

How well do molecular and pedigree relatedness correspond, in populations with variable mating systems, and types and quantities of molecular and demographic data?

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SUPPLEMENTARY INFORMATION

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Modelled Scenarios

The population size was kept constant using a Beverton-Holt function (Beverton and Holt 1957; Maynard Smith and Slatkin 1973; Bellows 1981). Mutations were not implemented in the simulation because effects of mutations are negligible for the time frame over which the simulations were run (Ellegren 2000).

Table S1: Parameter values used in the model. RCA Relatedness Category Assignment; MAF Minor Allele Frequency; PO parent-offspring; FS full siblings; R=0.25 avuncular, half sibs, grand-parent-grand offspring; R=0.125 full cousins, half avuncular; R=0.0625 half first cousins, first cousins once removed, double second cousins; unrel unrelated; No. number

Parameter	Classes	Value
Mating system scenarios	monogamy, polygyny, promiscuity	
No. of simulations/scenario	10	
No. of time steps/simulation before performing the RCA	100	
Initial population size	600	
No. of overlapping generations	3	
Age class at first reproduction	4	
Max. age class	12	
Overlapping generations	Mean no. of offspring per female/time step (Poisson distribution)	monogamy polygyny promiscuity
		age class 1
		age class 2-3
	Mortality rates	age class 4-6
		age class 7-9
		age class 10-12
	No. of SNP loci simulated	50, 100, 200, 400, 800, 1600, 3200 (single simulations with 50000)
No. of STR loci simulated	10, 20, 40, 80	
No. of SNP loci combined with 20 STR loci simulated	50, 100, 200, 400, 800, 1600, 3200 (single simulations with 50000)	
Mean MAF (SNP only) simulated	0.05, 0.25, 0.5	
Proportion of population sampled	1; for some simulations 0.5, 0.25, 0.125, 0.0625	

	Sex ratio at start of simulation/probability for male (female) offspring	1:1/ 0.5 (0.5)	
	mtDNA haplotypes known	yes, when indicated	
	No. of unifrequent mtDNA haplotypes	5	
	Age class known	yes, when indicated	
	Sex known	Yes, when mtDNA haplotype and/or age class known	
	Mating system scenarios	monogamy, polygyny, promiscuity	
	Relatedness categories used	PO, FS, R=0.25, R=0.125, unrel	
	No. of time steps/simulation before performing the RCA	10	
	No. of simulations/scenario	10	
	Initial population size	600	
	No. of overlapping generations	1	
	Age class at first reproduction	1	
	Max. age class	1	
Non-overlapping generations	Mean no. of offspring per / time step (Poisson distribution)	monogamy	4
		polygyny	4
		promiscuity	4
	Mortality rates	550-650 randomly chosen offspring survived each time step to produce the next generation in all mating system scenarios	
	No. of SNP loci simulated	50, 100, 200, 400, 800, 1600, 3200	
	No. of STR loci simulated	10, 20, 40, 80	
	No. of SNP loci combined with 20 STR loci simulated	50, 100, 200, 400, 800, 1600, 3200	
	Mean MAF (SNP only) simulated	0.05, 0.25, 0.5	
	Relatedness categories used	PO, FS, R=0.25, R=0.125, unrel	
	Proportion of population sampled	1	
	Sex ration at start of simulation/probability for male (female) offspring	1:1/ 0.5 (0.5)	
		mtDNA haplotypes known	no
	No. of unifrequent mtDNA haplotypes	n/a	
	Age class known	no	
	Sex known	no	

Table S2: Correct classification rate of relationship category assignment. For each category, the lowest number of loci (No. Loci) is shown, where the mean correct classification rate exceeded 0.95 (95% correct classification rate, Figures 1, S1, S2). Numbers are based on 10 independent simulations.

Mating System	Marker	MAF	PO				FS				R=0.25				unrel			
			min	max	Mdn	No Loci	min	max	Mdn	No Loci	min	max	Mdn	No Loci	min	max	Mdn	No Loci
Monogamy	SNP	0.05	0.988	1	0.993	3200	0.964	0.994	0.982	1600	0.929	0.977	0.950	3200	0.990	0.993	0.991	50
		0.25	0.964	0.984	0.976	200	0.933	0.980	0.965	200	0.960	0.990	0.976	1600	0.993	0.994	0.994	50
		0.5	0.941	0.979	0.969	100	0.939	0.983	0.967	200	0.958	0.988	0.976	1600	0.992	0.995	0.993	50
	STR	n/a	0.992	0.998	0.995	80	0.951	0.987	0.974	80	-	-	-	-	0.992	0.994	0.993	10
	SNP&STR	0.05	0.929	0.966	0.954	800	0.971	0.995	0.981	800	0.936	0.978	0.951	3200	0.995	0.996	0.995	50
		0.25	0.952	0.978	0.969	100	0.957	0.990	0.982	200	0.964	0.992	0.977	1600	0.995	0.997	0.996	50
0.5		0.982	0.995	0.989	100	0.947	0.993	0.979	200	0.958	0.991	0.975	1600	0.995	0.997	0.996	50	
Polygyny	SNP	0.05	0.959	0.989	0.983	1600	0.942	0.992	0.965	3200	0.976	0.985	0.982	3200	0.988	0.990	0.989	50
		0.25	0.986	1	0.994	200	0.922	1	0.966	800	0.940	0.961	0.953	800	0.992	0.993	0.992	50
		0.5	0.959	0.987	0.977	100	0.921	0.991	0.968	400	0.939	0.969	0.955	800	0.991	0.993	0.992	50
	STR	n/a	0.986	1	0.997	80	-	-	-	-	-	-	-	-	0.990	0.992	0.991	10
	SNP&STR	0.05	0.933	0.970	0.953	400	0.929	1	0.951	1600	0.946	0.960	0.956	1600	0.994	0.995	0.995	50
		0.25	0.968	0.993	0.979	100	0.907	1	0.966	800	0.949	0.967	0.955	800	0.995	0.996	0.995	50

		0.5	0.938	0.980	0.964	50	0.924	1	0.972	400	0.952	0.975	0.959	800	0.994	0.996	0.995	50
		0.05	0.978	0.993	0.982	800	-	-	-	-	0.972	0.982	0.979	3200	0.990	0.992	0.991	50
Promiscuity	SNP	0.25	0.985	1	0.996	200	-	-	-	-	0.973	0.992	0.982	1600	0.992	0.995	0.994	50
		0.5	0.984	1	0.993	100	-	-	-	-	0.977	0.994	0.981	1600	0.993	0.996	0.994	50
		n/a	0.964	0.992	0.977	40	-	-	-	-	-	-	-	-	0.991	0.993	0.993	10
	STR	0.05	0.937	0.971	0.957	200	-	-	-	-	0.972	0.985	0.979	3200	0.995	0.996	0.995	50
	SNP&STR	0.25	0.947	0.977	0.957	50	-	-	-	-	0.975	0.991	0.982	1600	0.996	0.997	0.996	50
		0.5	0.963	0.991	0.978	50	-	-	-	-	0.938	0.970	0.955	800	0.996	0.997	0.996	50

Min minimum correct classification rate, max maximum correct classification rate, Mdn median, MAF minor allele frequency, PO parent-offspring, R=0.25 avuncular, half sibs, grand-parent-grand offspring, unrel unrelated, SNP&STR number of SNP loci required when combined with 20 STR loci. Dashes indicate that the category could not be assigned with a >95% correct classification rate with the simulated number of loci.

Table S3: Not considering R=0.125: minimum number of SNP and/or STR loci required per category for a relatedness category assignment with a >95% (>80%) correct classification rate without considering the category R=0.125.

