



VARIABILITY OF CROSS-VALIDATION PREDICTION ERRORS: a statistical (machine) learning perspective



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Dairy Science

0. PHILOSOPHY OF PRESENTATION

- QUANTITATIVE TRAITS NOT WELL UNDERSTOOD (MECHANISTICALLY) IN ANIMAL AND PLANT BREEDING
- YET WE DO STUFF (PREDICT-SELECT), SEEMINGLY SUCCESSFULLY

“Would you refuse your dinner because you do not understand the digestive system?”

quote by British mathematician in
“The emperor of the maladies: a biography of cancer”, 2010, by
Siddhartha Mukherjee

PRE-DINNER: CAN ARGUE FROM PRE-CONCEIVED NOTIONS
POST-DINNER: CAN SAY WHETHER DINNER WAS GOOD OR BAD

"Clearly hypothesis testing and estimation as stressed in almost all statistics books involve parameters. . .this presumes the truth of the model and imparts an inappropriate existential meaning to an index or parameter. . .inferring about observables is more pertinent since they can occur and be validated to a degree that is not possible for parameters".

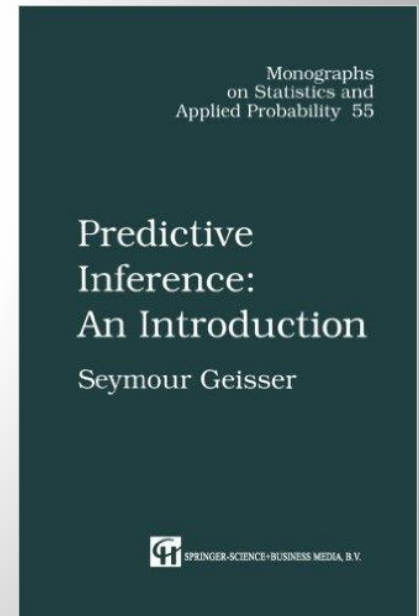
GEYSSER (1993)

Heritability: unobservable

Breeding values: unobservable

Prediction: statement about something yet-to-be observed, eventually observable

Phenotypes and functions thereof: observable



1. DISTRIBUTIONS OF ERRORS OF PREDICTION

(least-squares formulae but concepts carry to other methods)

1) Sampling over an infinite number of test sets, conditionally on training set and genotypes

$$\begin{aligned}
 E(PMSE|\mathbf{y}_{train}, \mathbf{X}_{train}, \mathbf{X}_{test}) &= \frac{1}{n_{test}} \left\{ \left(\boldsymbol{\mu}_{test} - \mathbf{X}_{test} \hat{\boldsymbol{\beta}} \right)' \left(\boldsymbol{\mu}_{test} - \mathbf{X}_{test} \hat{\boldsymbol{\beta}} \right) + tr [Var(\mathbf{y}_{test})] \right\} \\
 &= \frac{1}{n_{test}} \left[\left(\boldsymbol{\mu}_{test} - \mathbf{X}_{test} \hat{\boldsymbol{\beta}} \right)' \left(\boldsymbol{\mu}_{test} - \mathbf{X}_{test} \hat{\boldsymbol{\beta}} \right) + n_{test} \sigma_e^2 \right],
 \end{aligned}$$

2) Sampling over an infinite number of test and train sets, conditionally on genotypes

$$E(PMSE|\mathbf{X}_{train}, \mathbf{X}_{test}) = \frac{1}{n_{test}} \left\{ \boldsymbol{\delta}' \boldsymbol{\delta} + \sigma_e^2 tr[\mathbf{H}_{test,train}] + n_{test} \sigma_e^2 \right\}.$$

$$\begin{aligned}
 \boldsymbol{\delta} &= \boldsymbol{\mu}_{test} - \mathbf{X}_{test} E(\hat{\boldsymbol{\beta}}) = \boldsymbol{\mu}_{test} - \mathbf{X}_{test} (\mathbf{X}'_{train} \mathbf{X}_{train})^{-1} \mathbf{X}'_{train} \boldsymbol{\mu}_{train} \\
 &= \boldsymbol{\mu}_{test} - \mathbf{H}_{test,train} \boldsymbol{\mu}_{train}
 \end{aligned}$$

Pred. bias

It is unreasonable to dismiss prediction bias in more general settings because $\boldsymbol{\mu}_{test} \neq \mathbf{X}_{test} \boldsymbol{\beta}$ and $\boldsymbol{\mu}_{train} \neq \mathbf{X}_{train} \boldsymbol{\beta}$. Suppose now that the model is "wrong", that $n_{train} = n_{test}$, and that $\mathbf{X}_{test} = \mathbf{X}_{train} = \mathbf{X}$. In such a situation $\mathbf{H}_{test,train} = \mathbf{H}_{train,train}$, and (20) can be written as

$$E(PMSE|\mathbf{X}) = \frac{1}{n_{train}} \sum_{i=1}^{n_{train}} \delta_i^2 + \left(1 + \frac{p}{n_{train}} \right) \sigma_e^2, \quad (22)$$

Var-bias trade off

2) Sampling over an infinite number of test and train sets, AND genotypes

Observe that (22) gives the expected mean-squared error of prediction, conditionally on the realized values of \mathbf{X} . However, in genome-enabled prediction matrix \mathbf{X} has some distribution F that reflects linkage or linkage disequilibrium relationships (creating correlations among columns) as well as how genotypes are distributed in the target population, for example, a Hardy-Weinberg distribution. If the prediction model is to be applied repeatedly to a population, random variation of \mathbf{X} must be accommodated. The fully unconditional predictive mean-squared error is then

$$\begin{aligned} E(PMSE) &= \frac{1}{n_{train}} E \left[\sum_{i=1}^{n_{train}} \delta_i^2 \right] + \left(1 + \frac{p}{n_{train}} \right) \sigma_e^2 \\ &= \frac{1}{n_{train}} E \left[(\boldsymbol{\mu}_{test} - \mathbf{H} \boldsymbol{\mu}_{train})' (\boldsymbol{\mu}_{test} - \mathbf{H} \boldsymbol{\mu}_{train}) \right] \\ &\quad + \left(1 + \frac{p}{n_{train}} \right) \sigma_e^2. \end{aligned} \quad (23)$$

is $\mathbf{H} = \mathbf{X} (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}'$. Letting $E(\mathbf{H}) = \bar{\mathbf{H}}$

$$E(PMSE) = \left\{ \frac{1}{n_{train}} (\boldsymbol{\mu}_{test} - \bar{\mathbf{H}} \boldsymbol{\mu}_{train})' (\boldsymbol{\mu}_{test} - \bar{\mathbf{H}} \boldsymbol{\mu}_{train}) + tr [Var(\mathbf{H} \boldsymbol{\mu}_{train})] \right\} + \left(1 + \frac{p}{n_{train}} \right) \sigma_e^2. \quad (24)$$

Var-bias
trade off

The preceding implies that the contribution of bias (first part of the expression above) is a function of the unknown population means and of the distribution of genotypes in the population. Perhaps an elaborate model can palliate the adverse impact of bias on predictive performance, but the second part of the expression indicates that a highly parameterized model will produce predictions with larger variance than a "smaller" model. The upper limit of p is n_{train} (otherwise, the OLS estimator would not be unique), so the prediction error variance can almost double the residual variance in a model with many parameters. Unfortunately, the impact of model complexity on prediction bias is impossible to quantify in the absence of mechanistic knowledge.

2. DATA: PURE RANDOMNESS

- 599 LINES OF WHEAT PLANTED IN 3 ENVIRONMENTS
- GENOTYPED WITH DaRT MARKERS. TRAIT: GRAIN YIELD
- THINK OF ENVIRONMENT AS “COUNTRY”
- APPROXIMATE MULTIVARIATE ML: algorithm did not guarantee convergence inside of parameter space
- ➔ estimates “bent” to attain PD
- ➔ residual correlations between “countries” were 0.

> h2

[1] 0.5005951 0.4506505 0.4252388

> GENCOR

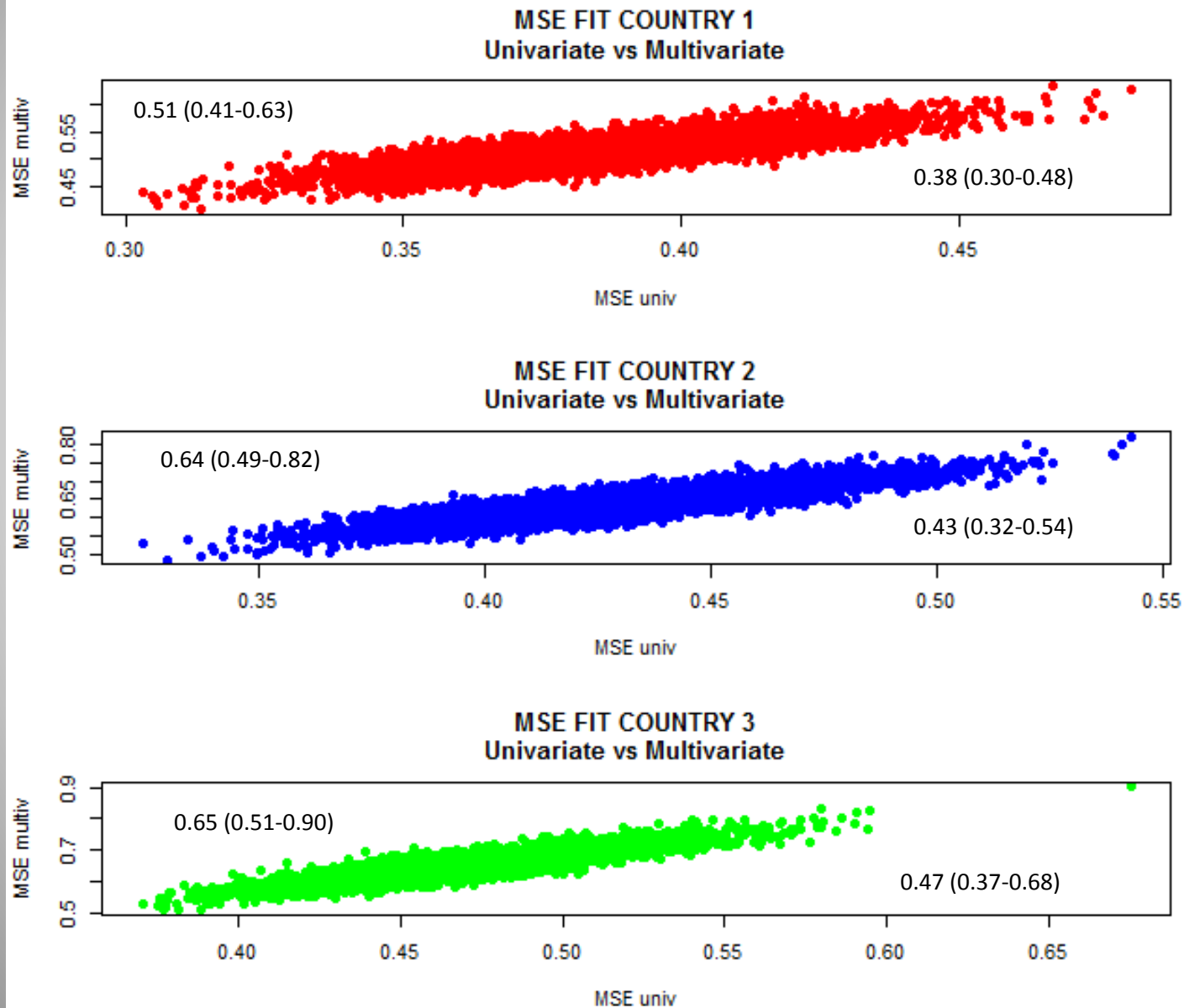
	[,1]	[,2]	[,3]
[1,]	1.0000000	-0.6379026	-0.5016693
[2,]	-0.6379026	1.0000000	-0.4210596
[3,]	-0.5016693	-0.4210596	1.0000000

IMPORTANT G X E SUGGESTED BY NEGATIVE GENETIC CORRELATIONS

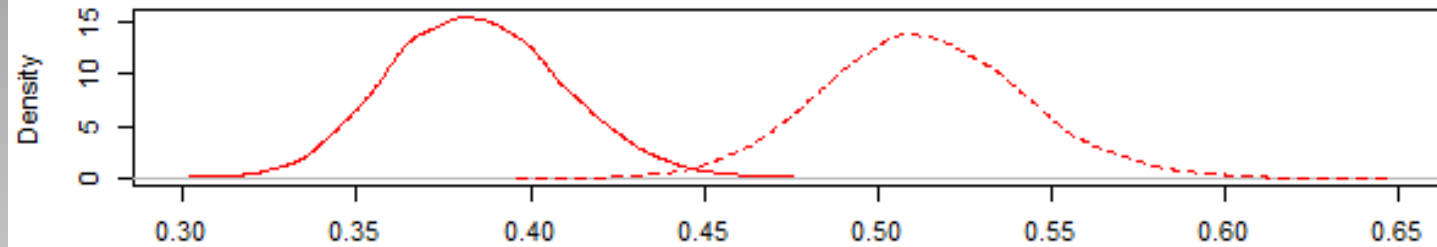
QUESTION: HOW DO WE MEASURE PREDICTION UNCERTAINTY FROM A SINGLE REALIZATION?

