On models and challenges in quantitative genetics and genomics

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UW–MADISON ANIMAL SCIENCES

Dairy Science

Coping with complexity

First assumption: there is a genetic signal and an environmental signal
Second assumption: the joint effect translates into a phenotye **y**

$$Y = f(G,E)$$

For some **UNKNOWN** function *f*

Huge number of possibilities for *f!*

Choices?

$$Y = G^E?$$
$$Y = E^G?$$
$$Y = G + E + GE?$$
$$Y = (G+E)^{GE}?$$
$$Y = G + E?$$

Is an assumption

(plant breeders very aware)

Is an even a stronger assumption

(animal breeders typically ignore it)

BIG-BANG OF WHOLE-GENOME REGRESSIONS

Cast

God: BLUP

Adam: Bayes A

Eve: Bayes B

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Prediction of Total Genetic Value Using Genome-Wide Dense Marker Maps

T. H. E. Meuwissen,* B. J. Hayes† and M. E. Goddard†,‡

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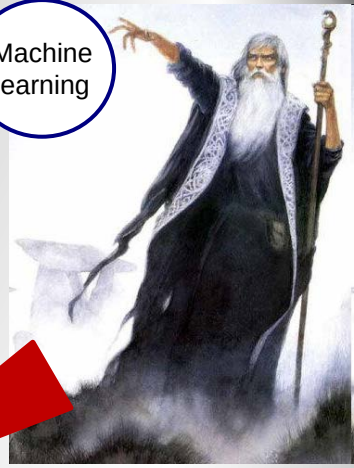
GENOMIC SELECTION: A DOMINANT RESEARCH AND DEVELOPMENT THEME

"The curse of the Bayesian Alphabet"

Bayes A, B, Bayes BLUPC, C-pi, D, Fast-B, L, R, RC, RS, TA, TB, TC, RKHS, NN…

A MACHINE LEARNING PERSPECTIVE

BLUP (1948, 1953,1959)
is
a linear UA



2011

Pattern recognition

Neural networks

Data mining

Universal approximators

2000

Cross-validation designs

Kernel methods

2006
2008

1991
1993

Random forest algorithms

2011

Sampling methods

Support vector machines

Ensemble Methods: bagging

Ensemble Methods: boosting

Non-parametric prediction

Bayesian networks

2011

2014

2010

2006

2009

LOOKING AHEAD

(entirely personal and subjective “shopping list”)

Area 1: Outlier detection, control and accommodation

Area 2: Genomic similarity matrix as estimand

Area 3: The Bayesian Alphabet marches on!

Area 4: On MCMC and “discovery”

Area 5: GE interactions and multi-omics

Area 6: Deep learners: experience so far

Area 1:
Outlier detection, control and accommodation

The problem is of concern…
(at least in Denmark and Finland)

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Short communication: Multivariate outlier detection for routine Nordic dairy cattle genetic evaluation in the Nordic Holstein and Red population

H. Gao,*[1] P. Madsen,* J. Pösö,† G. P. Aamand,‡ M. Lidauer,§ and J. Jensen*
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9-trait model: milk, fat, protein in 3 lactations
-Compute Mahalanobis intra year-lactation-DIM classes
for each record. Cut-offs for edits discarding outliers of increased stringency

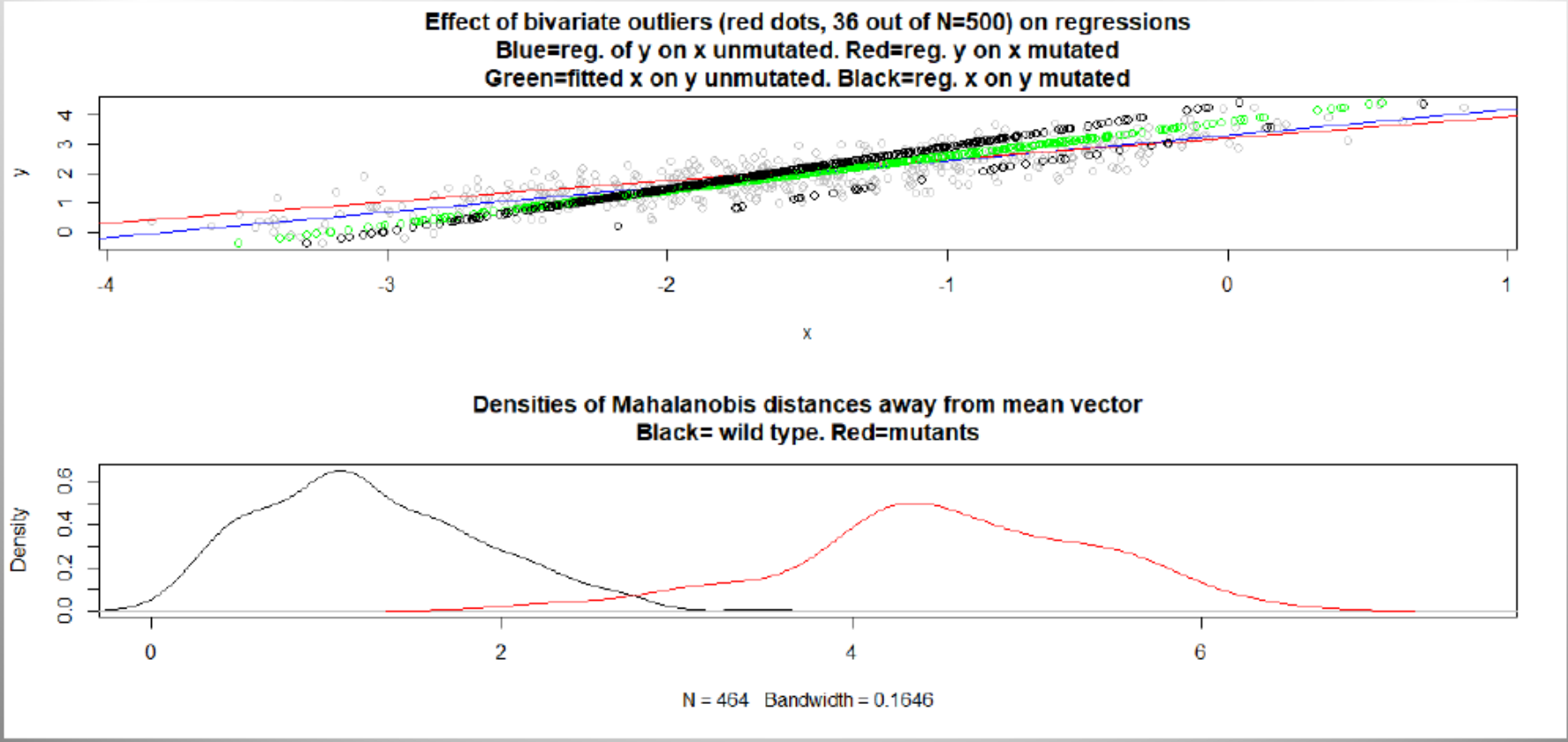
The results showed that, averaged over all scenarios, gains of 0.005 to 0.048 on prediction accuracy have been obtained by deleting the multivariate outliers. The improvements were more profound for progeny of young bulls compared with progeny of proven bulls. It is easy to implement this multivariate outlier-detection procedure in the routine genetic evaluation for different dairy cattle breeds; however, an optimal cutoff value for Mahalanobis distance needs to be defined to achieve

$$N = 500 \; bivariate \; normals \; N(0, \Sigma)$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} 0.8 & 0.7 \\ 0.7 & 0.8 \end{bmatrix} \quad \text{Prob(mutation)} = 0.08$$

$$Mutation \; adds \; \boldsymbol{\delta} = (1, -1)'$$

Would not appear as outliers in x or y axis



ACCOMODATING OUTLIERS CAN AUTOMATE?