Mating System	Marker	MAF	PO	FS	R=0.25	Unrel ¹
Monogamy	SNP	0.05	3200 (800)	1600 (800)	--	50
		0.25	200 (100)	200 (200)	--	50
		0.5	100 (100)	200 (100)	--	50
	STR	n/a	80 (40)	80 (40)	--	10
	SNP&STR ²	0.05	800 (100)	400 (100)	--	50
		0.25	100 (50)	200 (50)	--	50
0.5		100 (50)	100 (50)	--	50	
Polygyny	SNP	0.05	1600 (400)	3200 (1600)	--	50
		0.25	200 (100)	400 (400)	--	50
		0.5	100 (100)	400 (200)	--	50
	STR	n/a	80 (40)	- (80)	--	10
	SNP&STR	0.05	400 (100)	1600 (800)	--	50
		0.25	100 (50)	400 (200)	--	50
0.5		50 (50)	400 (200)	--	50	
Promiscuity	SNP	0.05	800 (400)	- -	--	50
		0.25	200 (100)	- -	--	50
		0.5	100 (100)	- -	--	50
	STR	n/a	40 (40)	- -	--	10
	SNP&STR	0.05	200 (50)	- -	--	50
		0.25	50 (50)	- -	--	50
0.5		50 (50)	- -	--	50	

Dashes indicate that the category could not be assigned with a >95% (80%) correct classification rate with the simulated number of loci. MAF minor allele frequency, PO parent-offspring, FS full siblings, R=0.25 avuncular, half sibs, grand-parent-grand offspring, unrel unrelated. ¹Note that with the population size and parameters used, more than >95% of individuals are unrelated, so even if all dyads were assigned to the category 'unrelated' the correct classification rate might be >95%. ²Number of SNP loci required when combined with 20 STR loci.

Table S4: Considering R=0.0625: minimum number of SNP loci or SNP loci combined with 20 STR loci required per category for a relatedness category assignment (RCA) with >95% (>80%) correct classification rates. For the simulations shown in this table the category R=0.0625 was assessed. STR only results are not shown because they did not change compared to simulations without R=0.0625 (Table 2).

Mating System	Marker	MAF	PO	FS	R=0.25	R=0.125 ¹	R=0.0625 ¹	unrel ²
Monogamy	SNP	0.05	3200 (800)	1600 (800)	3200 (1600)	- -	--	50
		0.25	200 (200)	200 (200)	1600 (800)	- -	--	50
		0.5	100 (100)	200 (100)	1600 (800)	- -	--	50
	SNP&STR ³	0.05	1600 (100)	800 (200)	3200 (1600)	- -	--	50
		0.25	100 (50)	200 (50)	1600 (800)	- -	--	50
		0.5	100 (50)	200 (50)	1600 (800)	- -	--	50
Polygyny	SNP	0.05	1600 (800)	3200 (1600)	3200 (800)	- -	--	50
		0.25	200 (100)	400 (400)	800 (400)	- (3200)	--	50
		0.5	100 (100)	400 (200)	800 (400)	- (3200)	--	50
	SNP&STR	0.05	800 (100)	1600 (800)	3200 (800)	- -	--	50
		0.25	100 (50)	400 (200)	800 (400)	- (3200)	--	50
		0.5	100 (50)	400 (200)	800 (400)	- (3200)	--	50
Promiscuity	SNP	0.05	800 (400)	- -	3200 (800)	- (3200)	--	50
		0.25	200 (100)	- -	1600 (400)	- (3200)	--	50
		0.5	100 (100)	- -	800 (400)	- (1600)	--	50
	SNP&STR	0.05	200 (50)	- -	3200 (800)	- (3200)	--	50
		0.25	100 (50)	- -	1600 (400)	- (1600)	--	50
		0.5	50 (50)	- -	800 (400)	- (1600)	--	50

Dashes indicate that the category could not be assigned with a >95% (80%) correct classification rate with the simulated number of loci. MAF minor allele frequency, PO parent-offspring, FS full siblings, R=0.25 avuncular, half sibs, grand-parent-grand offspring, R=0.125 full cousins, half avuncular, unrel unrelated. ¹Even though no number of tested loci led to a 95% correct classification rate for the R=0.125 and R=0.0625 categories

under the simulated population conditions these categories are part of this table because it may be important to include them in the RCA. ²Note that with the population size and parameters used, more than >95% of individuals are unrelated, so even if all dyads were assigned to the category 'unrelated' the correct classification rate might be >95%. ³Number of SNP loci required when combined with 20 STR loci.

Table S5: Effect of typing error: minimum number of SNP and/or STR loci with 2% typing error required per category for a relatedness category assignment with >95% correct classification rates.

Mating System	Marker	MAF	PO	FS	R=0.25	R=0.125 ¹	Unrelated ²	
Monogamy	SNP	0.05	-	3200	3200	-	50	
		0.25	400	400	3200	-	50	
		0.5	400	400	3200	-	50	
	STR	n/a	80	80	-	-	10	
	SNP&STR ³	0.05	1600	1600	3200	-	10	
		0.25	200	200	3200	-	50	
		0.5	200	200	1600	-	50	
	Polygyny	SNP	0.05	1600	-	1600	-	50
			0.25	400	800	1600	-	50
0.5			400	800	1600	-	50	
STR		n/a	40	-	-	-	10	
SNP&STR		0.05	400	-	1600	-	50	
		0.25	200	400	1600	-	50	
		0.5	200	800	1600	-	50	
Promiscuity		SNP	0.05	800	-	1600	-	50
			0.25	400	-	1600	-	50
	0.5		200	-	1600	-	50	
	STR	n/a	40	-	-	-	10	
	SNP&STR	0.05	400	-	1600	-	50	
		0.25	100	-	1600	-	50	
		0.5	100	-	1600	-	50	

Dashes indicate that the category could not be assigned with a >95% correct classification rate with the simulated number of loci. MAF minor allele frequency, PO parent-offspring, FS full siblings, R=0.25 avuncular, half sibs, grand-parent-grand offspring, R=0.125 full cousins, half avuncular. ¹Even though no number of tested loci led to a 95% correct classification rate for the R=0.125 category under the simulated population conditions; R=0.125 is part of this table because it is important to include it in the relatedness category assignment for the correct classification rate of R=0.25. ²Note that with the population size and parameters used, more than >95% of individuals are unrelated, so even if all dyads were assigned to the category 'unrelated' the correct classification rate might be >95%. ³Number of SNP loci required when combined with 20 STR loci.

Table S6: Non-overlapping generations: minimum number of SNP and/or SNP loci required per category for a relatedness category assignment with >95% correct classification rates.

Mating System	Marker	MAF	PO	FS	R=0.25	R=0.125 ¹	unrel ²
Monogamy	SNP	0.05	-	400	-	-	50
		0.25	-	200	-	-	50
		0.5	-	200	-	-	50
	STR	n/a	-	40	-	-	10
	SNP&STR ³	0.05	-	200	-	-	50
		0.25	-	50	-	-	50
0.5		-	50	-	-	50	
Polygyny	SNP	0.05	-	800	1600	-	50
		0.25	-	400	800	-	50
		0.5	-	200	800	-	50
	STR	n/a	-	-	-	-	10
	SNP&STR	0.05	-	800	1600	-	50
		0.25	-	200	800	-	50
0.5		-	200	800	-	50	
Promiscuity	SNP	0.05	-	3200	800	-	50
		0.25	-	800	400	-	50
		0.5	-	800	400	-	50
	STR	n/a	-	-	-	-	10
	SNP&STR	0.05	-	3200	800	-	50
		0.25	-	800	400	-	50
0.5		-	800	400	-	50	

Dashes indicate that the category could not be assigned with a >95% correct classification rate with the simulated number of loci. MAF minor allele frequency, PO parent-offspring, FS full siblings, R=0.25 avuncular, half sibs, grand-parent-grand offspring, R=0.125 full cousins, half avuncular, unrel unrelated. ¹Even though no number of tested loci led to a 95% correct classification rate for the R=0.125 and R=0.0625 categories under the simulated population conditions these categories are part of this table because it may be important to include them in the relatedness category assignment. ²Note that with the population size and parameters used, more than >95% of individuals are unrelated, so even if all dyads were assigned to the category 'unrelated' the correct classification rate might be >95%. ³Number of SNP loci required when combined with 20 STR loci.

