Table S1: Root mean square error (RMSE) for 6 HGDP data sets as a function of the regularization parameter.

| | α | 0 | 1 | 10 | 100 | 1000 |
|--|----------|----------------|----------------|----------------|----------------|-----------------|
| | RMSE | 0.046 | 0.044 | 0.041 | 0.041 | 0.055 |
| | | [0.035, 0.064] | [0.035, 0.057] | [0.035, 0.052] | [0.031, 0.061] | [0.033, 0.095] |

| Table S2: | Choice | of <i>K</i> | for | sNMF | using t | he cr | oss-entrop | ру | criterion | (simulated | data). |
|-----------|--------|--------------------|-----|------|---------|-------|------------|----|-----------|------------|--------|
| | | | | | | | | | | | |

| | $\operatorname{Dir}(1,1,1)$ | Dir(.5, .5, .5) | Dir(.1, .1, .1) | Dir(.2, .2, .05) | Dir(.2, .2, .5) | Dir(.05, .05, .01) |
|-------|-----------------------------|-----------------|-----------------|------------------|-----------------|--------------------|
| K = 2 | 0.713 | 0.703 | 0.682 | 0.662 | 0.706 | 0.645 |
| K = 3 | 0.707 | 0.691 | 0.660 | 0.642 | 0.697 | 0.624 |
| K = 4 | 0.708 | 0.692 | 0.661 | 0.644 | 0.699 | 0.626 |
| K = 5 | 0.710 | 0.694 | 0.663 | 0.645 | 0.700 | 0.628 |

Dir: Dirichlet distribution used to simulate "true" admixture coefficients using 3 ancestral populations.



Figure S1. Run-times for sNMF. Time is expressed in unit of minutes. A) Run-time analysis for Harvard HGDP panel 01224 (10.6K SNPs). B) Run-time analysis for Harvard HGDP panel 00778 (78K SNPs). C) Run-time analysis for the HGDP-CEPH data (660K SNPs).



Figure S2. Values of the cross-entropy criterion for sNMF algorithms. Minimal values of the cross-entropy criterion over 5 runs of the sNMF program for A-E) 5 Harvard HGDP panel, F) the HGDP-CEPH data, and G) The 1000 Genomes Project data set. The number of clusters ranged from 5 to 10, and the values of the regularization parameter ranged from 0 to 10,000.



Figure S3. Graphical representation of admixture estimates for European populations of A. thaliana. Estimated admixture coefficients using sNMF using K = 3 and $\alpha = 100$ (crossentropy = 0.483).



Figure S4. Accuracy of ADMIXTURE and sNMF in the presence of linkage disequilibrium. RMSEs between estimated Q matrices without and with linkage disequilibrium for ADMIXTURE and sNMF using K = 5 based on subsets of SNPs sampled from the 1000 Genome Project data set.



Figure S5. Accuracy of ADMIXTURE and sNMF in the presence of related individuals. Cross-entropy criterion for ADMIXTURE and for sNMF. Simulations mimicked the population structure of European populations of *Arabidopsis thaliana*. A-B) Moderate levels of inbreeding, $F_{\rm IS} = 25 - 50\%$, C-D) Strong levels of inbreeding, $F_{\rm IS} = 75 - 100\%$.