires Gaussian data

We suspect the benefits extend beyond the Gaussian case

The algorithms but maybe not the theory extend to binary responses

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