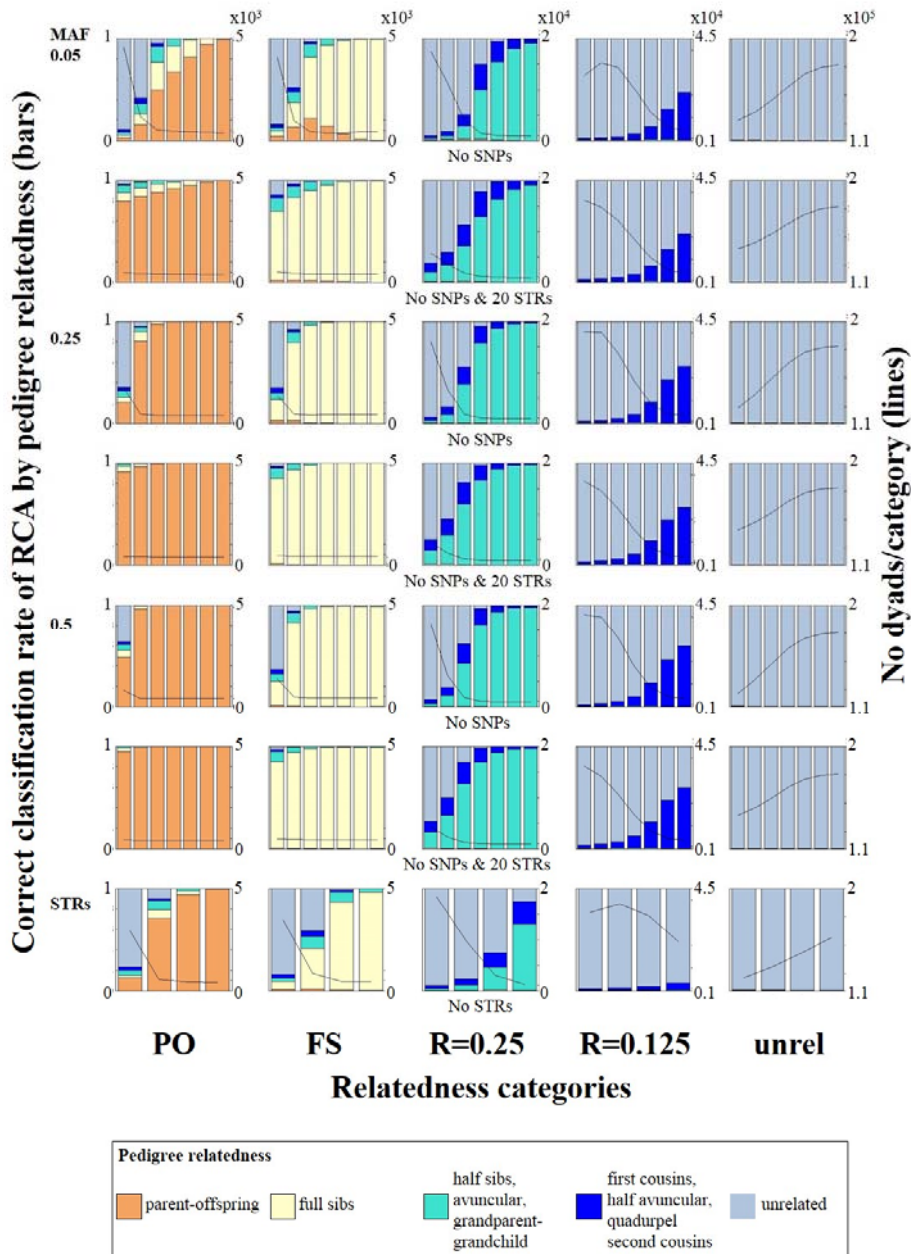


Figure S1: Monogamy: correct classification rates of relatedness category assignment (RCA) in a monogamous population (average over 10 simulations). Three different minor allele frequencies (MAF) for SNPs, seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. On the left vertical axes, the proportion of the correct pedigree relatedness color in each category (PO: parent-offspring; FS: full sibs; unrel: unrelated) indicates the correct classification rate of the category-assignment based on the genetic loci. Other colors indicate source of erroneously assigned categories. The right vertical axes, and the lines, indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The orders of magnitude at the top of the No dyads/category scale of the first row applies to all No dyads/category scales below it. Figures 1 and S2 show the same plots for other mating systems. The variability between the 10 independent simulations is presented in Table S2.

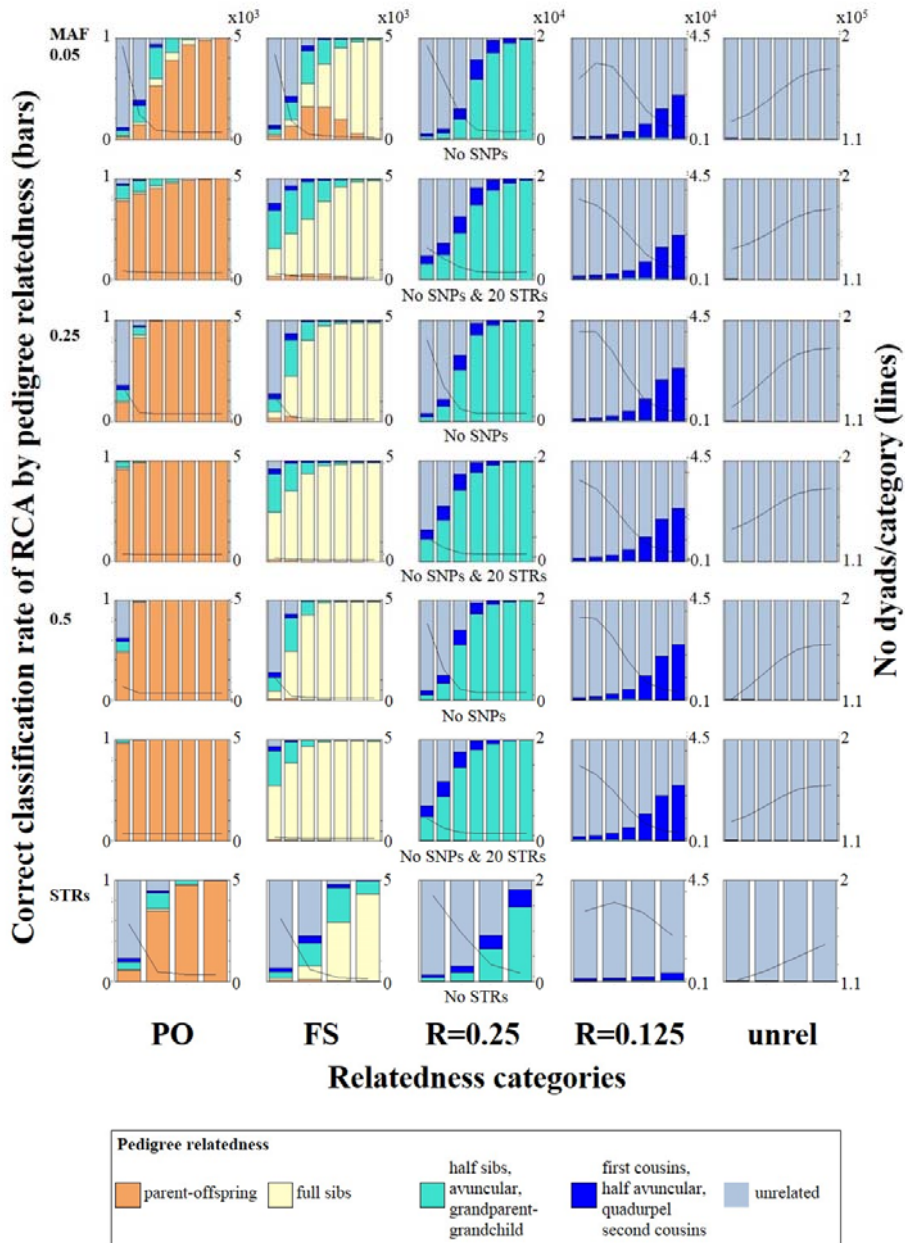


Figure S2: Polygyny: correct classification rates of relatedness category assignment (RCA) in a polygynous population (average over 10 simulations). Three different minor allele frequencies (MAF) for SNPs, seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. On the left vertical axes, the proportion of the correct pedigree relatedness color in each category (PO: parent-offspring; FS: full sibs; unrel: unrelated) indicates the correct classification rate of the category-assignment based on the genetic loci. Other colors indicate source of erroneously assigned categories. The right vertical axes, and the lines, indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The orders of magnitude at the top of the No dyads/category scale of the first row applies to all No dyads/category scales below it. Figures 1 and S1 show the same plots for other mating systems. The variability between the 10 independent simulations is presented in Table S2.