3. PURE RANDOMNESS: GOODNESS OF FIT

- UNIVARIATE G-BLUPS: “COUNTRIES” 1-2-3
- MULTIVARIATE G-BLUP: ACROSS COUNTRIES
- **MSE FIT**: 5000 bootstrap samples of residuals → median (min-max)



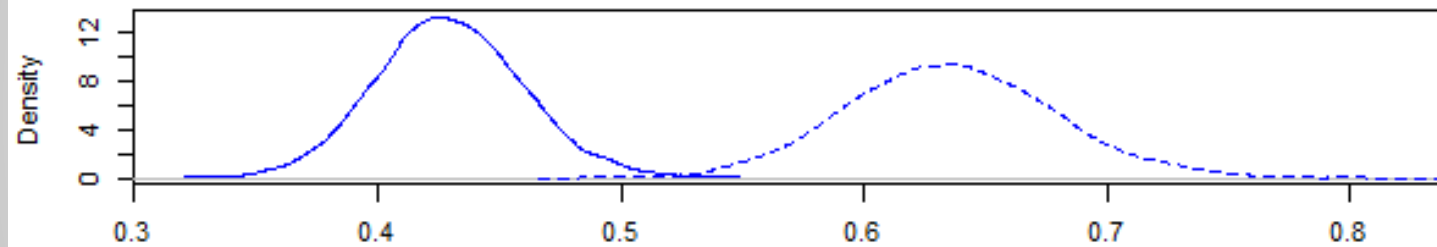
MSE FIT COUNTRY 1 b=5000
UNI= solid MULTI= dashed



N = 5000 Bandwidth = 0.004144

SMALLER MSE: BETTER FIT

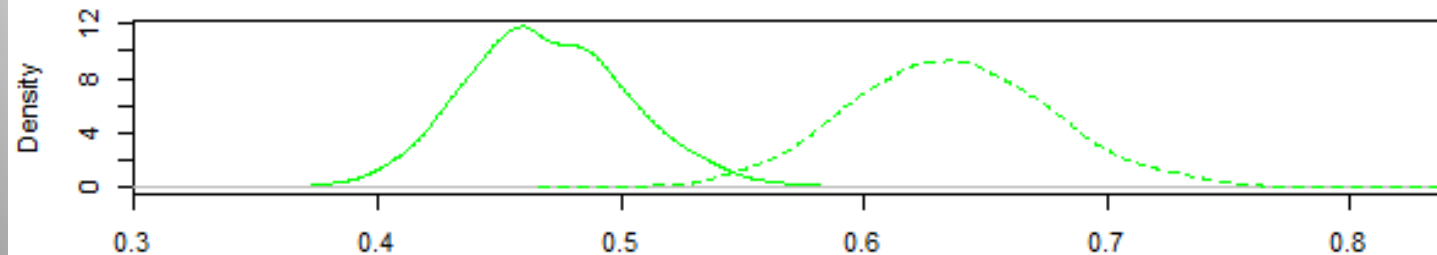
MSE FIT COUNTRY 2 b=5000
UNI= solid MULTI= dashed



N = 5000 Bandwidth = 0.004908

SMALLER MSE: BETTER FIT

MSE FIT COUNTRY 3 b=5000
UNI= solid MULTI= dashed



SMALLER MSE: BETTER FIT N = 5000 Bandwidth = 0.005585

Message 1

- “Bigger” model (MULTI) described data worse (larger MSE) than “smaller” mode(UNI)
- “Bigger” model produced more variable results
- Single analysis does not inform on variability.
- May suggest room for action, but cannot be used as basis for decision
- Resampling emulates a supply of training-testing sets

4. PURE RANDOMNESS: PREDICTIVE ABILITY OF UNIVARIATE MODELS

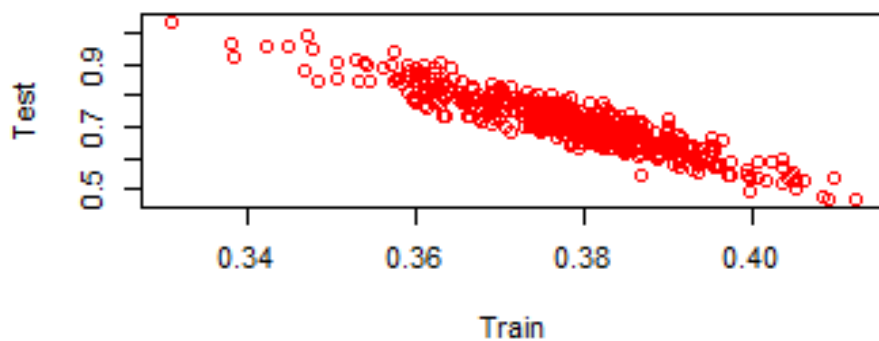
$$n=599$$

$$n_{Train} = 499$$

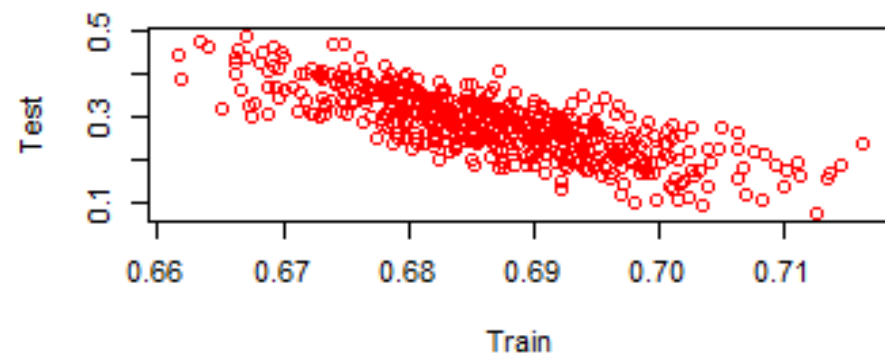
$$n_{Test} = 100$$

500 randomly reconstructed
training-testing sets

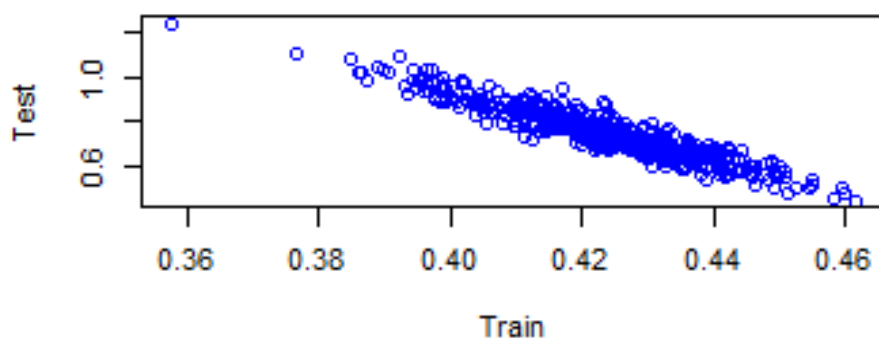
**MSE Train vs MSE Test
COUNTRY 1**



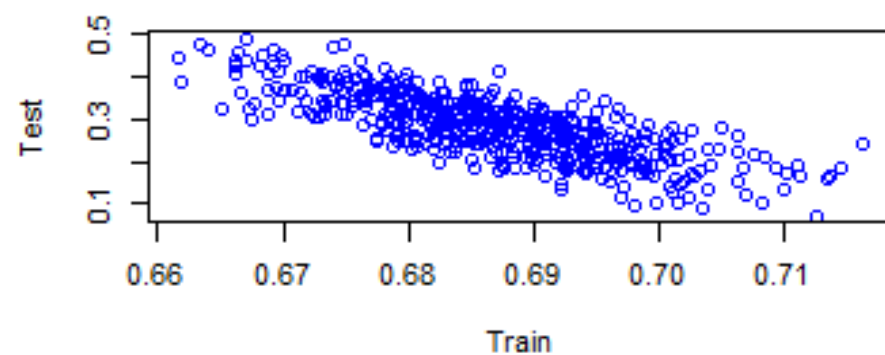
**R2 Train vs R2 Test
COUNTRY 1**



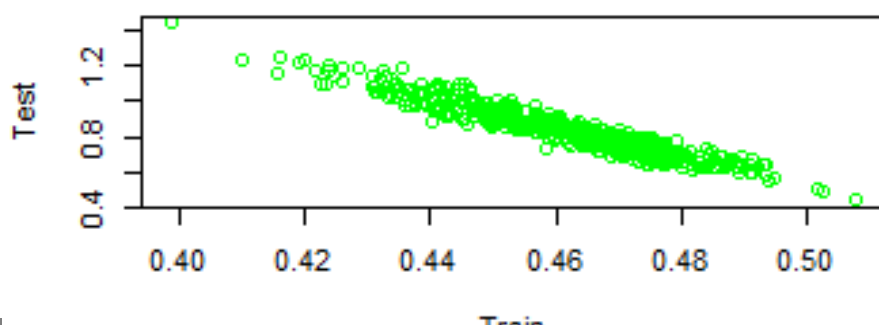
**MSE Train vs MSE Test
COUNTRY 2**



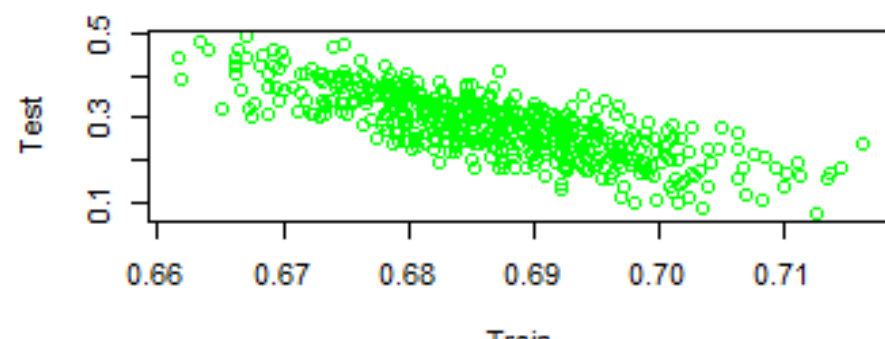
**R2 Train vs R2 Test
COUNTRY 2**



**MSE Train vs MSE Test
COUNTRY 3**



**R2 Train vs R2 Test
COUNTRY 3**



Message 2

- The closer the fit (MSE train) the poorer the predictions (MSE test)
- R^2 in test sets mildly associated with closeness (MSE)
- THE FOLLOWING IS A COMMERCIAL
- R^2 (predictive) seldom used in machine learning.
 1. It does not reflect bias
 2. Gives false idea about reproducibility





simplystats

ABOUT

CONFERENCE

COURSES

INTERVIEWS

12
AUG

Correlation is not a measure of reproducibility

POSTED BY RAFAEL IRIZARRY / UNCATEGORIZED

**Professor of Biostatistics,
T.H. Chan School of Public Health
Harvard University**

Suppose you have collected data from an experiment

$$x_1, x_2, \dots, x_n$$

and want to determine if a second experiment replicates these findings

$$y_1 = x_1 + d_1, y_2 = x_2 + d_2, \dots, y_n = x_n + d_n.$$

For us to claim reproducibility we want the differences

to be as small as possible $d_1 = y_1 - x_1, d_2 = y_2 - x_2, \dots, d_n = y_n - x_n$