- DISCARD DATA USING AD-HOC RULES (no account for exclusion uncertainty and arbitrariness in rules—GAO et al. 2018 recognized the issue)

- FIT ROBUST RESIDUAL DISTRIBUTION TO (Andrews and Mallows, 1974):
  ➔ATTENUATE ABERRANT (W.R. TO THE MODEL) OBSERVATIONS

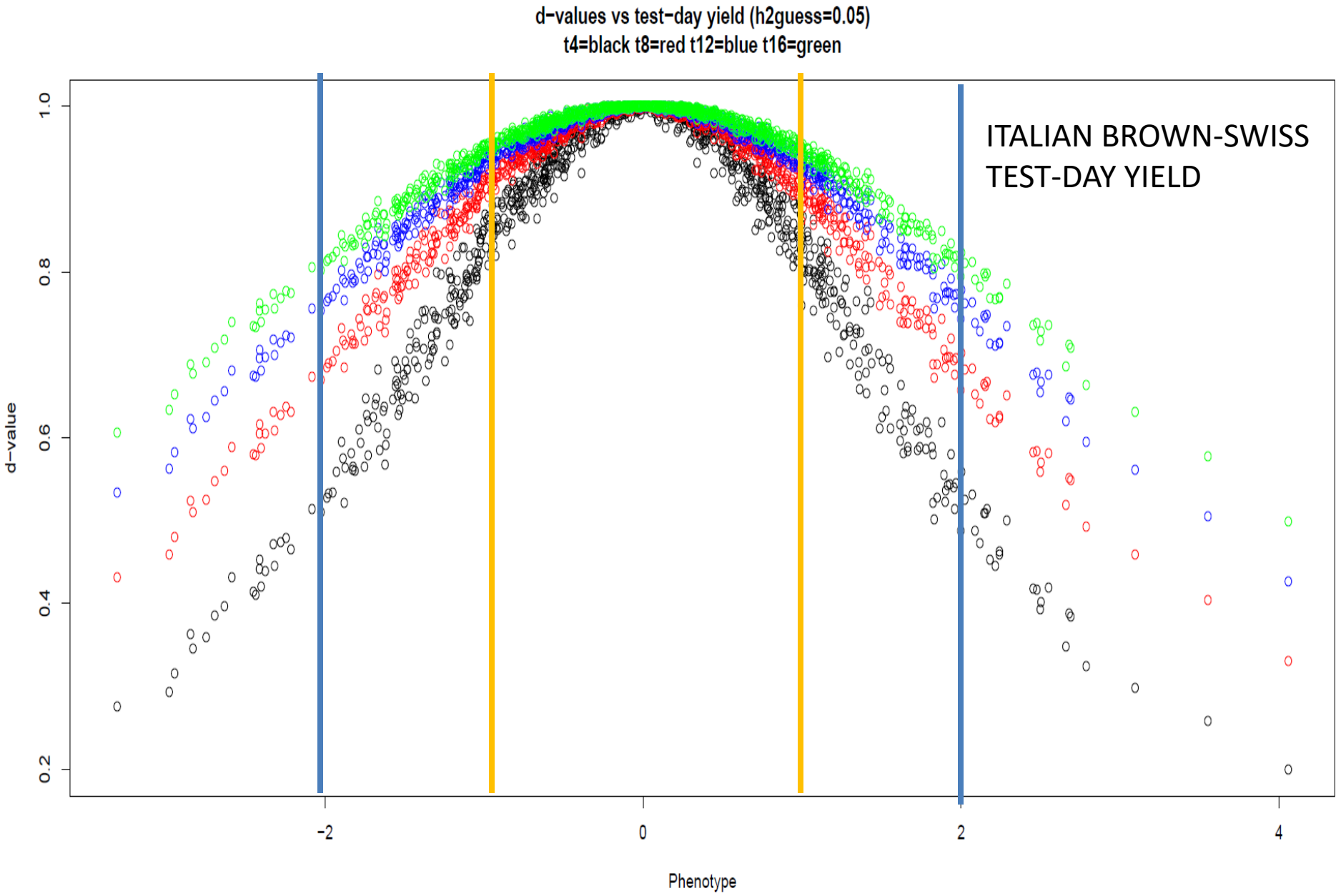
- ANIMAL BREEDERS HAVE DONE IT FOR INFERENCE, NOT PREDICTION!

-STRANDEN AND GIANOLA (1998, 1999)
-ROSA ET AL. (2003, 2004)
-KIZILKAYA ET A. (2003)
-CARDOSO ET AL. (2006)

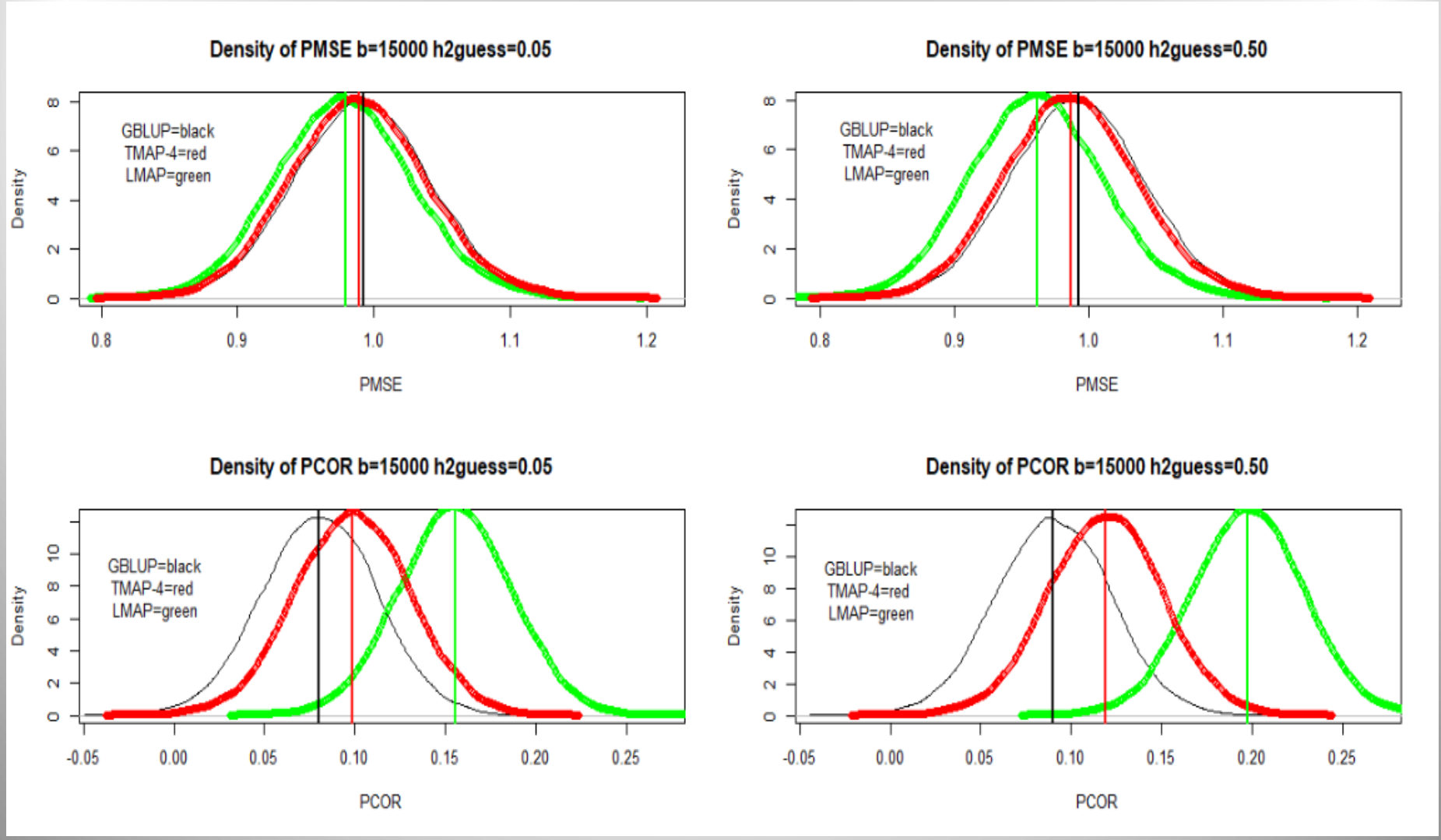
} t-distributions (MCMC)

-GIANOLA ET AL. (2018)➔ t and Laplace distributions: “Iterative GBLUP”

OUTLIERS IN TMAP: weights assigned automatically



Bootstrap distribution (b=15,000 samples) of predictive mean-squared error (PMSE) and predictive correlation (PCOR) for GBLUP, TMAP (df=4) and LMAP at selected genomic heritability values (guesses of 0.05 and 0.50 produced MINQUE estimates of 0.07 and 0.15, respectively): test-day milk yield in Brown-Swiss cows.



