File S1

Supplementary Information

Data sets

In this study we used two published wheat and two published maize data sets. The first data set consisted of 599 wheat lines genotyped by 1,447 Diversity Array Technology (DArT) markers in the CIMMYT Global Wheat Breeding Program (Crossa *et al.* 2010). Genotypic and phenotypic data were downloaded from the corresponding supplementary materials.

The second data set comprised 254 advanced wheat breeding lines from the CIMMYT wheat breeding program, genotyped using a genotyping-by-sequencing approach (Poland *et al.* 2012). Genotypic and phenotypic data were downloaded from the corresponding supplementary materials. 1,576 Single Nucleotide Polymorphism (SNP) markers with lowest missing rate (<0.15%) were selected in this study. Remaining missing values were imputed based on marginal allele frequencies.

The third data set consisted of 300 maize lines from the Drought Tolerance Maize for Africa project of CIMMYT Global Maize Program genotyped with 1,148 SNP markers (Crossa *et al.* 2010). Genotypic and phenotypic data were downloaded from the corresponding supplementary materials. In this study we focused on grain yield, which was examined for 264 lines.

The forth data set comprised two large half-sib maize panels from the flint and dent heterotic pools generated within the European PLANT-KBBE CornFed project (Bauer *et al.* 2013). The dent (flint) panel consisted of 10 (11) half-sib families with 847 (833) doubled haploid (DH) lines. Genomic data were downloaded from the website of National Center for Biotechnology Information (NCBI) Gene

Expression Omnibus as data set GSE50558 (http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE50558).

After quality control for missing rate and minor allele frequency, the number of SNP markers used in this study was 31,498 for dent lines and 29,466 for flint lines. Field trials were described in Lehermeier *et al.* (2014) and the phenotypic data were downloaded from the corresponding supplementary materials.

Simulation study

The simulation was based on the first wheat data set (599 wheat lines with 1,447 markers, Crossa *et al.* 2010) and the dent panel of the second maize data set (847 lines with 31,498 markers, Bauer *et al.* 2013).

For each data set we simulated traits in two scenarios: In the LE scenario, we randomly selected 100 markers with pairwise LD (r^2) less than 0.06 as the causal QTL contributing to the trait. The additive effects of the 100 QTL were independently sampled as a normally distributed random variable with mean 0 and variance 1. Then, we randomly sampled 100 pairs (among 5,050 pairs) of markers as causal epistatic QTL pairs. The epistatic effects were independently sampled as a normally distributed random variable with mean 0 and variance 0.5. Setting the heritability to be 0.7, we calculated the variance of environmental errors and the error terms for each genotype were independently sampled as a normally distributed random variable. Finally, we obtained the simulated trait values by summing up the additive values, epistatic values and environmental errors. In the LD scenario, we just randomly sampled 100 markers as causal QTL without considering LD and all other procedures are the same as the independent case. For each data set and each scenario, the simulation was repeated 50 times.

Evaluating prediction accuracies

The prediction accuracies of the three genomic prediction models were evaluated by five-fold cross-validation with 20 replications. For experimental data sets, the Pearson product-moment correlation between predicted and observed total genotypic values of the individuals in the test set was used as the measure of prediction accuracy. For simulated data sets, the prediction accuracy was defined as the correlation between predicted and true genotypic values of the individuals in the test set. Standard errors of prediction accuracies were estimated based on a bootstrap approach following Rutkoski *et al.* (2012). All models were implemented using the R package BGLR (Pérez and de los Campos 2014).

Supplementary References

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- Crossa, J., G. de Los Campos, P. Pérez, D. Gianola, J. Burgueño *et al.*, 2010 Prediction of genetic values of quantitative traits in plant breeding using pedigree and molecular markers. Genetics 186: 713-724.
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