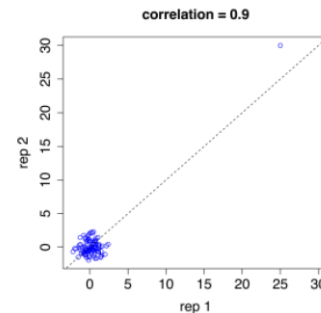
But aren't correlations and distances directly related? Sort of, and this actually brings up another problem. If the x and y are standardized to have average 0 and standard deviation 1 then, yes, correlation and distance are directly related:

$$\frac{1}{2n} \text{dist}(x, y)^2 = 1 - \text{cor}(x, y)$$

However, if instead x and y have different average values, which would put into question reproducibility, then distance is sensitive to this problem while correlation is not. If the standard deviation is 1, the formula is:

$$\frac{1}{2n} \text{dist}(x, y)^2 = 1 + \frac{1}{2} \{ \text{avg}(y) - \text{avg}(x) \}^2 - \text{cor}(x, y)$$

Add one point to uncorrelated data: 0.9 →

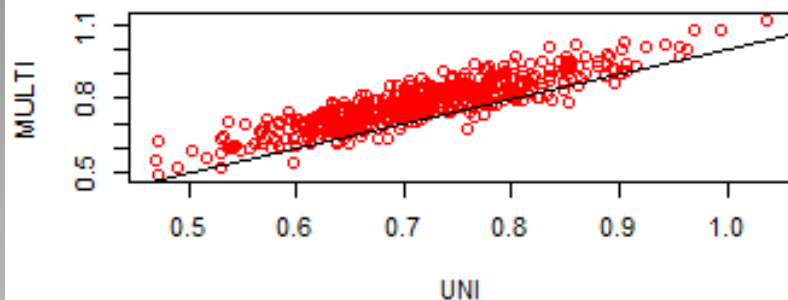


La-la Land

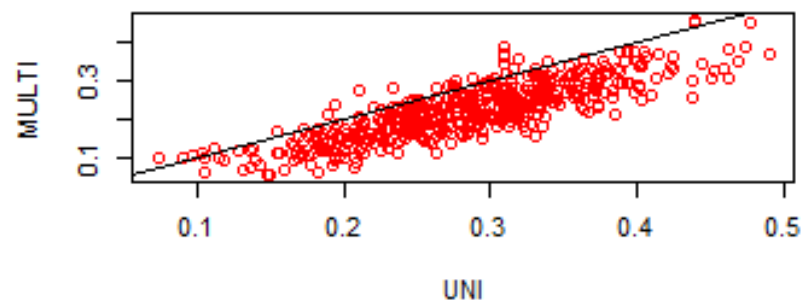
Hacksaw ridge

5. PURE RANDOMNESS: PREDICTIVE ABILITY OF MULTIVARIATE VERSUS UNIVARIATE

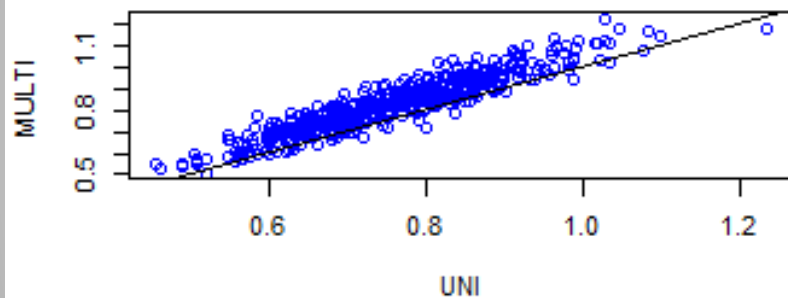
**MSE Test UNI VS MULTI
COUNTRY 1**



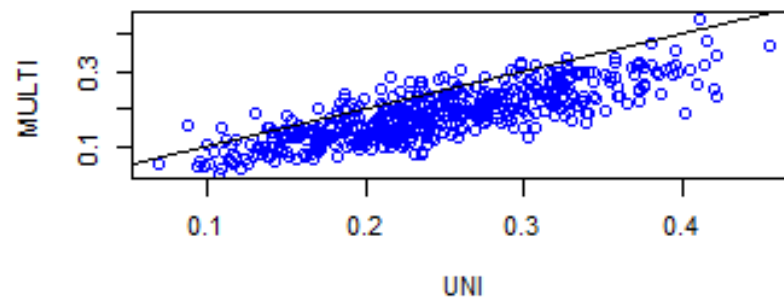
**R2 Test UNI VS MULTI
COUNTRY 1**



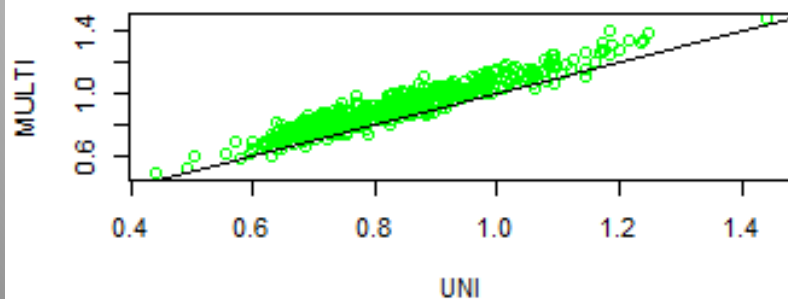
**MSE Test UNI VS MULTI
COUNTRY 2**



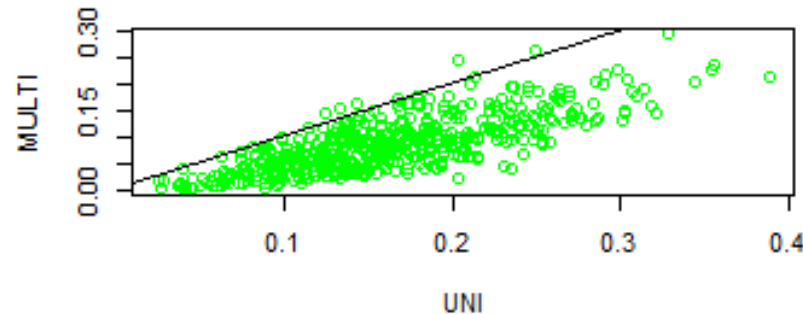
**R2 Test UNI VS MULTI
COUNTRY 2**



**MSE Test UNI VS MULTI
COUNTRY 3**



**R2 Test UNI VS MULTI
COUNTRY 2**



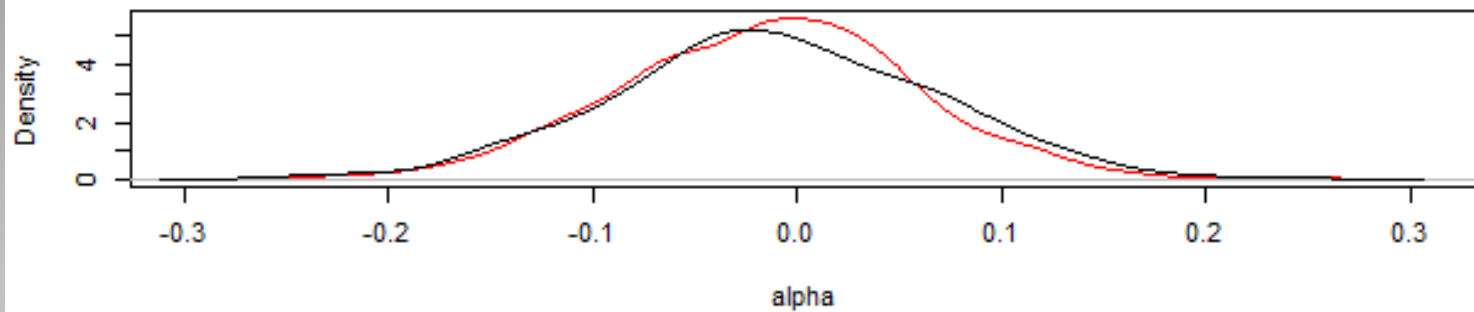
Message 3

- “Bigger” model (MULTI) predicted data worse (larger MSE) than “smaller” mode(UNI)
- “Bigger” model captured less variation in test sets (predictive R2 metric)
- MULTI predictions more variable in the predictive MSE sense and less variable in the predictive R2 sense
- Again, resampling emulated supply of training-testing sets, leading to clear+empirical measures of uncertainty

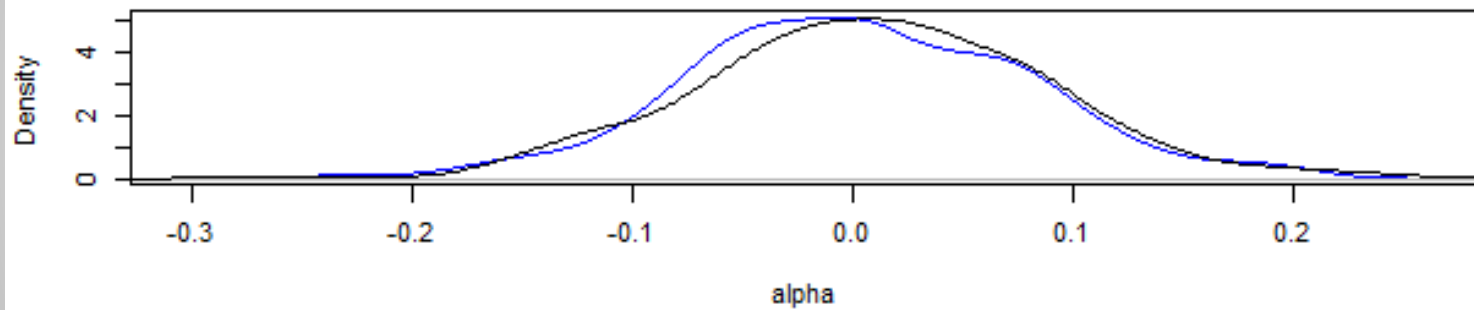
6. PURE RANDOMNESS: DEALING WITH
PREDICTION “BIAS” VIA THE
ALPHABETA TEST

(regression of predictand on prediction)