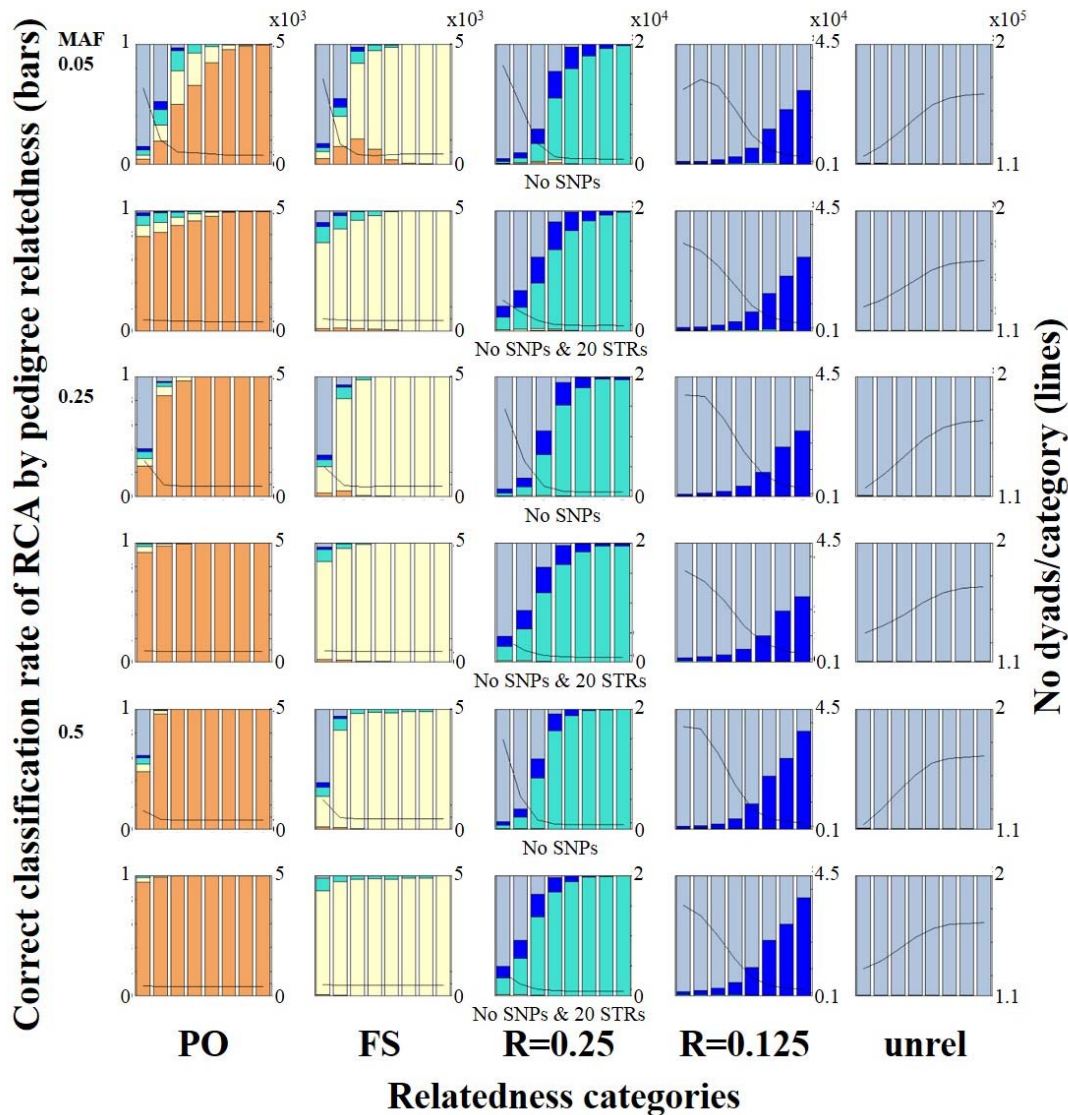


Figure S3: 50 000 SNP loci/monogamy: correct classification rates of relatedness category assignment (RCA) in a monogamous population (results of a single simulation shown). Three different minor allele frequencies (MAF) for SNPs, eight different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200, 50 000) and a combination of SNP with 20 STR loci were simulated. On the left vertical axes, the proportion of the correct pedigree relatedness color in each category (PO: parent-offspring; FS: full sibs; unrel: unrelated) indicates the correct classification rate of the category-assignment based on the genetic loci. Other colors indicate source of erroneously assigned categories. The right vertical axes, and the lines, indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The orders of magnitude at the top of the No dyads/category scale of the first row applies to all No dyads/category scales below it.