LMAP "BEST" FOLLOWED BY TMAP4 AND THEN BY GBLUP

EXTENSION TO MULTIVARIATE OUTLIERS NEEDED

-FOUNDATION: STRANDEN (1996) FOR T-DISTRIBUTION (MCMC)

-WORK IN PROGRESS FOR NON-MCMC T AND LAPLACE DISTRIBUTIONS

Area 2: Learning similarity matrices among individuals (**G**) as an estimation problem

Van Raden proposed marker-based similarity matrix (acts as hype-parameter):

$$G_{VR}=\frac{XX'}{\sum_{i=1}^{p} 2p_i(1-p_i)},$$

Inferring similarity among individuals from molecular markers and phenotypes with Bayesian regression

Daniel Gianola[a,b,c] and Rohan L. Fernando[c]

$$Var(\mathbf{g}|\mathbf{X}) = \mathbf{XDX}' = \mathbf{G}\sigma^2_g$$

Model specific genomic variance

A diagonal matrix

An unknown matrix

$$p(G|X) = prior\ distribution\ based\ on\ markers$$
$$y = vector\ of\ phenotypes\ (single\ or\ multiple - traits)$$
$$p(G|X,y) = posterior\ distribution\ informed\ by\ markers\ and\ phenotypes$$

HAVE DEVELOPED A FORMALISM FOR BAYES A, B, C, Cπ, R

EXAMPLE: BAYES A

$$\sigma^2_{gBA} = \sum_{i=1}^{p} 2p_i(1-p_i)S^2_\beta \frac{\nu_\beta}{\nu_\beta - 2}.$$

$$\mathbf{G}_{BA} = \frac{1}{\sigma^2_{gBA}}\mathbf{X}\mathbf{D}_{BA}\mathbf{X}'.$$

$$\mathbf{D}_{BA} = diag\left\{\sigma^2_{\beta_j}\right\}$$

Sample from prior → Prior distribution of G_{BA}

Sample from posterior → Posterior distribution of G_{BA}

EXAMPLE: BAYES B

Prob. non-null effect

$$\sigma^2_{gBB} = \sum_{i=1}^{p} 2p_i(1-p_i)S^2_\beta \frac{\nu_\beta}{\nu_\beta - 2}\pi.$$

Sample from prior → Prior distribution of G_{BB}

$$\mathbf{G}^{(s)}_{BB} = \frac{1}{\sigma^2_{gBB}}\mathbf{X}\mathbf{D}_{BB}\mathbf{X}'^{(s)}; s = 1, 2, ..., S.$$

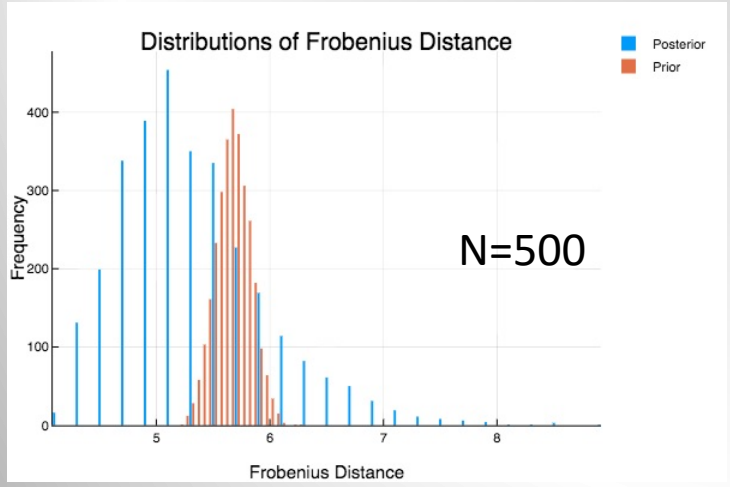
Sample from posterior → Posterior distribution of G_{BB}

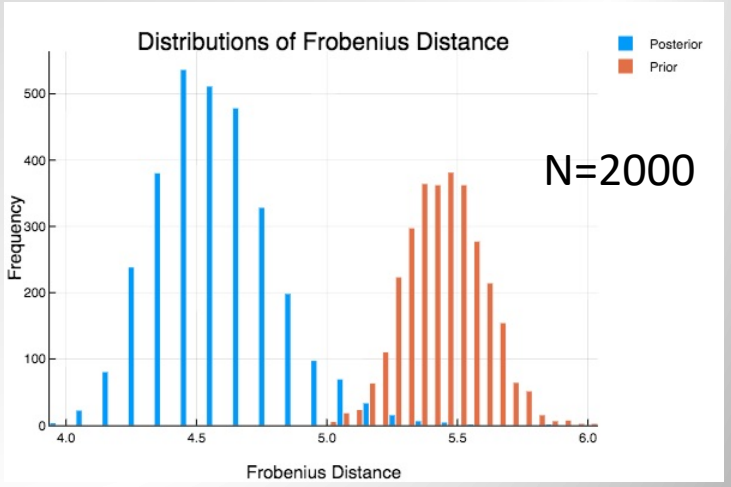
$\mathbf{D}_{BB}$ is a diagonal matrix containing either $\sigma^2_{\beta_j}$ or 0 in position j

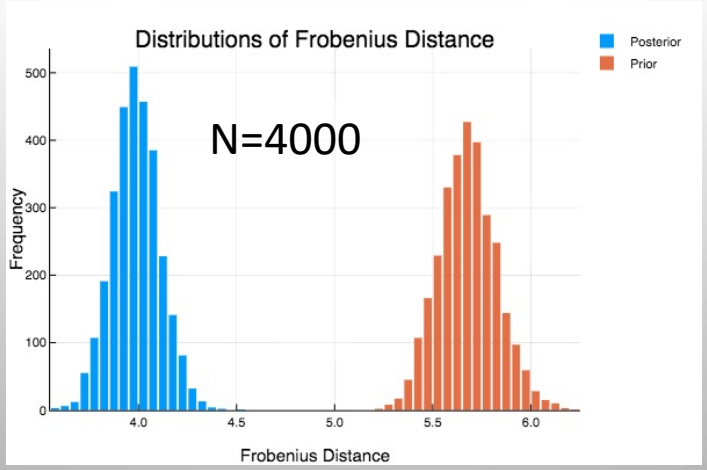
EXTENT TO TO WHICH PHENOTYPES INFORM ABOUT SIMILARITY:

Frobenius distances between TRUE QTL G and their prior and posteriors

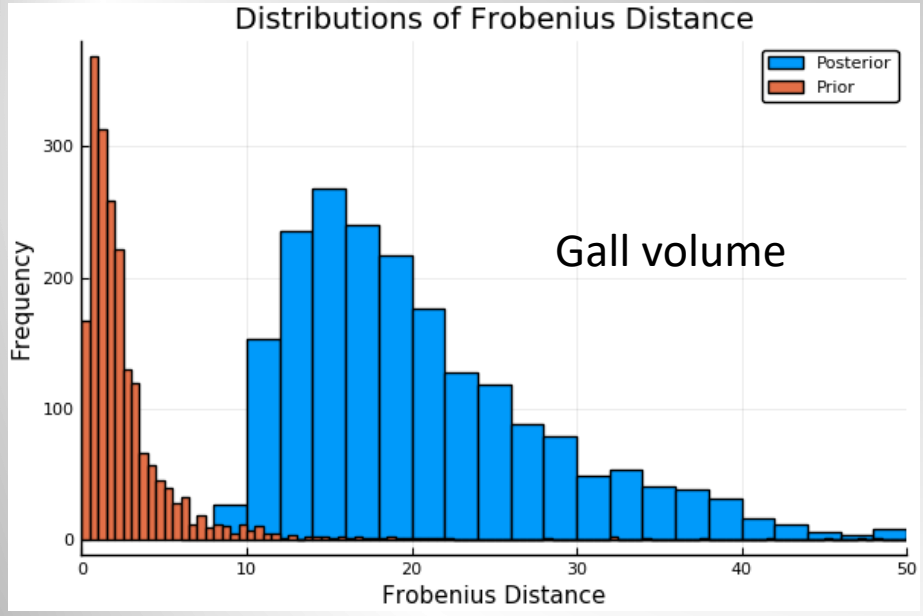
10 chromosomes- 2000 SNP (100 QTL)- Bayes Cπ