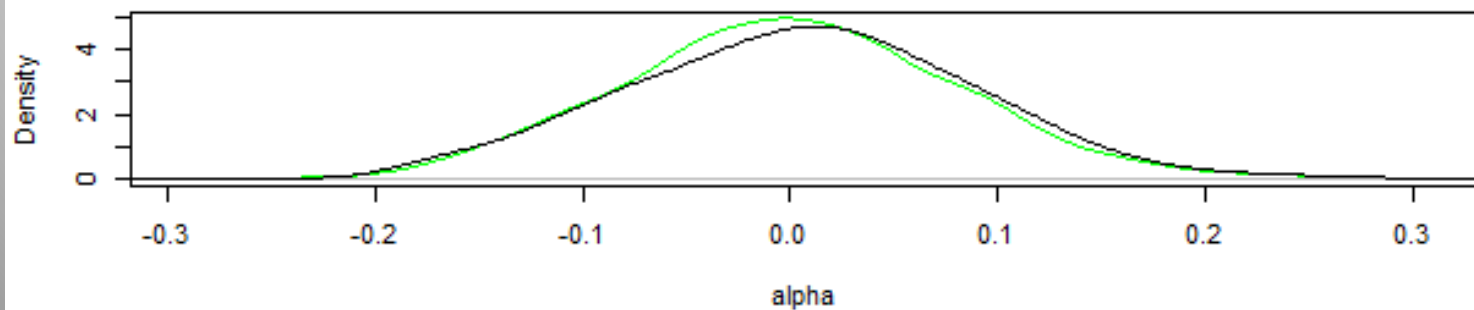
**ALPHA Test UNI (RED) VS MULTI (BLACK)
COUNTRY 1**



**ALPHA Test UNI (BLUE) VS MULTI (BLACK)
COUNTRY 2**

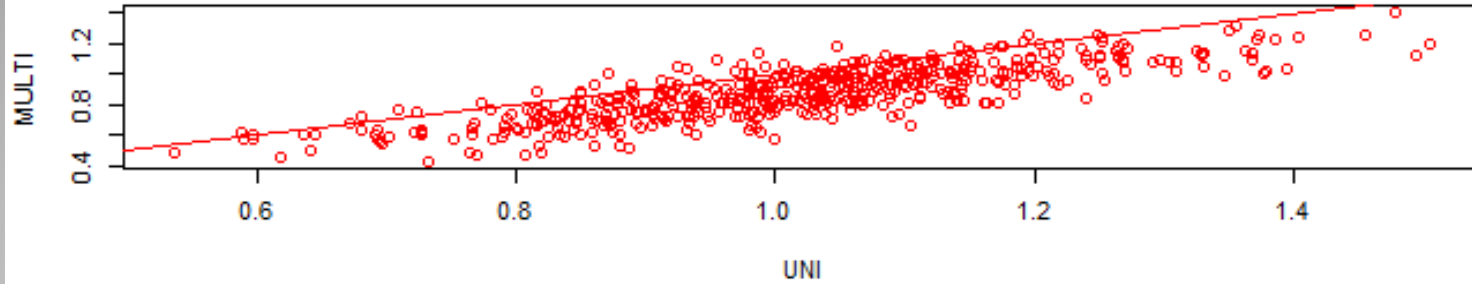


**ALPHA Test UNI (GREEN) VS MULTI (BLACK)
COUNTRY 3**

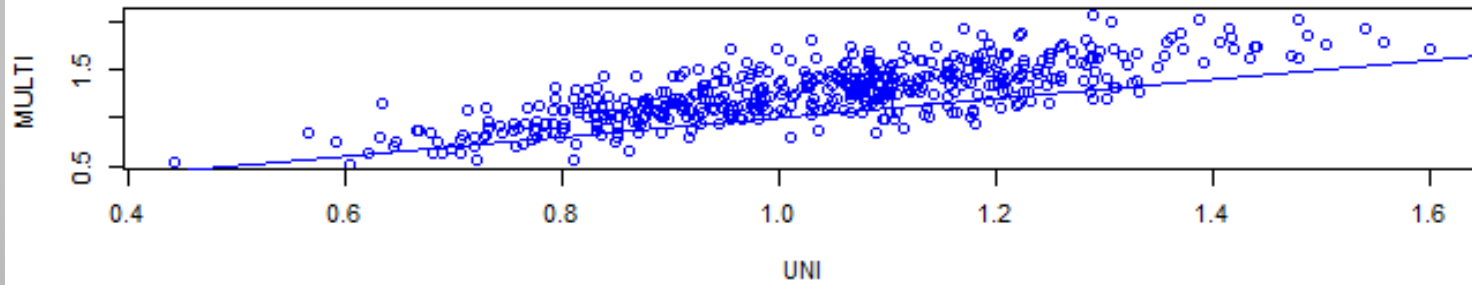


BETAS LOWER FOR MULTI IN COUNTRY 1 AND HIGHER IN COUNTRY 2
PERHAPS SOMETHING GOING ON HERE?

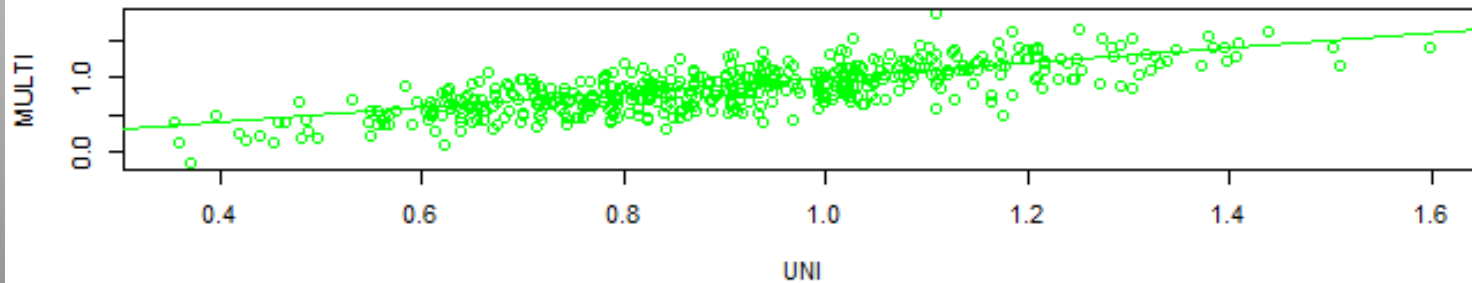
BETA Test UNI (RED) VS MULTI (BLACK)
COUNTRY 1



BETA Test UNI (RED) VS MULTI (BLACK)
COUNTRY 2

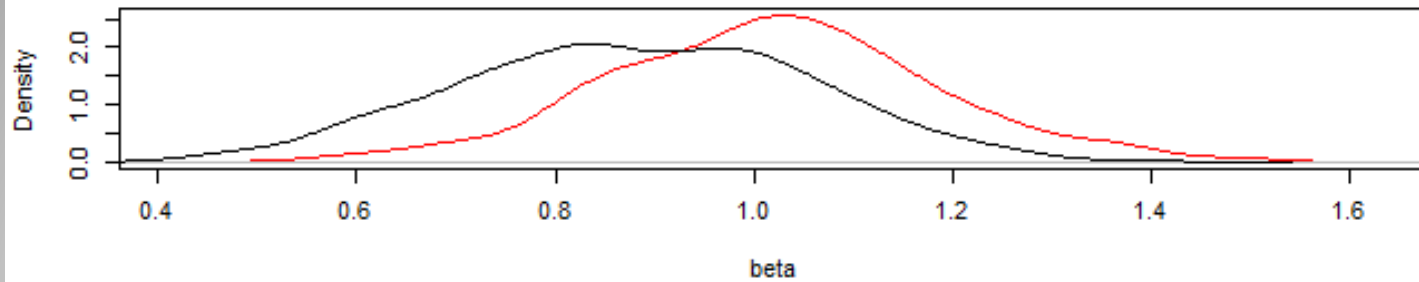


BETA Test UNI (RED) VS MULTI (BLACK)
COUNTRY 3

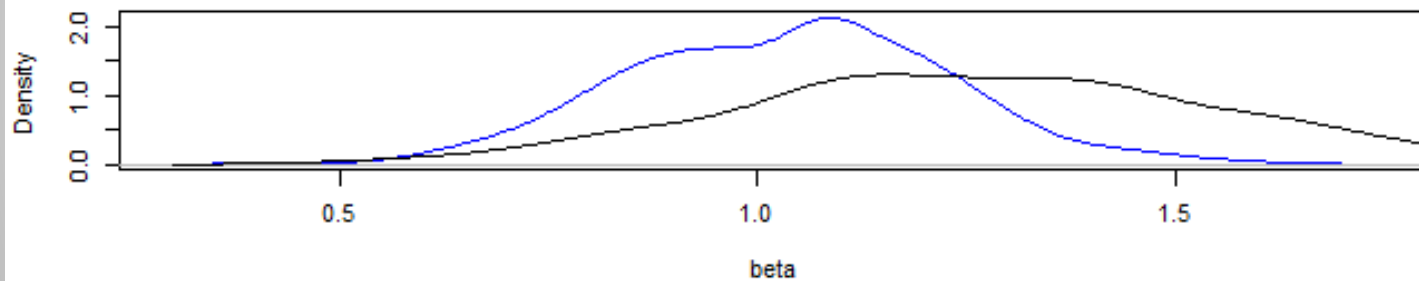


OBSERVE SPREAD AND DENSITY SHAPES. 500 RE-SAMPLES NOT ENOUGH

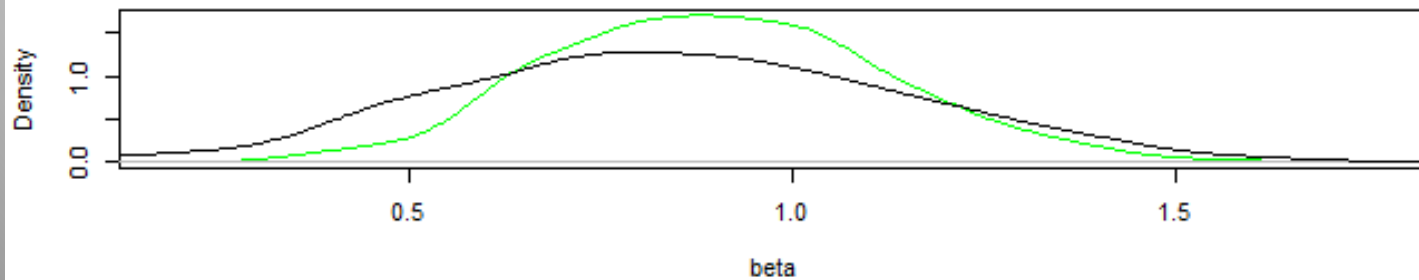
BETA Test UNI (RED) VS MULTI (BLACK)
COUNTRY 1



BETA Test UNI (BLUE) VS MULTI (BLACK)
COUNTRY 2



BETA Test UNI (GREEN) VS MULTI (BLACK)
COUNTRY 3

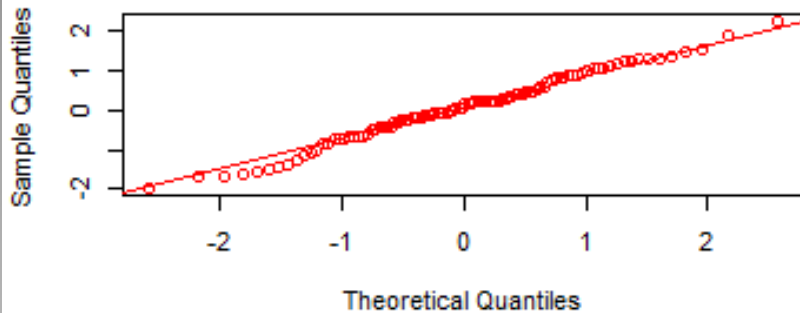


7A. CREATING BIAS ARTIFICIALLY

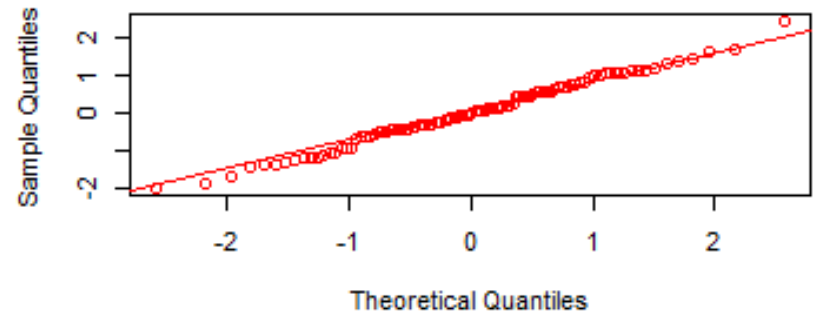
- MODEL TRAINED IN POPULATION 1 WITH **BEST** 499 LINES
- POPULATIONS 2 AND 3 WITH 499 RANDOM LINES
- UNIVARIATE MODELS+ MULTI-TRAIT MODEL
- 5000 BOOTSTRAP SAMPLES OF THE TESTING SET DISTRIBUTION

CAN WE DIAGNOSE SOMETHING FROM THE DISTRIBUTION OF PREDICTION ERRORS?