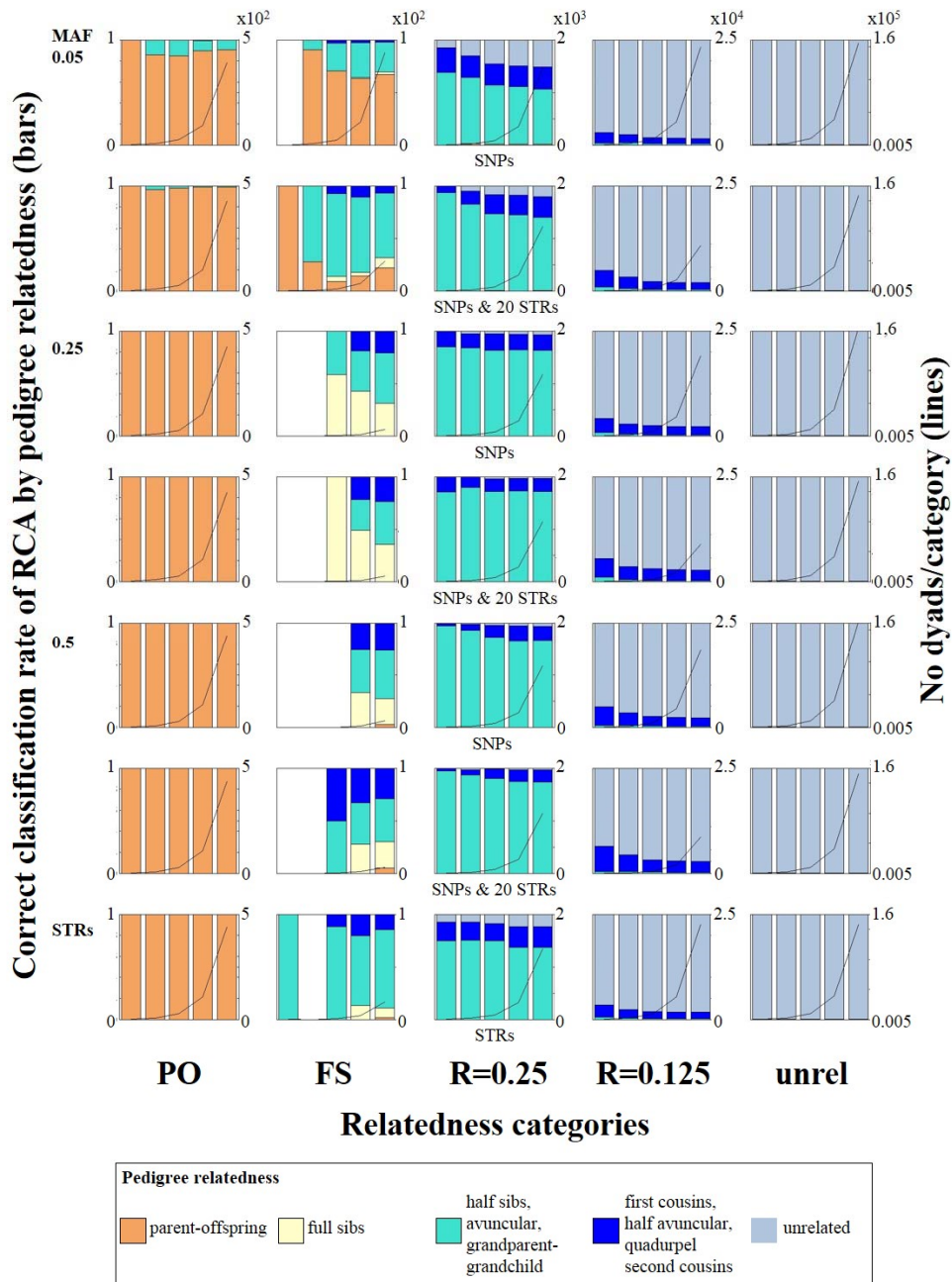


Figure S4: Subsampling/promiscuity: correct classification rates of relatedness category assignment (RCA) with subsampling of a promiscuous population based on 400 SNPs, 400 SNPs & 20 STRs, and 80 STRs, respectively (average over 10 simulations). Five different proportions of the population were sampled (individual bars from left to right within each subplot: 0.0625, 0.125, 0.25, 0.5, 1). Three different minor allele frequencies (MAF) for SNPs were simulated. On the left vertical axes, the proportion of the correct pedigree relatedness color in each category (PO: parent-offspring; FS: full sibs; unrel: unrelated) indicates the correct classification rate of the category-assignment based on the genetic loci. Other colors indicate source of erroneously assigned categories. The right vertical axes, and the lines, indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rate were achieved). No bar means that no dyads were assigned to the category. The order of magnitudes at the top of the No dyads/category scale of the first row apply to all No dyads/category scales below it.

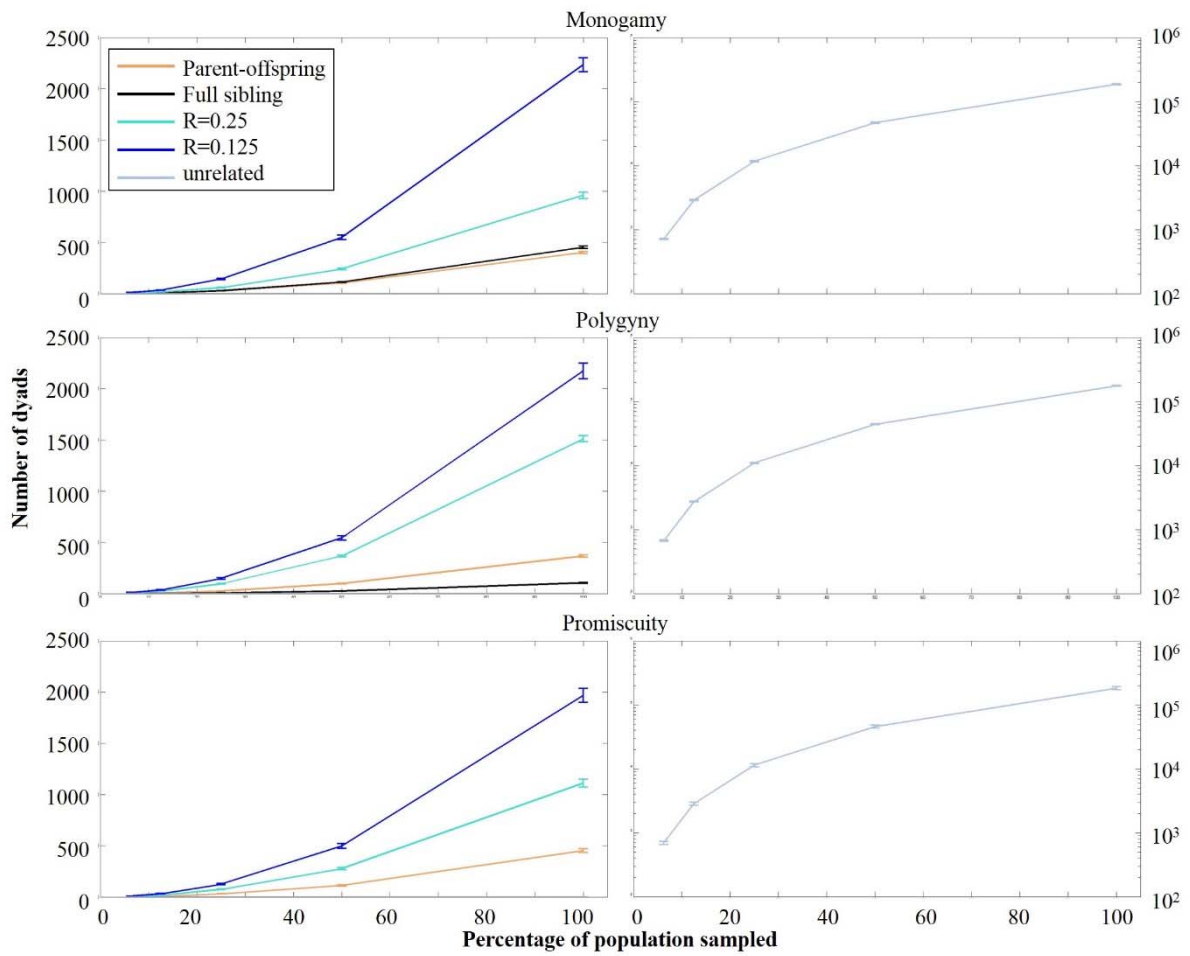


Figure S5: Number of pedigree dyads in subsamples of the population. Error bars indicate standard errors across 10 independent simulations. Note the log scale for plots containing the results of unrelated dyads.