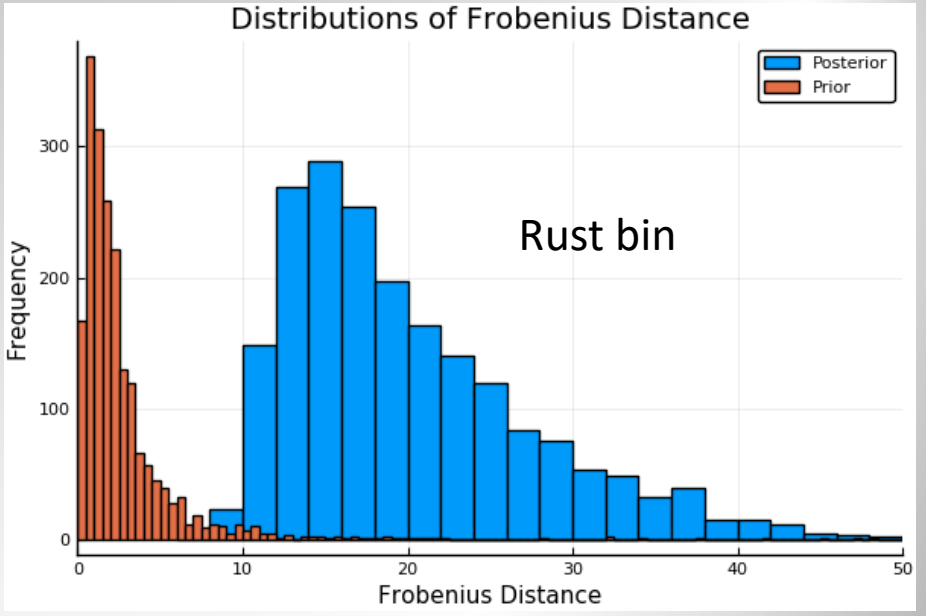


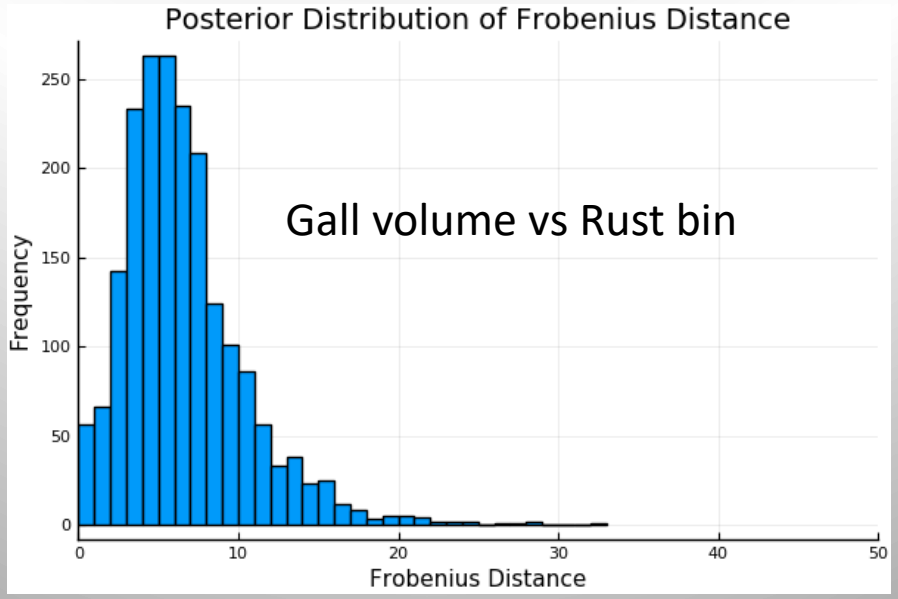




Pinus taeda: N=807 p=4828 Bayes Cπ bivariate analysis (only 100 pairs of individuals)







Basis for deciding whether trait-specific Similarities exist

Area 3: The Bayesian Alphabet marches on!

A multiple-trait Bayesian Lasso for genome-enabled association and prediction of complex traits

Daniel Gianola[a,b,c,d] Rohan L. Fernando and Chris-Carolin Schön[d]

[a] Department of Animal Sciences, University of Wisconsin-Madison, USA;

[b] Department of Dairy Science, University of Wisconsin-Madison, USA;

[c]Department of Animal Science, Iowa State University, USA

[d] Department of Plant Sciences, Technical University of Munich,

TUM School of Life Sciences, Germany.

2.1.2 Multivariate Laplace prior distribution (MLAP) for marker effects

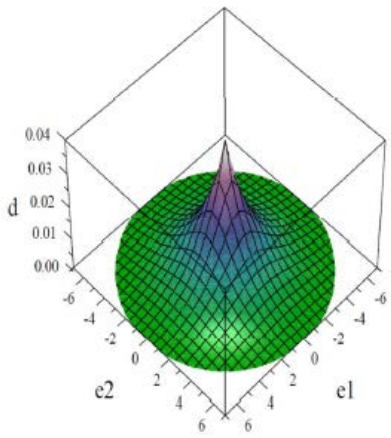
Independent T-variate Laplace prior distributions with a null mean vector will be assigned to each of the $T \times 1$ vectors $\boldsymbol{\beta}_j$ $(j = 1, 2, ..., p)$. Gómez et al. (2007) presented a multi-dimensional version of the power exponential (PE) family of distributions; one special case is the multivariate Laplace distribution (MLAP). The density of the MLAP distribution with a zero-mean vector used here has form

$$p(\boldsymbol{\beta}_j|\boldsymbol{\Sigma}) = \frac{T\Gamma\left(\frac{T}{2}\right)}{|\boldsymbol{\Sigma}|^{\frac{1}{2}}\,\pi^{\frac{T}{2}}\Gamma\left(1+T\right)2^{(1+T)}} \exp\left(-\frac{1}{2}\sqrt{\boldsymbol{\beta}_j'\boldsymbol{\Sigma}^{-1}\boldsymbol{\beta}_j}\right);\ j = 1, 2, ..., p, \tag{8}$$

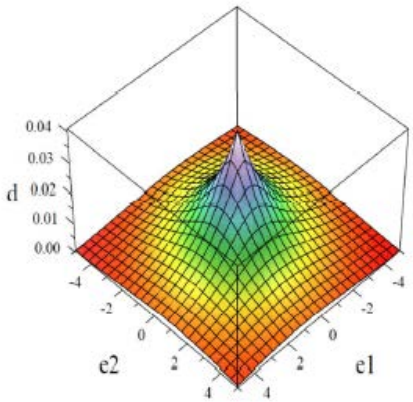
where $\boldsymbol{\Sigma} = \{\Sigma_{kk'}\}$ is a $T \times T$ positive-definite scale matrix. The variance-covariance matrix of the distribution is

$$Var(\boldsymbol{\beta}_j|\boldsymbol{\Sigma}) = 4\left(T+1\right)\boldsymbol{\Sigma} = \mathbf{B}; \tag{9}$$

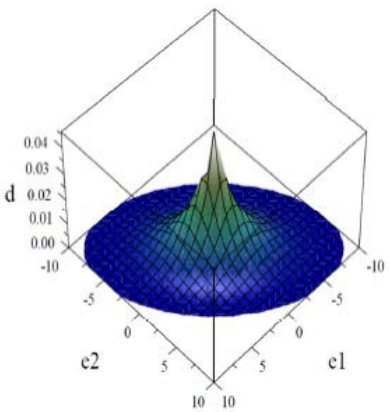
a) Density of two uncorrelated bivariate Laplace random variables with null means and unit scales. e1 and e2 are coordinates of bivariate vectors.



b) Density of two positively correlated bivariate Laplace random variables with null means and unit scales. e1 and e2 are coordinates of bivariate vectors