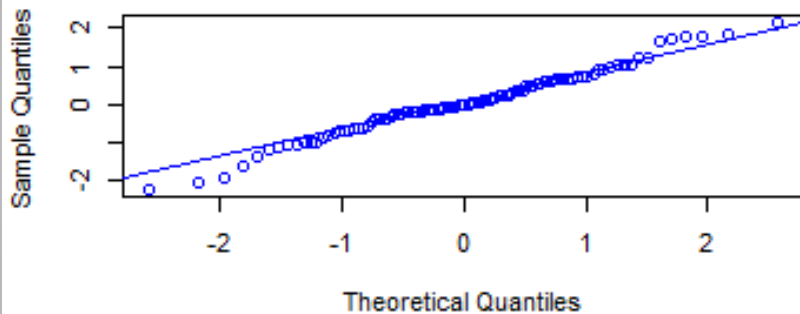
**TEST SET PREDICTION ERRORS
UNIVARIATE COUNTRY 1: RED**



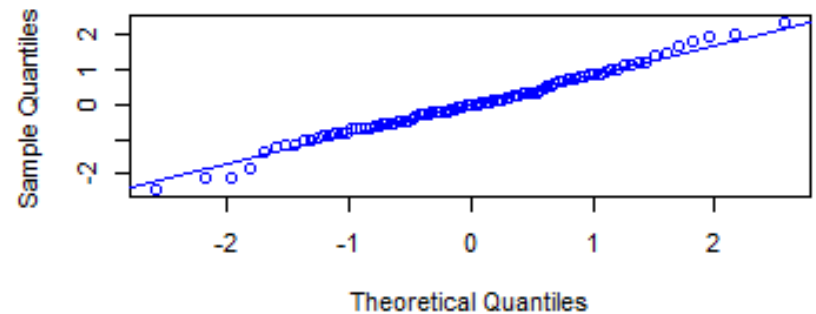
**TEST SET PREDICTION ERRORS
MULTIVARIATE COUNTRY 1: RED**



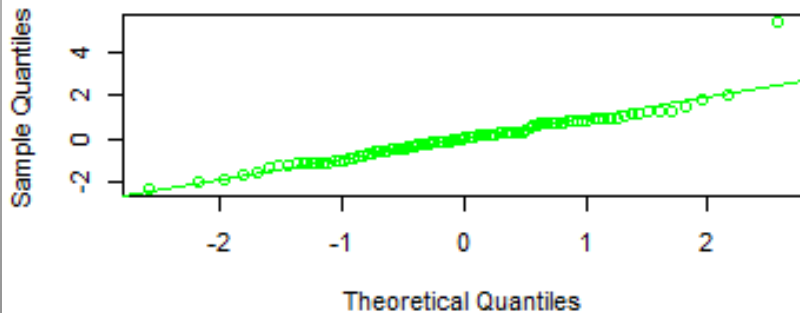
**TEST SET PREDICTION ERRORS
UNIVARIATE COUNTRY 2: BLUE**



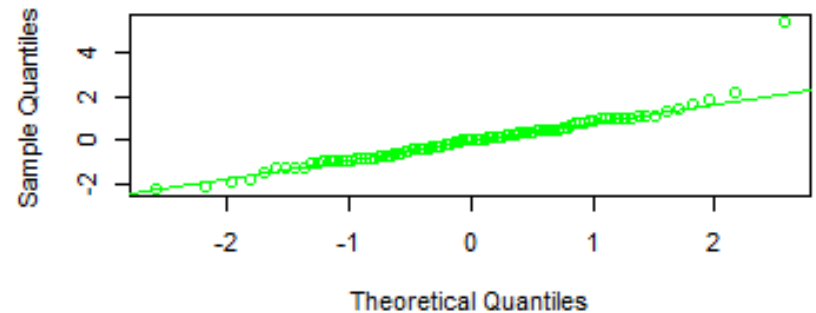
**TEST SET PREDICTION ERRORS
MULTIVARIATE COUNTRY 2: BLUE**



**TEST SET PREDICTION ERRORS
UNIVARIATE COUNTRY 3: GREEN**



**TEST SET PREDICTION ERRORS
MULTIVARIATE COUNTRY 1: GREEN**

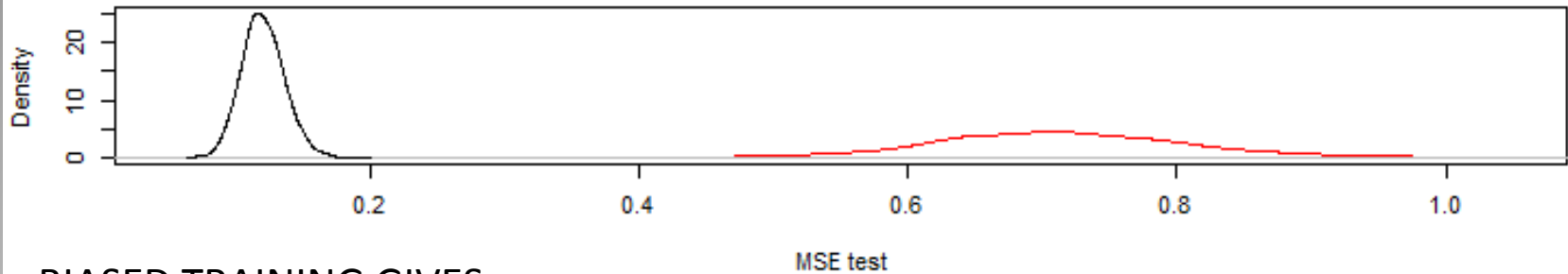


Message 4

MULTI-TRAIT MODEL “IMPROVES” CONFORMITY OF THE
PREDICTION ERROR DISTRIBUTION WITH GAUSSIAN PROCESS
...BY SOME

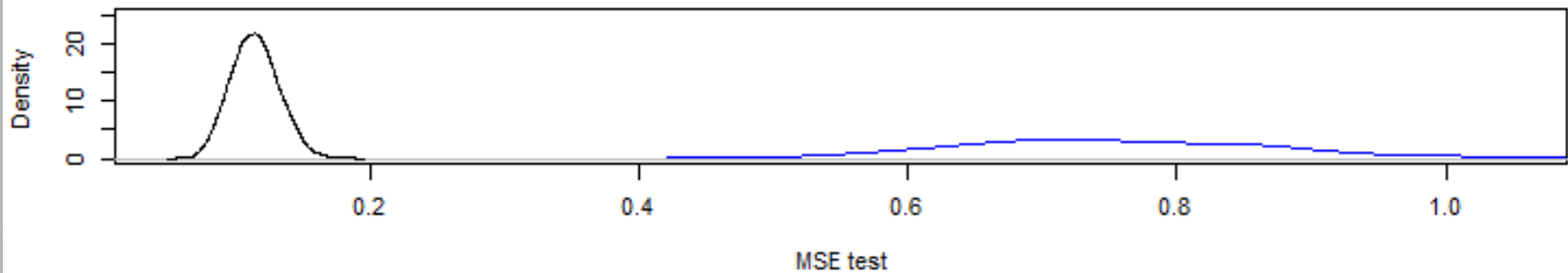
MOST IMPROVEMENT IS FOR POPULATION IN WHICH TRAINING
BIAS OCCURS

MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
UNIVARIATE COUNTRY 1: red

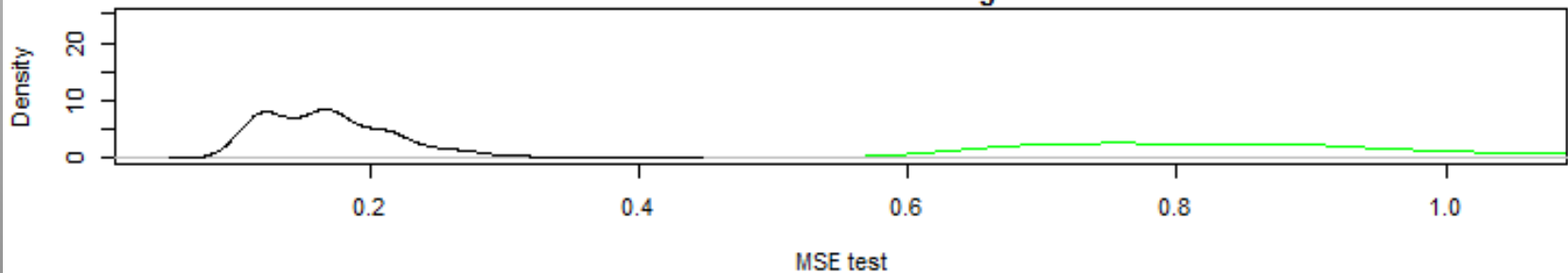


BIASED TRAINING GIVES
"CLOSER" PREDICTIONS

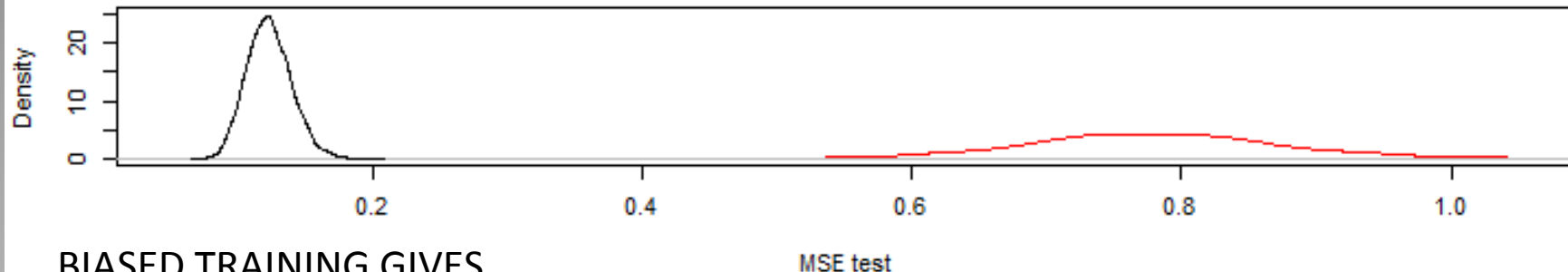
MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
UNIVARIATE COUNTRY 2: blue



MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
UNIVARIATE COUNTRY 3: green