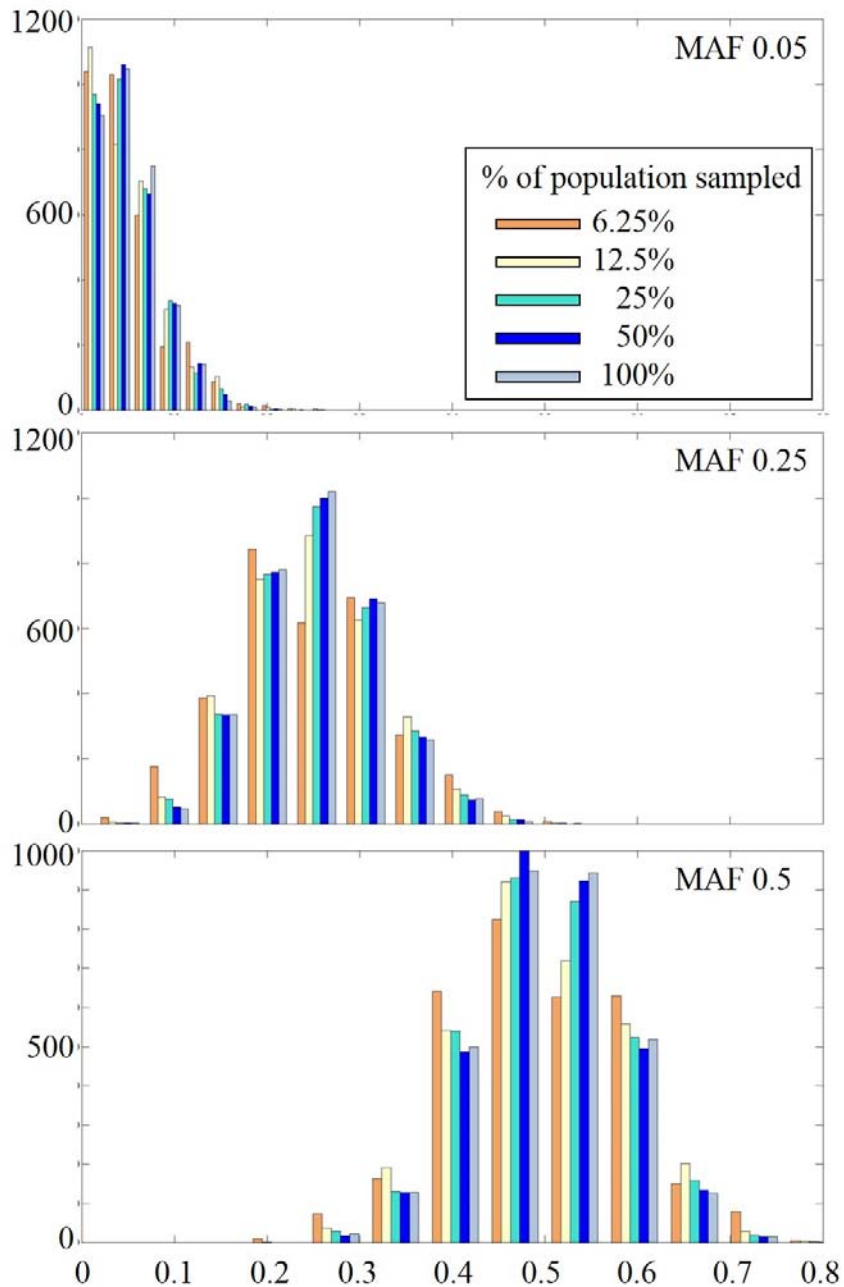


Figure S6: Allele frequency distribution after 100 time steps of the SNP allele with indicated minor allele frequency (MAF) at the start of the simulations. Results of single simulations are shown (3200 SNP loci, promiscuous population). Different colors represent allele frequency estimates of different proportions of the population sampled.

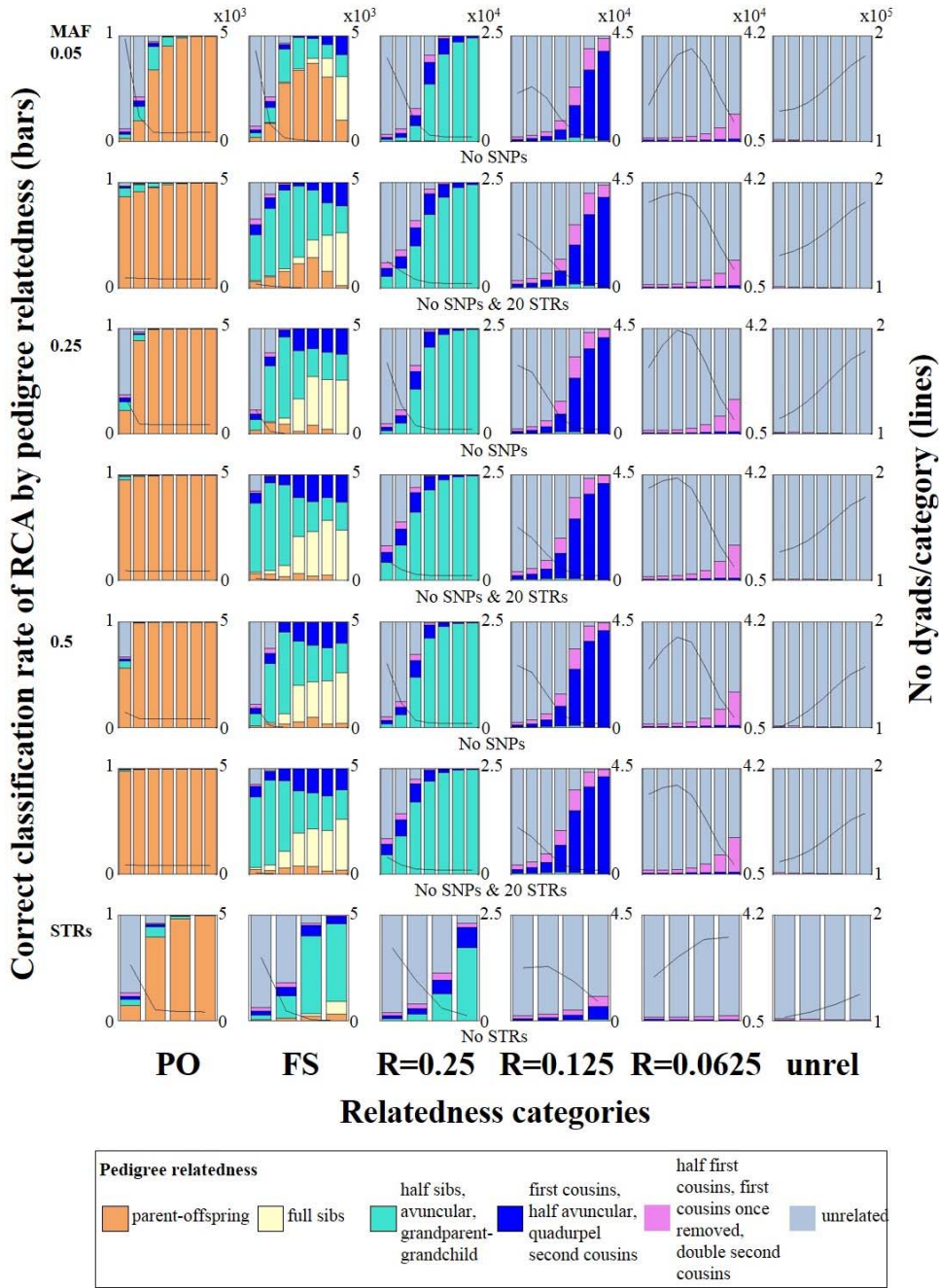


Figure S7: Considering $R=0.0625$ /promiscuity: correct classification rates of relatedness category assignment (RCA) including the category $R=0.0625$ in a promiscuous population (average over 10 simulations). Three different minor allele frequencies (MAF), seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. The proportion of the pedigree relatedness color in each category indicates the correct classification rate of the category-assignment based on the genetic markers. Other colors indicate source of erroneously assigned categories. Lines indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The order of magnitudes at the top of the No dyads/category scale of the first row apply to all No dyads/category scales below it.