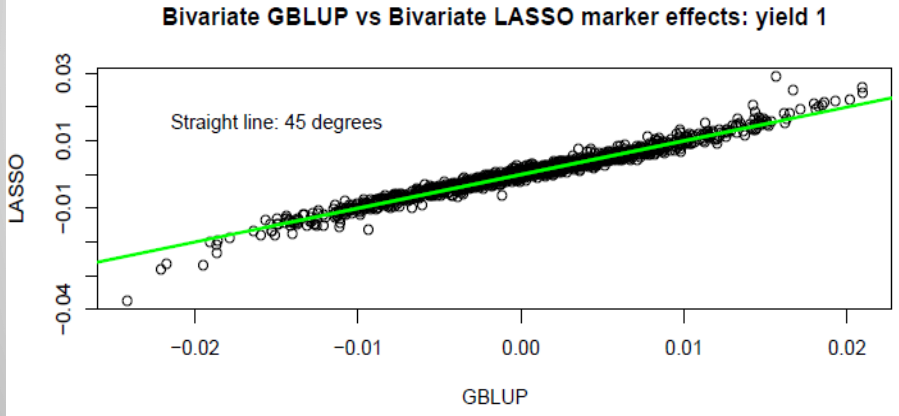


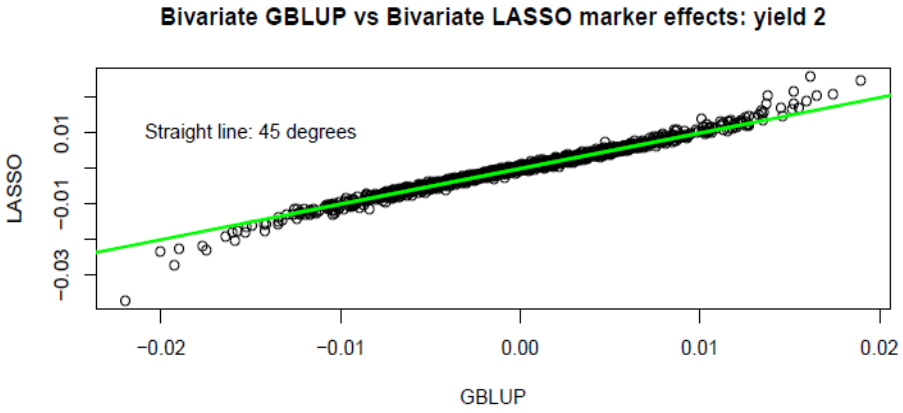
c) Density of two negatively correlated bivariate Laplace random variables with null means and unit scales. e1 and e2 are coordinates of bivariate vectors

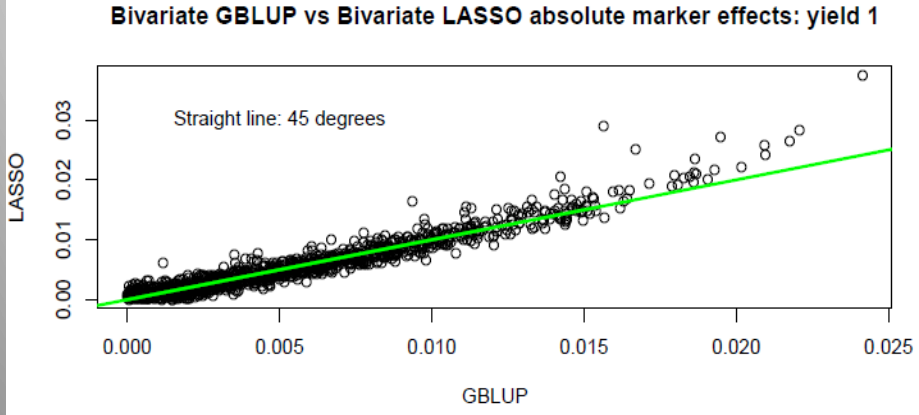


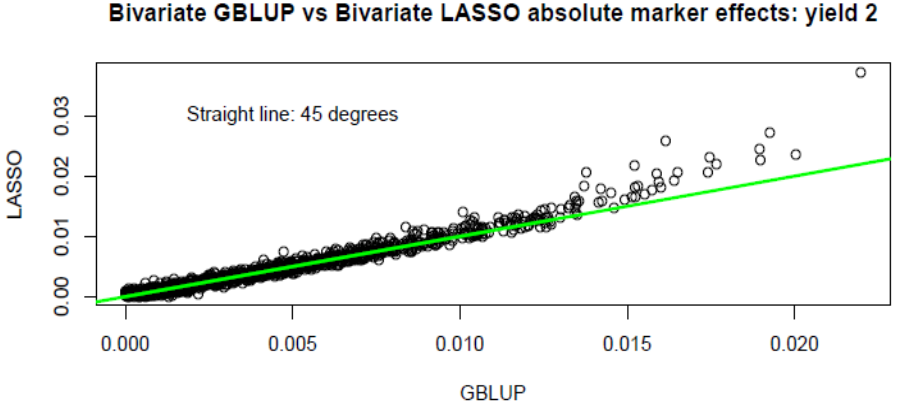
Analysis of wheat data set

- n=599 inbred lines
- p=1279 DaRT markers
- Traits: grain yield in environments 1 and 2
- Bivariate GBLUP (maximum likelihood for variance components)
- Bivariate Lasso
- Six chains of 1500 iteration each (evaluate MCMC)
- Gelman's R-statistics+ Geweke's batching for convergence assessment
- Six chains of 2000 samples post-burn in: 12000 samples used for inference


Bivariate GBLUP vs Bivariate LASSO marker effects: yield 1
Straight line: 45 degrees
LASSO
GBLUP
−0.04
−0.01
0.01
0.03
−0.02
−0.01
0.00
0.01
0.02

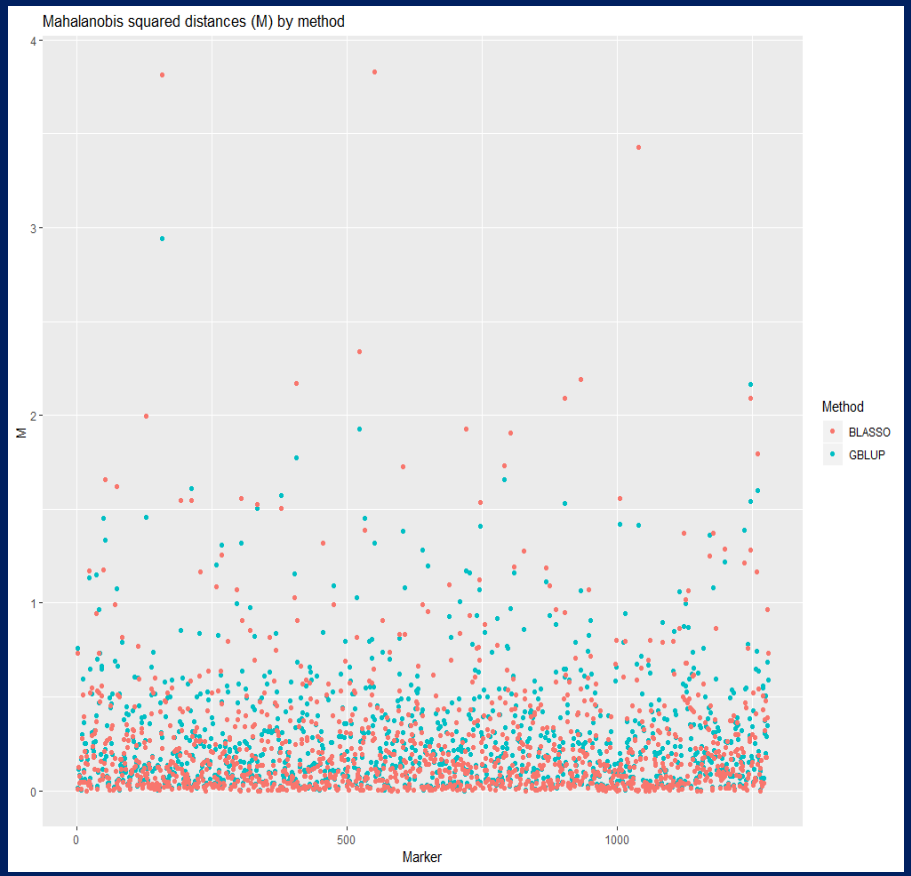

Bivariate GBLUP vs Bivariate LASSO marker effects: yield 2
Straight line: 45 degrees
LASSO
GBLUP
−0.03
−0.01
0.01
−0.02
−0.01
0.00
0.01
0.02