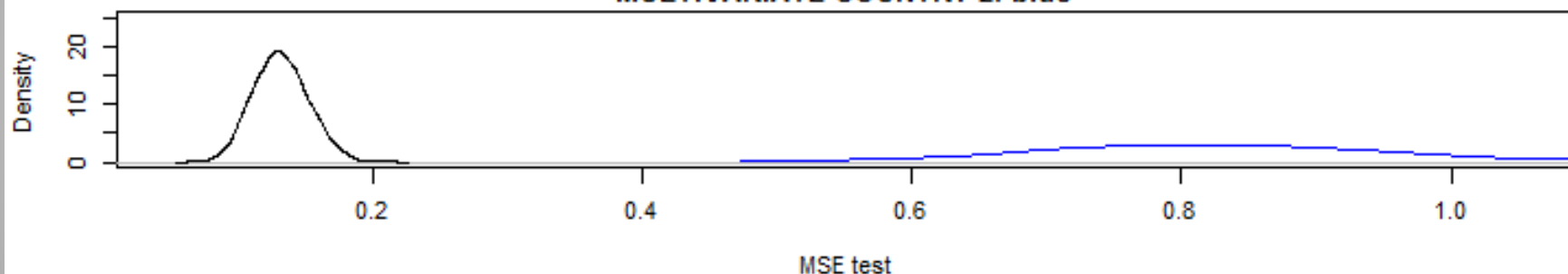


MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red

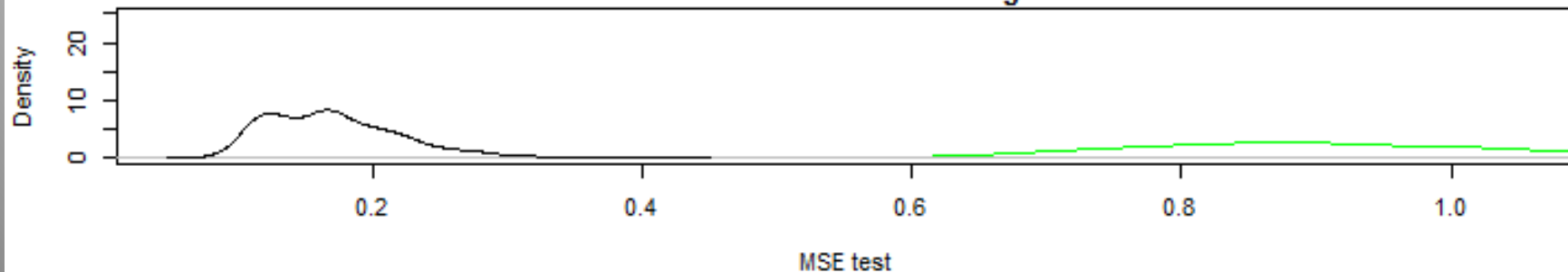


BIASED TRAINING GIVES
"CLOSER" PREDICTIONS

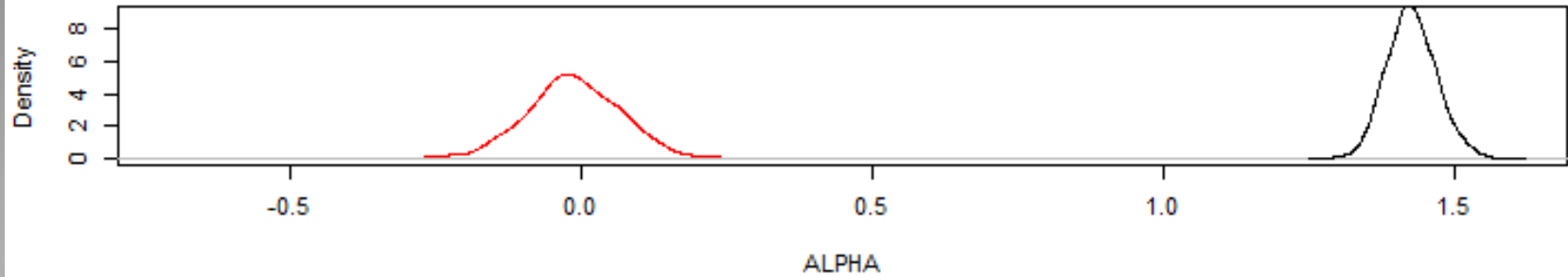
MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue



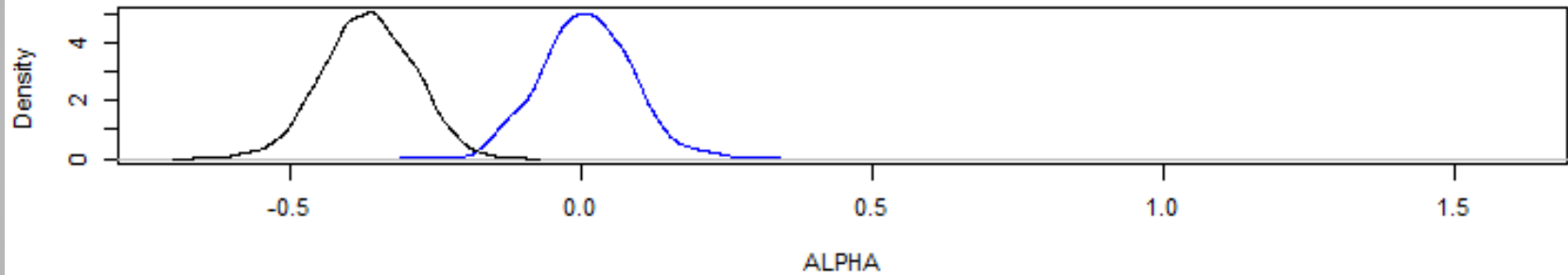
MSE test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green



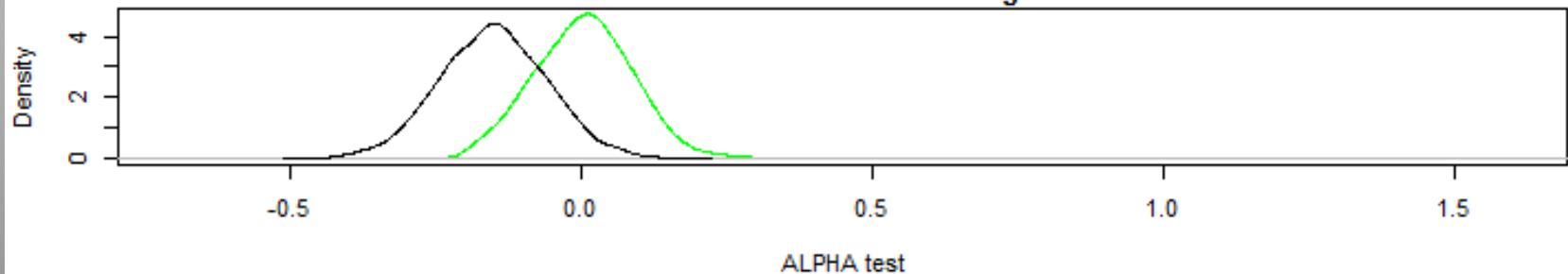
ALPHA test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red



ALPHA test random (blue) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue

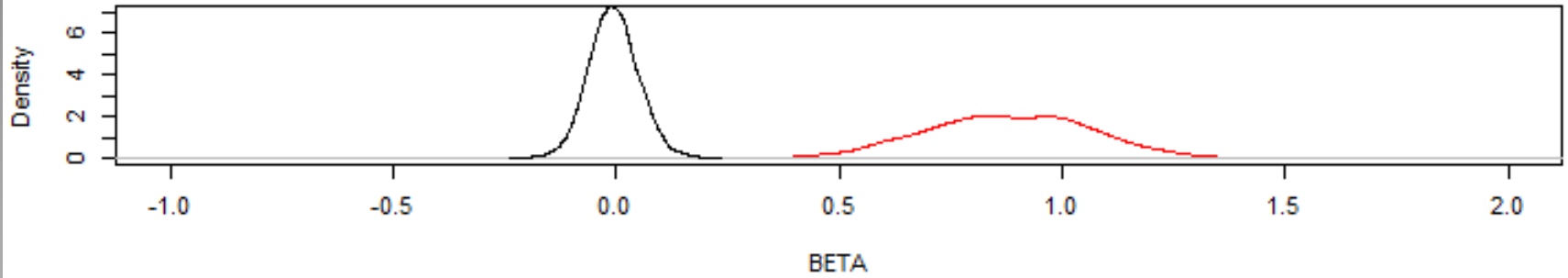


ALPHA test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green

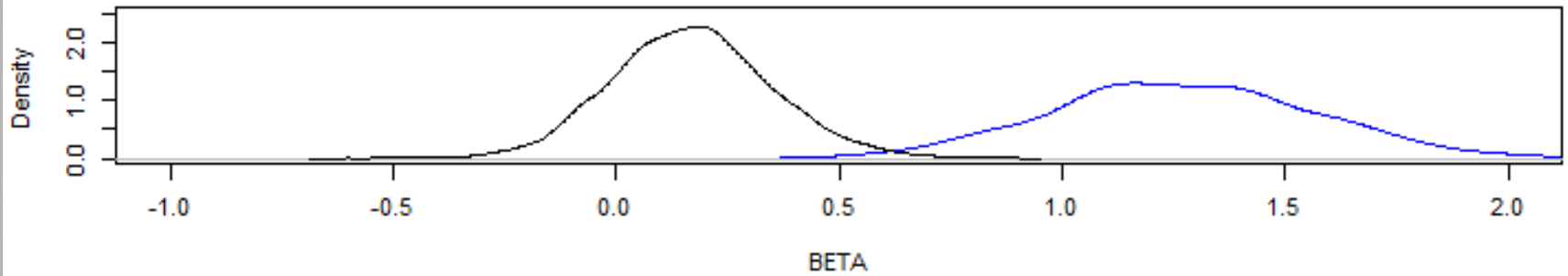


ALPHA TEST CAPTURES BIAS: EASIER TO DIAGNOSE IN "BAD HOMBRES" COUNTRY

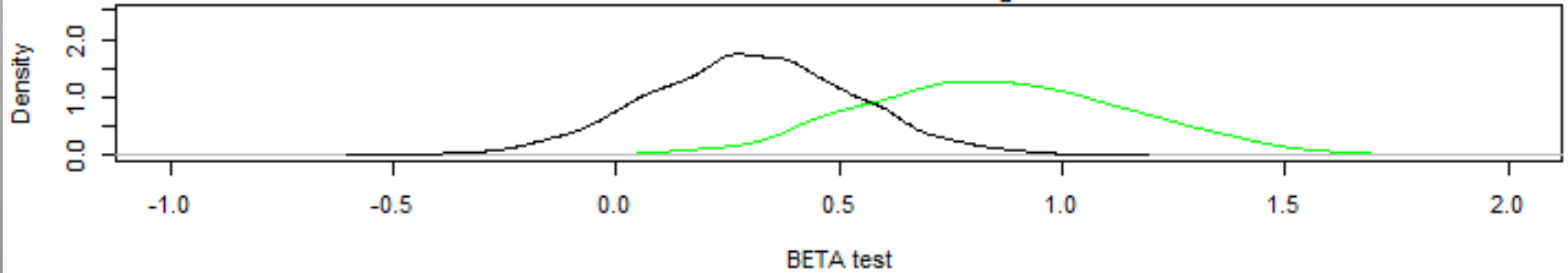
BETA test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red



BETA test random (blue) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue



BETA test random (red) vs biased sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green