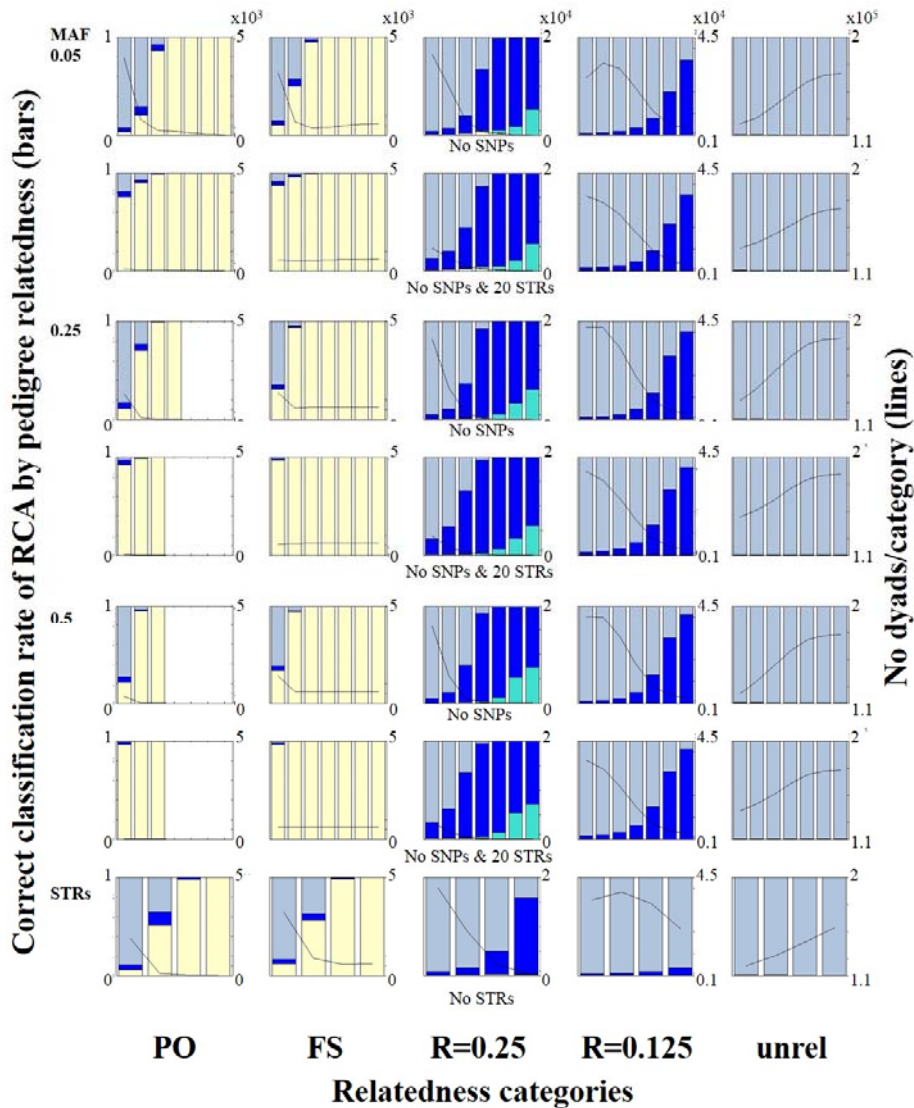


Figure S8: Non-overlapping generations/monogamy: correct classification rates of relatedness category assignment (RCA) in a monogamous population without overlapping generations (average over 10 simulations). Three different minor allele frequencies (MAF), seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. The proportion of the pedigree relatedness color in each category indicates the correct classification rate of the category-assignment based on the genetic markers. Other colors indicate source of erroneously assigned categories. Lines indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rate were achieved). Because neither half sibs, avuncular nor grandparent-grandchild would be expected under these conditions the turquoise bars represent quadruple second cousins. S9 and S10 show the same plot but for other mating systems.

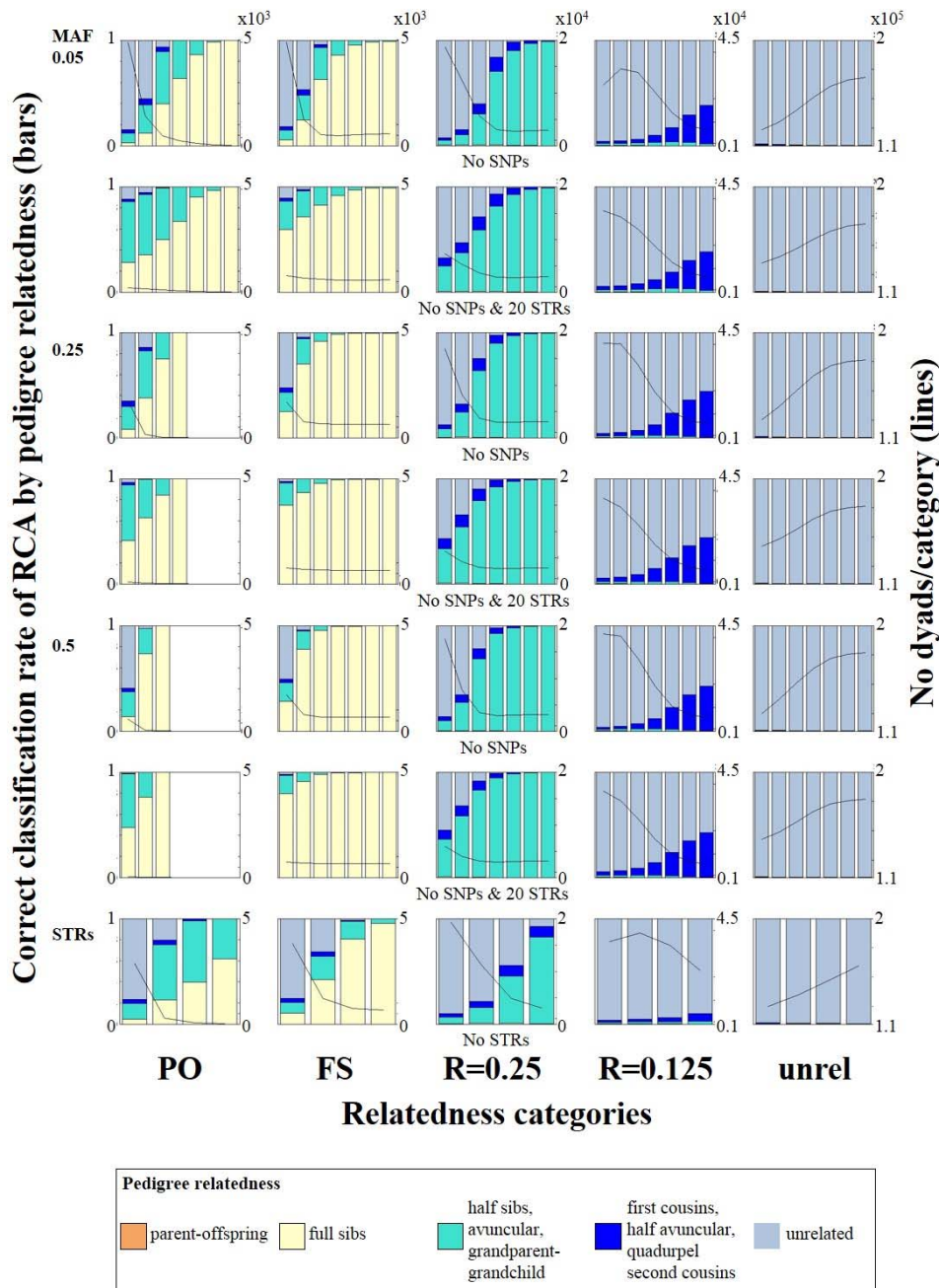


Figure S9: Non-overlapping generations/polygyny: correct classification rates of relatedness category assignment (RCA) in a polygynous population without overlapping generations (average over 10 simulations). Three different minor allele frequencies (MAF), seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. The proportion of the pedigree relatedness color in each category indicates the correct classification rate of the category-assignment based on the genetic markers. Other colors indicate source of erroneously assigned categories. Lines indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The order of magnitudes at the top of the No dyads/category scale of the first row apply to all No dyads/category scales below it. Figures S8 and S10 show the same plot but or other mating systems.