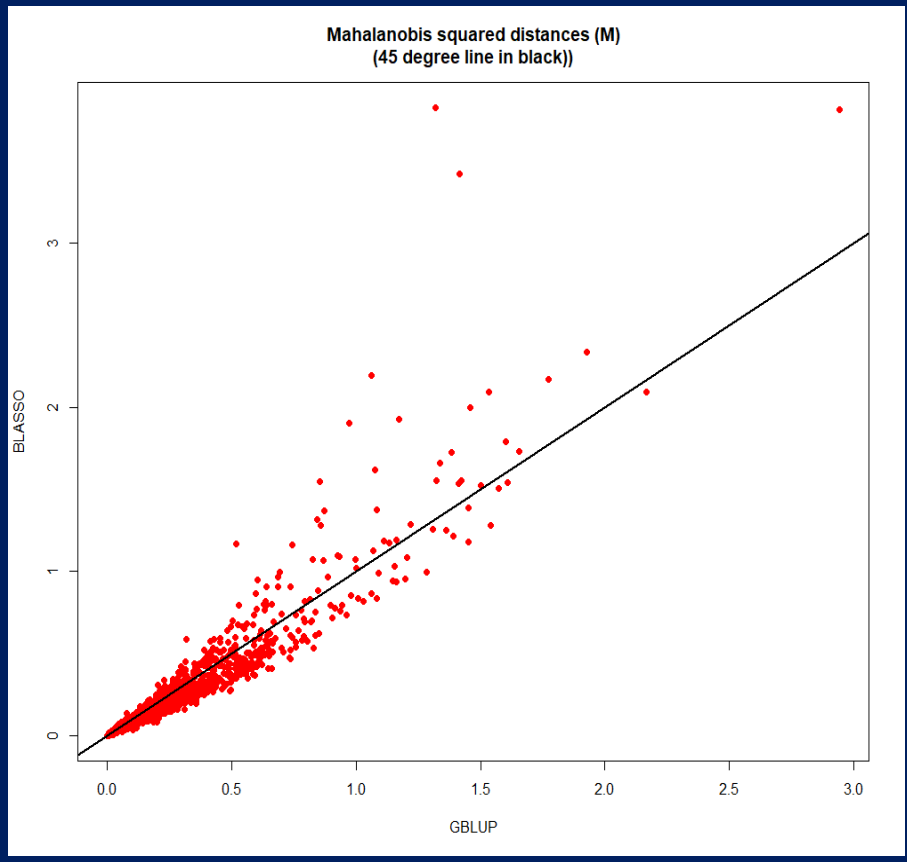

Bivariate GBLUP vs Bivariate LASSO absolute marker effects: yield 1
Straight line: 45 degrees
LASSO
GBLUP
0.00
0.01
0.02
0.03
0.000
0.005
0.010
0.015
0.020
0.025


Bivariate GBLUP vs Bivariate LASSO absolute marker effects: yield 2
Straight line: 45 degrees
LASSO
GBLUP
0.00
0.01
0.02
0.03
0.000
0.005
0.010
0.015
0.020

MUMA PLOTS
(MULTIVARIATE MANHATTAN)

$$\sqrt{\beta_j' \Sigma^{-1} \beta_j}$$





Area 4: On MCMC and “discovery”

MCMC-Based Inference in the Era of Big Data:
A Fundamental Analysis of the Convergence Complexity
of High-Dimensional Chains

Bala Rajaratnam and Doug Sparks
Stanford University

August 28, 2015

Variational distance between posterior π and estimate of (distribution) at iterate *k*

$$d_{TV}(P_{x_0}^k, \Pi) \leq M_{x_0} r^k$$

"Starting distance"

$0 < r < 1$

Convergence rate

Ranges in 0-1
1 when the two distributions differ

AUTHORS:

In summary, our theoretical and numerical analysis above indicates that regardless of the type or form of regression (standard regression, lasso, elastic net, or spike-and-slab), there is a universal geometric convergence rate of the form $r = p/(n + p - 2)$.

ITERATIONS REQUIRED TO REDUCE STARTING VARIATIONAL DISTANCE T0 10^{-7}

GENOTYPIC VALUES

n	p	Parameterization in n
1000	50000	23
	800000	23
	20×10^6	23
5000	50000	23
	800000	23
	20×10^6	23

MARKER EFFECTS

n	p	Parameterization in n	Parameterization in p
1000	50000	23	816
	800000	23	12886
	20×10^6	23	322350
5000	50000	23	169
	800000	23	2587
	20×10^6	23	64664

MARKER EFFECTS

n	p	Parameterization in n	Parameterization in p	Parameterization in $4p$
1000	50000	23	816	3235
	800000	23	12886	51986
	20×10^6	23	322350	$1.611\,8 \times 10^6$
5000	50000	23	169	653
	800000	23	2587	10324
	20×10^6	23	64664	$2.686\,3 \times 10^5$

Area 5: Multi-omics and GE

RESEARCH ARTICLE

Genetic Epidemiology

OFFICIAL JOURNAL INTERNATIONAL GENETIC EPIDEMIOLOGY SOCIETY www.geneticepi.org

Poly-Omic Prediction of Complex Traits: OmicKriging

Heather E. Wheeler,[1] Keston Aquino-Michaels,[2] Eric R. Gamazon,[2] Vassily V. Trubetskoy,[2] M. Eileen Dolan,[1] R. Stephanie Huang,[1] Nancy J. Cox,[2] and Hae Kyung Im[3]*

[1]Section of Hematology/Oncology, Department of Medicine, University of Chicago, Chicago, Illinois, United States of America; [2]Section of Genetic Medicine, Department of Medicine, University of Chicago, Chicago, Illinois, United States of America; [3]Department of Health Studies, University of Chicago, Chicago, Illinois, United States of America

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HIGHLIGHTED ARTICLE
GENETICS | GENOMIC SELECTION

Increased Proportion of Variance Explained and Prediction Accuracy of Survival of Breast Cancer Patients with Use of Whole-Genome Multiomic Profiles

Ana I. Vazquez,*,[1] Yogasudha Veturi,† Michael Behring,*,[6] Sadeep Shrestha,‡ Matias Kirst,**,[11] Marcio F. R. Resende, Jr.,**,[11] and Gustavo de los Campos*,[11]
*Department of Epidemiology and Biostatistics, Michigan State University, East Lansing, Michigan 48824, †Biostatistics Department, ‡Comprehensive Cancer Center, and §Department of Epidemiology, University of Alabama at Birmingham, Alabama 35294, **School of Forest Resources and Conservation and ††University of Florida Genetics Institute, University of Florida, Gainesville, Florida 32611, and ‡‡Statistics Department, Michigan State University, East Lansing, Michigan 48824

ABSTRACT Whole-genome multiomic profiles hold valuable information for the analysis and prediction of disease risk and progression. However, integrating high-dimensional multilayer omic data into risk-assessment models is statistically and computationally challenging. We describe a statistical framework, the Bayesian generalized additive model ((BGAM), and present software for integrating multilayer high-dimensional inputs into risk-assessment models. We used BGAM and data from The Cancer Genome Atlas for the analysis and prediction of survival after diagnosis of breast cancer. We developed a sequence of studies to (1) compare predictions based on single omics with those based on clinical covariates commonly used for the assessment of breast cancer patients (COV), (2) evaluate the benefits of combining COV and omics, (3) compare models based on (a) COV and gene expression profiles from oncogenes with (b) COV and whole-genome gene expression (WGGE) profiles, and (4) evaluate the impacts of combining multiple omics and their interactions. We report that (1) WGGE profiles and whole-genome methylation (METH) profiles offer more predictive power than any of the COV commonly used in clinical practice (*e.g.*, subtype and stage), (2) adding WGGE or METH profiles to COV increases prediction accuracy, (3) the predictive power of WGGE profiles is considerably higher than that based on expression from large-effect oncogenes, and (4) the gain in prediction accuracy when combining multiple omics is consistent. Our results show the feasibility of omic integration and highlight the importance of WGGE and METH profiles in breast cancer, achieving gains of up to 7 points area under the curve (AUC) over the COV in some cases.

HIGHLIGHTED ARTICLE
GENETICS | GENOMIC SELECTION

Prediction of Plant Height in *Arabidopsis thaliana* Using DNA Methylation Data

Yaodong Hu,*,[1] Gota Morota,† Guilherme J. M. Rosa,*,‡ and Daniel Gianola*,‡,§
*Department of Animal Sciences, ‡Department of Biostatistics and Medical Informatics, and §Department of Dairy Science, University of Wisconsin, Madison, Wisconsin 53706, and †Department of Animal Science, University of Nebraska, Lincoln, Nebraska 68583

Theor Appl Genet (2014) 127:595–607
DOI 10.1007/s00122-013-2243-1

ORIGINAL PAPER

A reaction norm model for genomic selection using high-dimensional genomic and environmental data

Diego Jarquín · José Crossa · Xavier Lacaze · Philippe Du Cheyron · Joëlle Daucourt · Josiane Lorgeou · François Piraux · Laurent Guerreiro · Paulino Pérez · Mario Calus · Juan Burgueño · Gustavo de los Campos

RKHS FOR GENOTYPE X ENVIRONMENT INTERACTION

J. Dairy Sci. 100:2042–2056
https://doi.org/10.3168/jds.2016-11543
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Genotype by environment (climate) interaction improves genomic prediction for production traits in US Holstein cattle

F. Tiezzi,*[1] G. de los Campos,† K. L. Parker Gaddis,‡ and C. Maltecca*
*Department of Animal Science, North Carolina State University, Raleigh 27695
†Department of Epidemiology and Biostatistics, Michigan State University, East Lansing 48828
‡Council on Dairy Cattle Breeding, Bowie, MD 20716