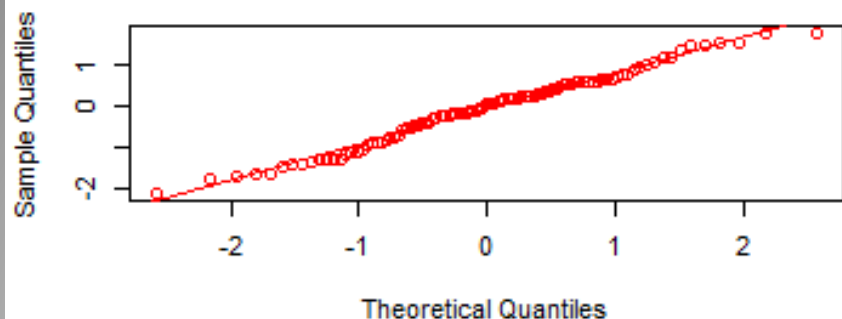
BETA TEST CAPTURES BIAS: EASIER TO DIAGNOSE IN "BAD HOMBRES" COUNTRY

7A. CREATING BIAS ARTIFICIALLY

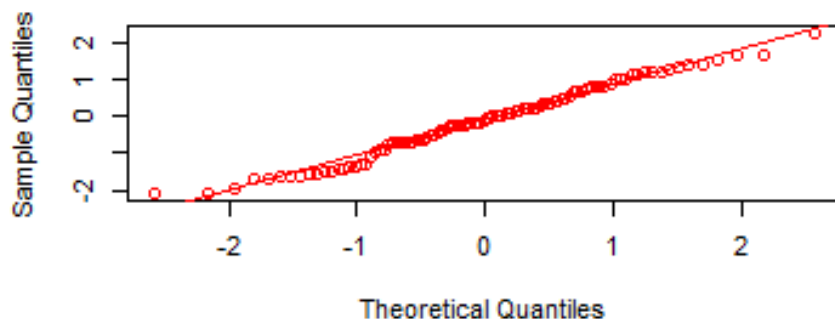
- ➔ MODEL TRAINED IN POPULATION 1 WITH **WORST** 499 LINES
- ➔ POPULATIONS 2 AND 3 WITH 499 RANDOM LINES
- ➔ UNIVARIATE MODELS+ MULTI-TRAIT MODEL
- ➔ 5000 BOOTSTRAP SAMPLES OF THE TESTING SET DISTRIBUTION

CAN WE DIAGNOSE SOMETHING FROM THE DISTRIBUTION OF PREDICTION ERRORS?

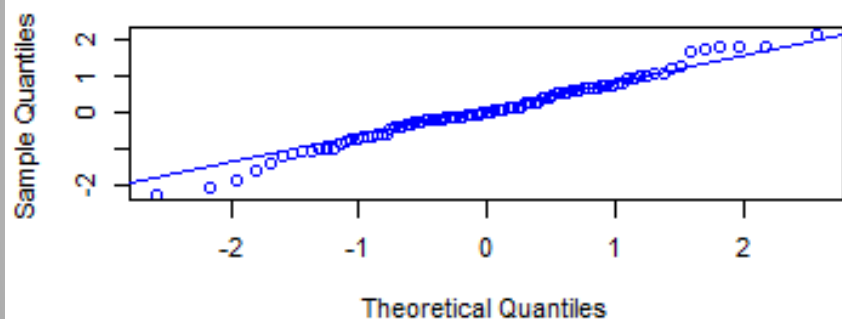
TEST SET PREDICTION ERRORS SEL DOWN
UNIVARIATE COUNTRY 1: RED



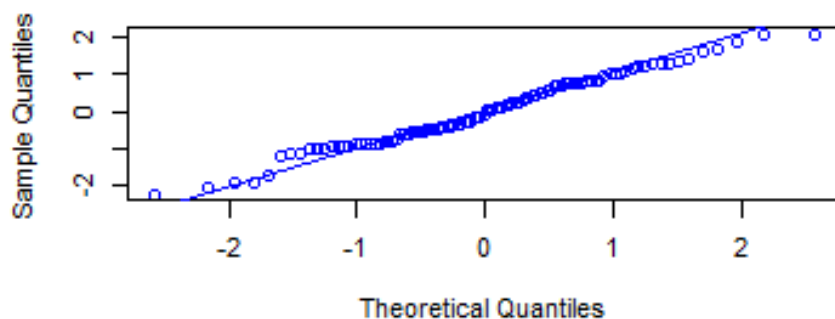
TEST SET PREDICTION ERRORS SEL DOWN
MULTIVARIATE COUNTRY 1: RED



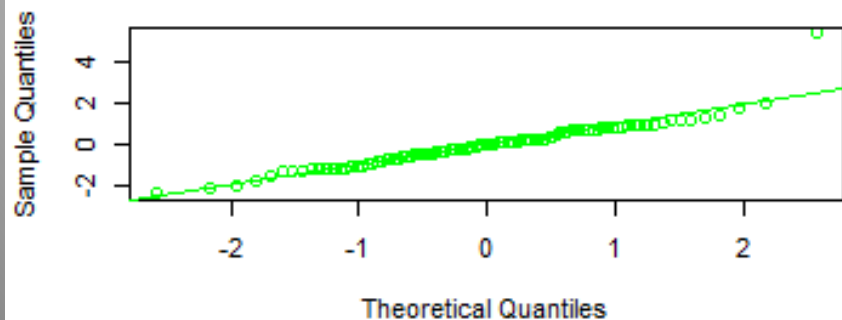
TEST SET PREDICTION ERRORS SEL DOWN
UNIVARIATE COUNTRY 2: BLUE



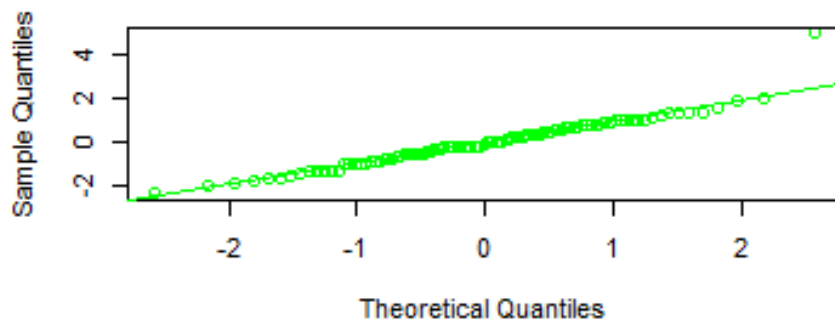
TEST SET PREDICTION ERRORS SEL DOWN
MULTIVARIATE COUNTRY 2: BLUE



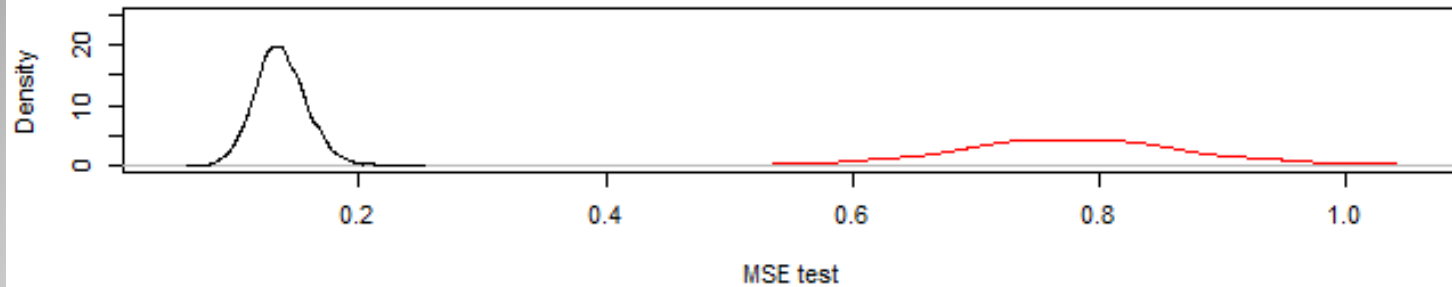
TEST SET PREDICTION ERRORS SEL DOWN
UNIVARIATE COUNTRY 3: GREEN



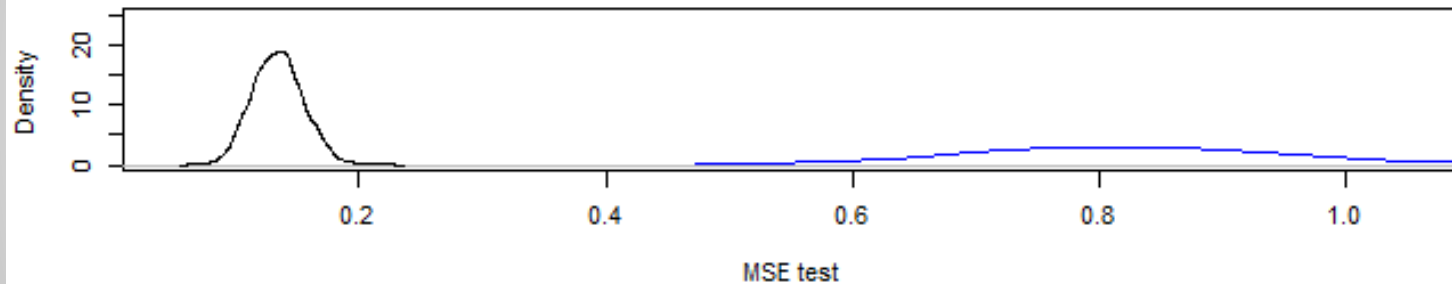
TEST SET PREDICTION ERRORS SEL DOWN
MULTIVARIATE COUNTRY 1: GREEN



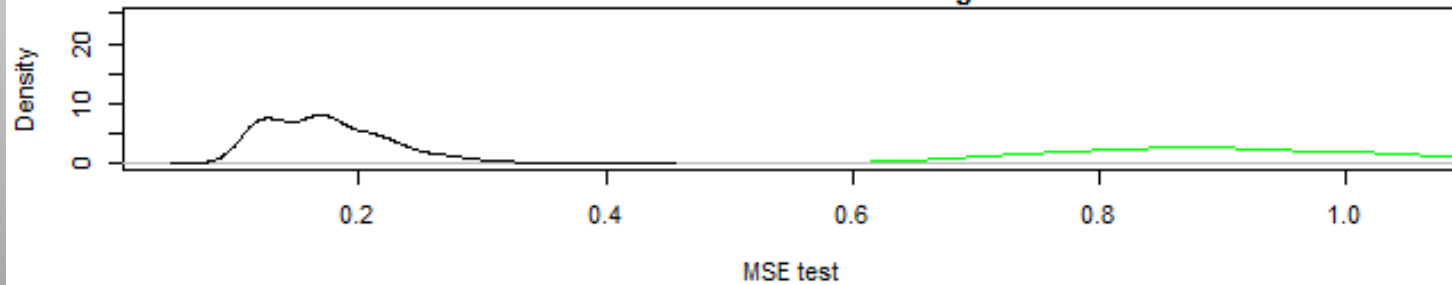
MSE test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red



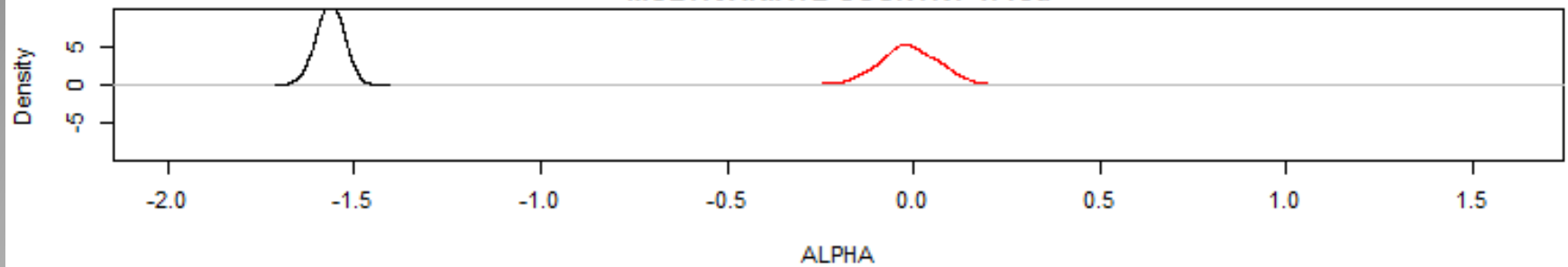
MSE test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue