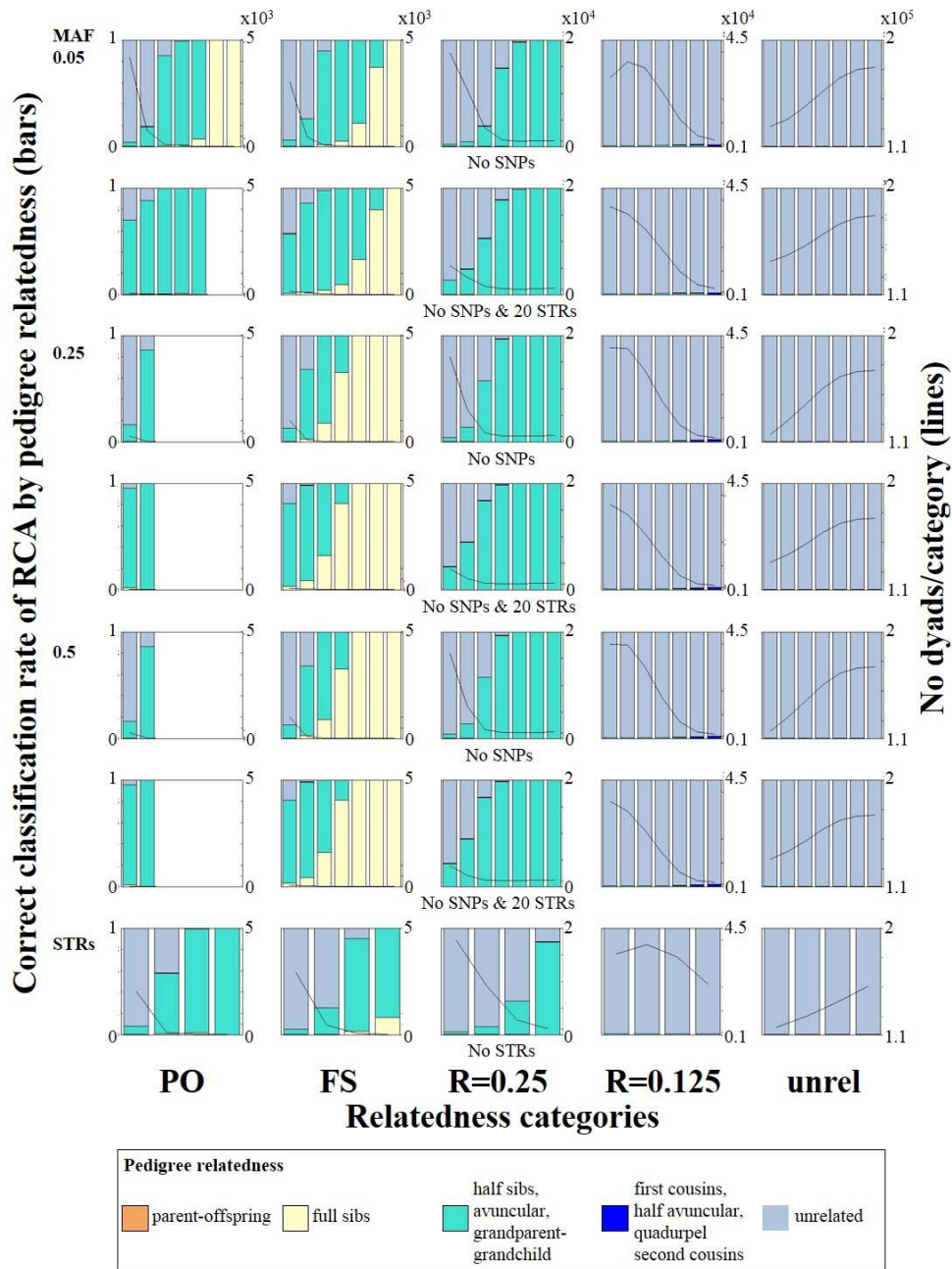


Figure S10: Non-overlapping generations/promiscuity: correct classification rates of relatedness category assignment (RCA) in a promiscuous population without overlapping generations (average over 10 simulations). Three different minor allele frequencies (MAF), seven different number (No) of SNP loci (individual bars from left to right: 50, 100, 200, 400, 800, 1600, 3200), four different numbers of STR loci (from left to right: 10, 20, 40, 80), and a combination of SNP with 20 STR loci were simulated. The proportion of the pedigree relatedness color in each category indicates the correct classification rate of the category-assignment based on the genetic markers. Other colors indicate source of erroneously assigned categories. Lines indicate the number of dyads that were assigned to each category (the true number of dyads can be inferred where almost 100% correct classification rates were achieved). The order of magnitudes at the top of the No dyads/category scale of the first row apply to all No dyads/category scales below it. Figures S8 and S9 show the same plot but for other mating systems.

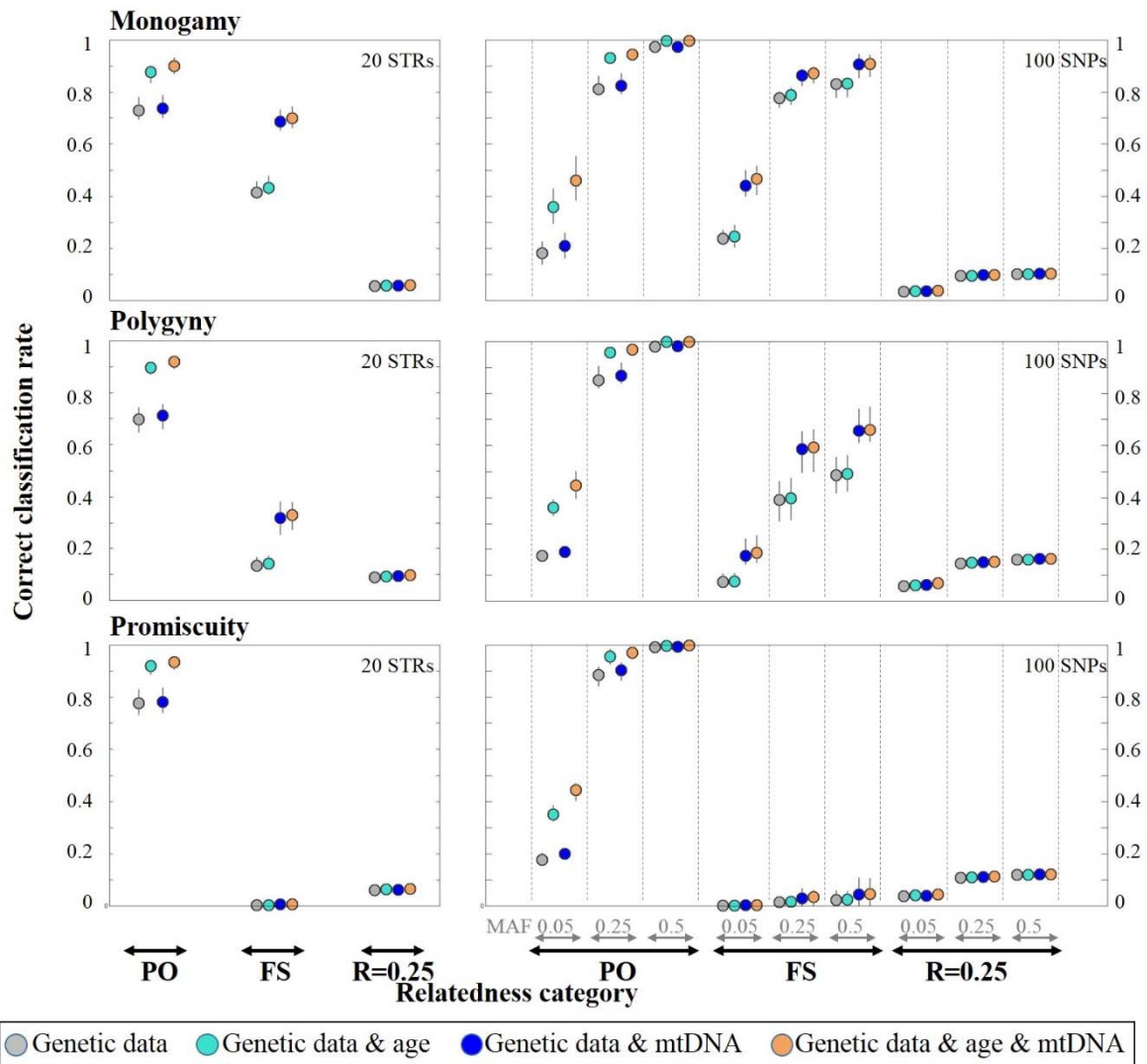


Figure S11: Effect of additional data on correct classification rates of relatedness category assignment in three different mating systems using 20 STR and 100 SNP loci, respectively. In addition to age and/or mtDNA haplotype the sex of the individuals was known too. Plotted are mean and range of correct classification rates based on 10 independent simulations.

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