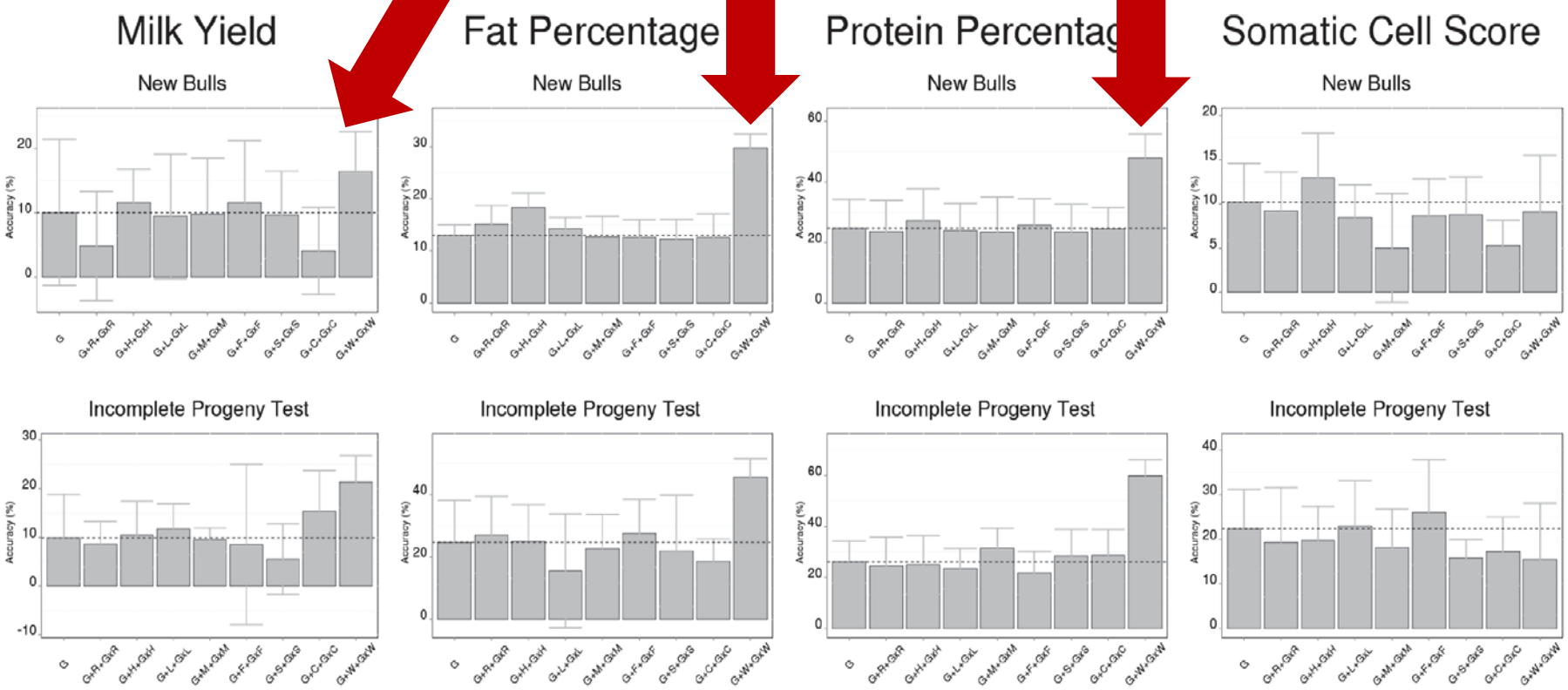

Figure 3. Accuracy of prediction for the new bulls and incomplete progeny test cross-validation scenarios. Models included genomic effect (G), geographical region effect (R), herd effect (H), latitude and longitude effects (L), herd management effects (M), herd fertility effects (F), service-sire choice effects (S), culling descriptors effects (C), and climate variables effects (W). Histograms (error bars) report the average (SD) over the 4 folds used in the cross-validation.

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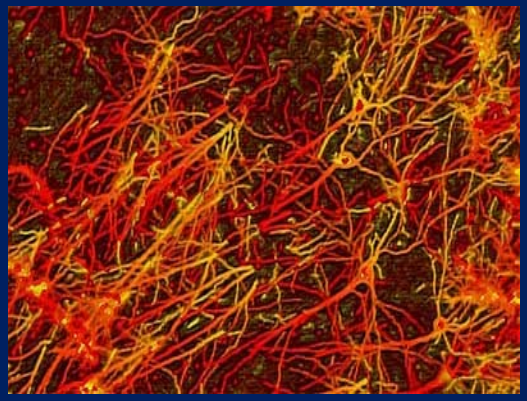
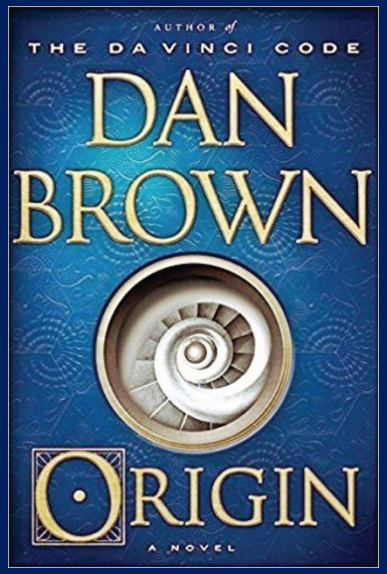
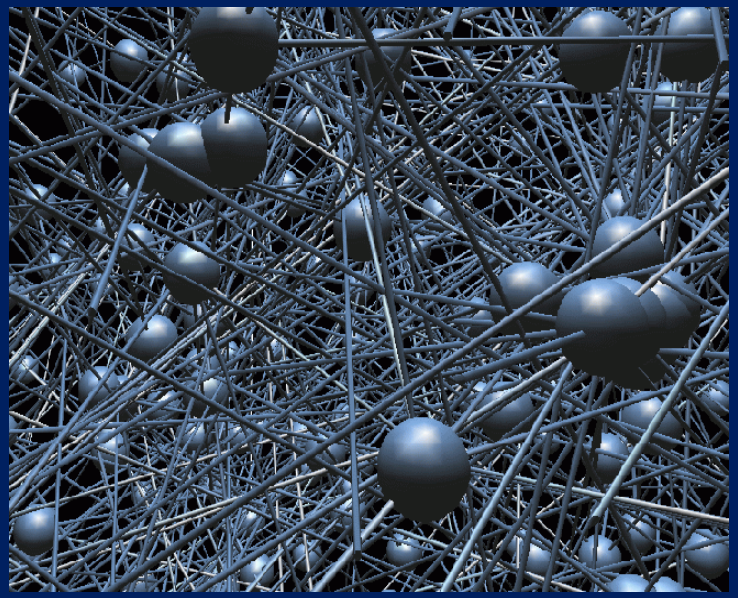
Predicting Growth and Carcass Traits in Swine Using Metagenomic Data and Machine Learning Algorithms

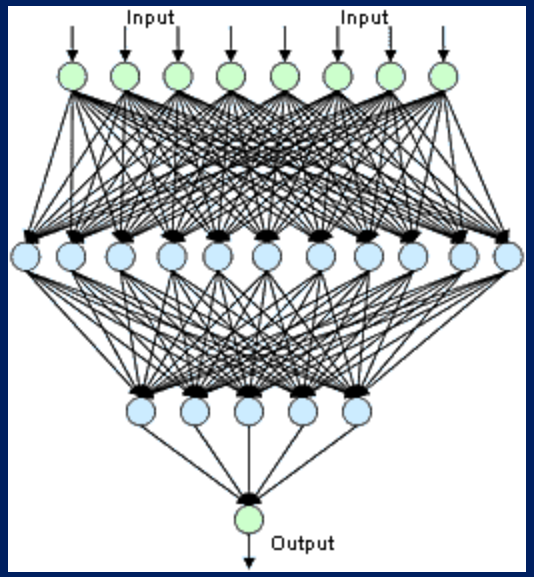
Christian Maltecca[1,*,+], Duc Lu[1,+], Costantino Schillebeeckx[2], Nathan P McNulty[2], Clint Schwab[3], Caleb Schull[3], and Francesco Tiezzi[1,+]

Area 6: Deep learners: experience so far









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Prediction of maize phenotype based on whole-genome single nucleotide polymorphisms using deep belief networks