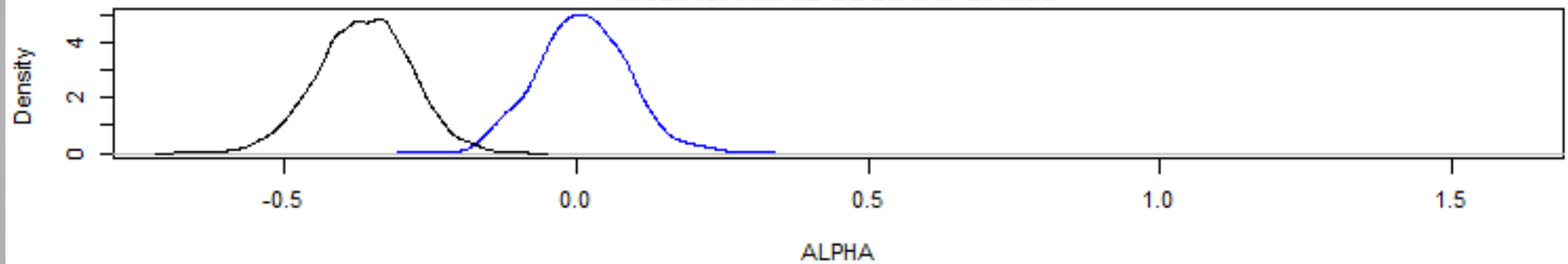
MSE test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green



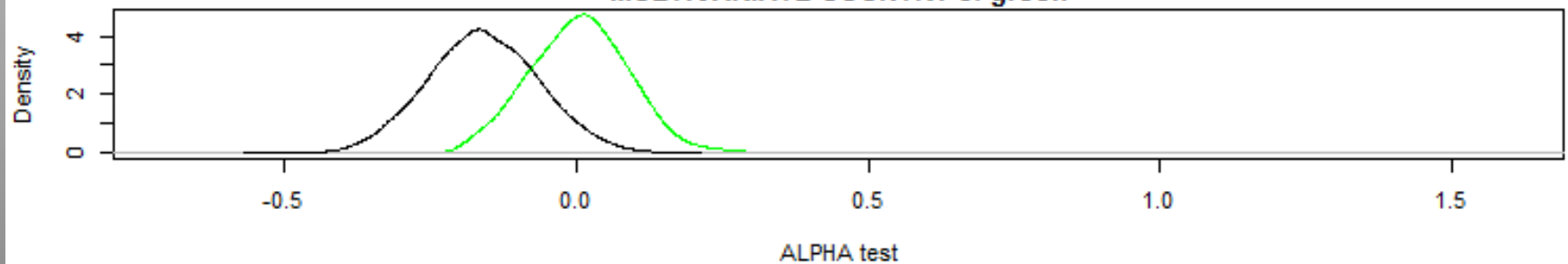
ALPHA test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red



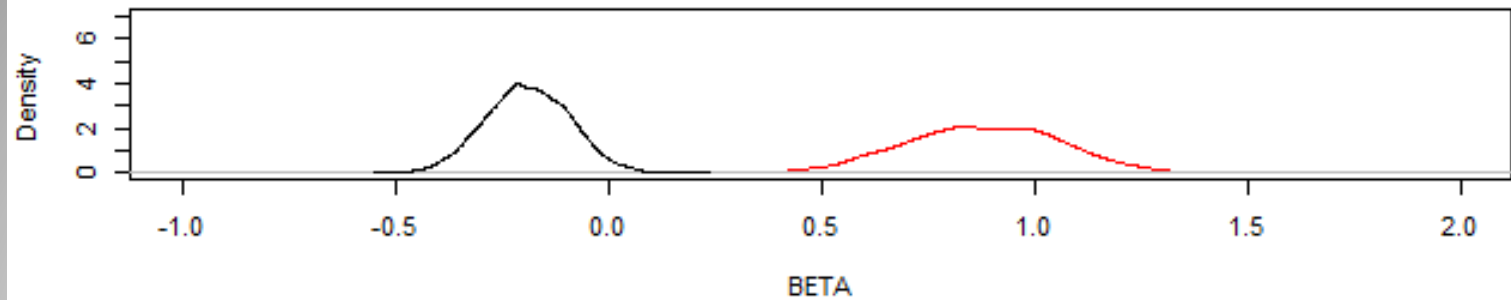
ALPHA test random (blue) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue



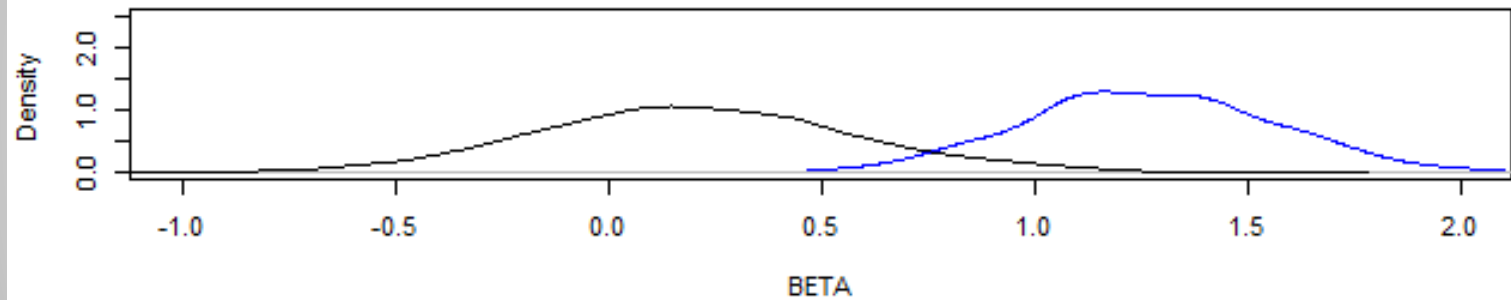
ALPHA test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green



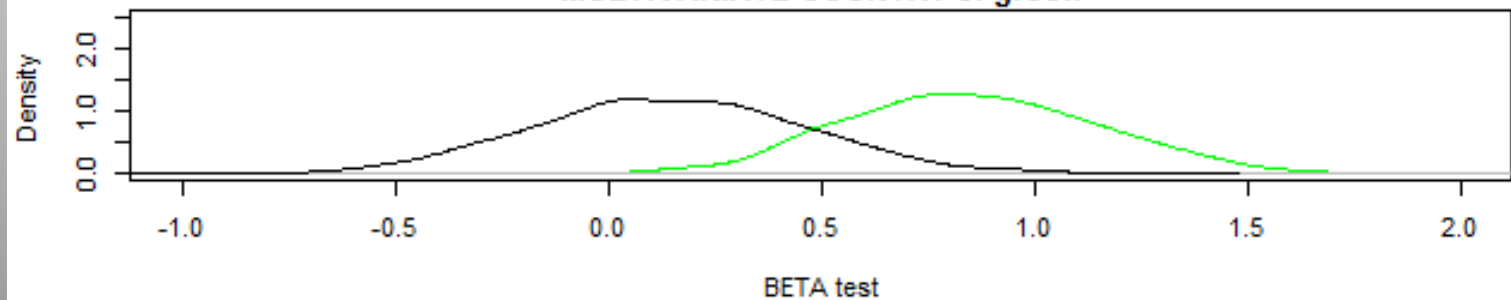
BETA test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 1: red



BETA test random (blue) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 2: blue



BETA test random (red) vs biased down sampling (black)
5000 bootstrap samples
MULTIVARIATE COUNTRY 3: green



POTENTIALLY USEFUL APPROACH: “ROBUST” REGRESSION

TGBLUP: GENOMIC BLUP WITH t -DISTRIBUTED RESIDUALS

(basic ideas for single trait model presented here)

I. Strandén and D. Gianola. 1998 Attenuating effects of preferential treatment with Student- t mixed linear models: a simulation study. *Genetics, Selection, Evolution* 30:565-583.

I. Strandén and D. Gianola. 1999. Mixed effects linear models with t -distributions for quantitative genetic analysis: a Bayesian approach. *Genetics, Selection, Evolution* 31: 25-42.

G. J. M. Rosa, C. R. Padovani and D. Gianola. 2003. Robust linear mixed models with normal/independent distributions and Bayesian MCMC implementation. *Biometrical Journal* 45: 573-590.

G. J. M. Rosa, D. Gianola and C. R. Padovani. 2004. Bayesian longitudinal data analysis with mixed models and thick-tailed distributions using MCMC. *Journal of Applied Statistics* 31, 855-873.

$$\mathbf{y} = \mathbf{g} + \mathbf{e}$$

$$\mathbf{g} \sim N(\mathbf{0}, \mathbf{G}\sigma_g^2)$$

$$e_i \sim t(0, \sigma_e^2, \nu)$$

$$p(\mathbf{g}|\mathbf{y}, \sigma_e^2, \sigma_g^2) \propto \prod \left[1 + \frac{(y_i - g_i)^2}{\sigma_e^2 \nu} \right]^{-\left(\frac{1+\nu}{2}\right)} \exp \left[-\frac{1}{2\sigma_g^2} \mathbf{g}'\mathbf{g} \right]$$

$$\left(\mathbf{D}^{-1[t]} + \frac{1}{\sigma_g^2} \mathbf{G}^{-1} \right) \mathbf{g}^{[t+1]} = \mathbf{D}^{-1[t]} \mathbf{y}$$

$$\begin{aligned} \mathbf{D}^{-1} &= \left\{ \frac{1}{\sigma_e^2 + \frac{(y_i - g_i)^2}{\nu}} \right\} = \frac{1}{\sigma_e^2} \left\{ \frac{1}{1 + \frac{(y_i - g_i)^2}{\nu \sigma_e^2}} \right\} \\ &= \frac{1}{\sigma_e^2} \mathbf{W} \end{aligned}$$

$$\left(\mathbf{W}^{[t]} + \frac{1 - h_g^2}{h_g^2} \mathbf{G}^{-1} \right) \mathbf{g}^{[t+1]} = \mathbf{W}^{[t]} \mathbf{y}$$

DEBIASING PREDICTIONS



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Machine Learning, 45, 261–277, 2001

Using Iterated Bagging to Debias Regressions

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CONCLUSION

- RESAMPLING USEFUL TO ESTIMATE DISTRIBUTIONS OF PREDICTION ERRORS
- BOOTSTRAPPING EMULATES DISTRIBUTIONS UNDER NON-RANDOM SAMPLING
- EXTENSIVE TESTING REQUIRED FOR FIRM DIAGNOSIS
- DO NOT WANT OVER-DIAGNOSIS AND TREATMENT
- DO NOT WANT TO REMAIN PASSIVE IN THE PRESENCE OF PROBLEMS
- MAIN ISSUE IS SCREWY DATA
- ANOTHER PROBLEM IS HOW SCREWY IT IS, AND WHO-WHY (selection) SCREWED IT!
- ROBUST REGRESSION METHODS TEMPER SCREWY DATA
- DEBIASING METHODS AVAILABLE: PAY VARIANCE PENALTY
- METHODS ARE COMPUTATIONALLY INTENSIVE BUT IS THIS A SERIOUS ISSUE AT THE TIMES OF MONSTROUS COMPUTERS, ARTIFICIAL INTELLIGENCE AND DEEP LEARNING?