H Rachmatia*, W A Kusuma, and L S Hasibuan
Department of Computer Science, Bogor Agricultural University, Indonesia

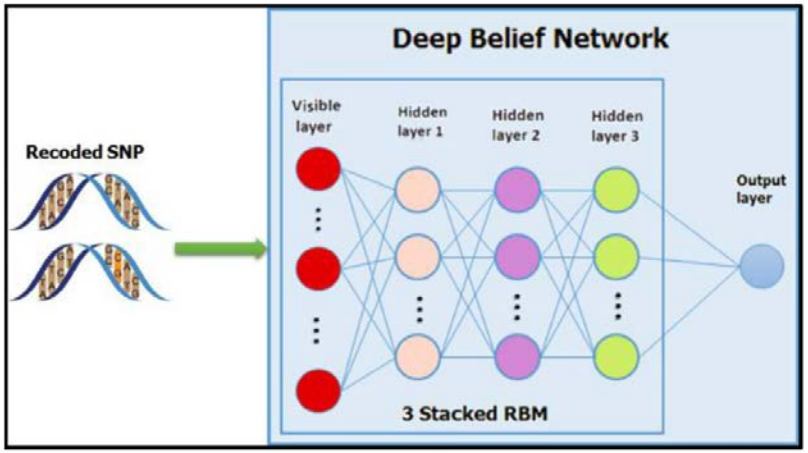

Figure 1. The DBN architecture for genomic prediction

Table 1. Cross-validation (cv) correlation between predicted and observed phenotypes

Trait–environment	Model[a]			
	RKHS	BL	BLUP	DBN
MFL – WW	0.607	0.790	—[b]	0.295
MFL – SS	0.674	0.778	0.464	0.325
FFL – WW	0.588	0.781	—[b]	0.270
FFL – SS	0.648	0.774	0.521	0.370
ASI – WW	0.547	0.513	0.469	**0.559**
ASI – SS	0.572	0.517	0.481	**0.579**
GY – WW	0.514	0.525	0.515	0.445
GY – SS	0.453	0.415	0.442	0.383

Four models were fitted to each trait (FFL, MFL, ASI, and GY) and environment (SS, severe drought stress; WW, well watered) combination.

[a] Models were molecular marker (SNPs) using reproducing kernel Hilbert space (RKHS) regression, Bayesian LASSO (BL), best linear unbiased predictor (BLUP), and our proposed method deep belief network (DBN).

[b] BLUP were not computed because the estimated genetic variances were negligible [9].

RESULTS: NO CONVINCING EVIDENCE OF SUPERIORITY OF DBN

Can Deep Learning Improve Genomic Prediction of Complex Human Traits?

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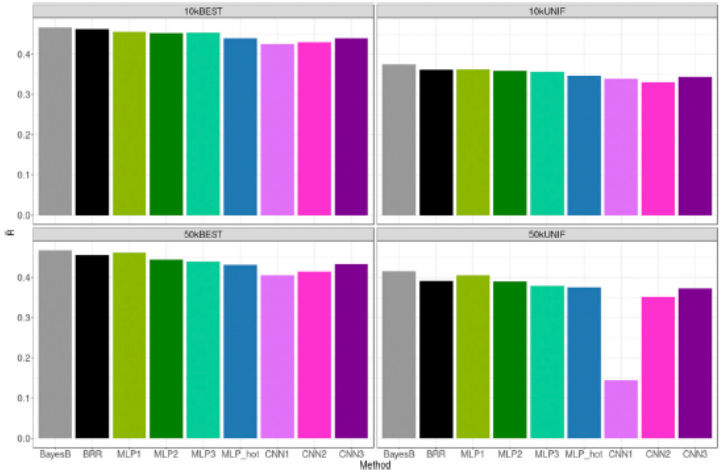

Figure 4 Prediction performance across methods and SNP sets for height. Gray, green, blue, and magenta bars correspond to linear, MLP, one-hot encoding MLP, and CNN methods, respectively. Average SE of R's were ~3×10^{-3}. BEST, set with the 10k or 50k top most-associated SNPs; BRR, Bayesian Ridge Regression; CNN, Convolutional Neural Network; MLP, Multilayer Perceptron; UNIF, set in which the genome was split in windows of equal physical length and the most-associated SNP within each window was chosen.

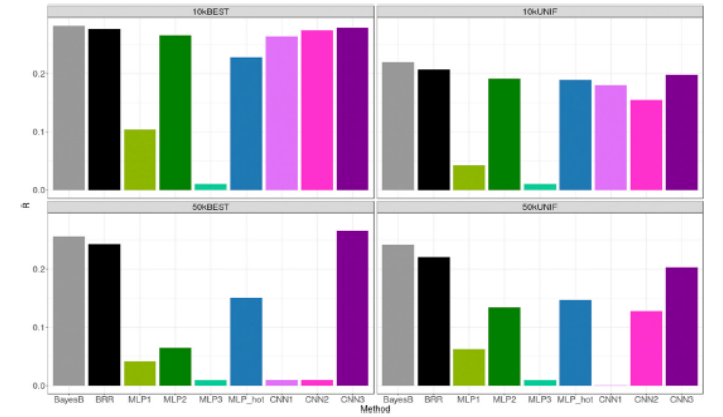

Figure 5 Prediction performance across methods and SNP sets for bone heel mineral density. Gray, green, blue, and magenta bars correspond to linear, MLP, one-hot encoding MLP, and CNN methods, respectively. Very low bar means method not converging. Average SE of R's were ~3×10^{-3}. BEST, set with the 10k or 50k top most-associated SNPs; BRR, Bayesian Ridge Regression; CNN, Convolutional Neural Network; MLP, Multilayer Perceptron; UNIF, set in which the genome was split in windows of equal physical length and the most-associated SNP within each window was chosen.

STATURE

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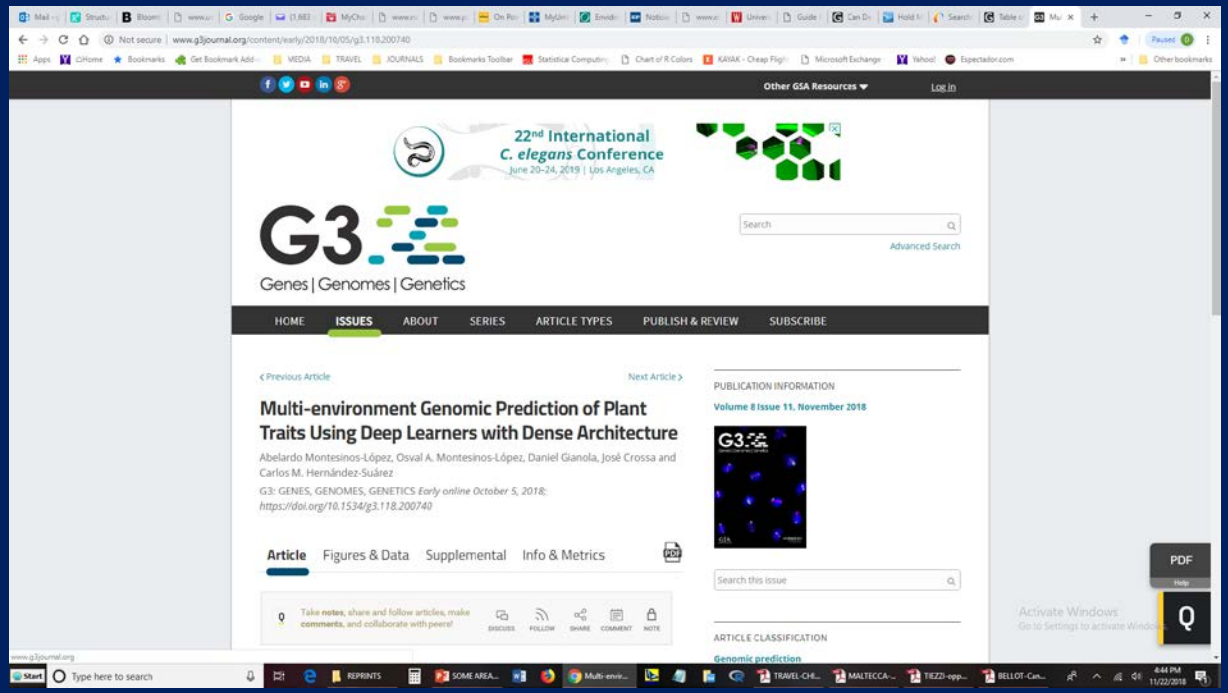
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CONCLUSION

Draw your own conclusions!