Table S1 Summary of phenotype and genotype in this study

Species	Trait[a]	Sample Size	Genotype (# SNPs)
White-feathered broiler chicken	NGG	4511	112502
	AGG	4511	112502
Yellow-feathered broiler chickens A	SW	7256	230031
	BW	7256	230031
	DP	7256	230031
Yellow-feathered broiler chickens B	TW	1881	124683
Duroc pig	TPD	2610	124679
	BF	2549	124679
	LMD	2549	124679
	TPV	2610	124679
	FR	2610	124679
	LMA	2549	124679
	FPV	2610	124679
	ADFI	2610	124679
	AGE	2549	124679
	NVD	2610	124679
Horse	HC	480	54000
Maize	SSK	2631	681257
	YKW	1595	681257
	GDD	2279	681257

[a] Trait including NGG, number of eggs qualified at 300 days of age; AGG, age at first egg; SW, slaughter weight at 91 days of age; BW, body weight at 90 days of age; DP, dressed percentage; TW, testicular weight at 90 days of age; YWK, yellow or white kernels; SSK, sweet or starchy kernels; GDD, growing degree days; AGE, age to 100 kg live weight; LMA, loin muscle area at 100 kg live weight; LMD, loin muscle depth at 100 kg live weight; BF, back fat thickness at 100 kg live weight; ADFI, average daily feed intake; NVD, number of visits to feeder per day; TPD, time spent to eat per day; TPV, time spent to eat per visit; FPV, feed intake per visit; FR, feed intake rate; HC, horse color.

Table S2 Average predictive accuracy across 12 machine learning and two traditional methods

Traits		Sample Size	GBLUP	BayesR	OLS Regression			Nonlinear		Bagging		Boosting				
Category	Abbr.				Linear (Logistic)	Ridge	Elastic Net	KNN	SVM	Random Forest	Decision Tree	GBDT	XGBoost	AdaBoost	LightGBM	CatBoost
I	SSK	2631	0.9357	0.7945	0.9412	-[a]	-	0.9393	0.9374	0.9374	0.8956	0.9108	0.9374	0.9374	0.9374	**0.9412**[c]
	YKW	1595	0.7485	0.7620	0.7649	-	-	0.6708	0.7994	0.7962	0.6865	0.7241	0.7806	**0.8056**	0.7868	0.7962
	GDD	2279	0.5021	0.8862	0.8920	0.8951	0.8909	0.8720	0.7534	0.8632	0.8620	0.8740	0.8755	0.8620	0.8858	**0.9001**
	HC	480	0.6813	0.8125	0.6729	-	-	0.6458	0.6438	0.7729	0.7375	0.8333	0.8583	0.7708	0.8604	**0.8667**
II	TW	1881	0.2259	**0.2584**	0.1593	0.1724	0.1633	0.0525	0.1029	0.0918	0.0842	0.0761	0.0643	0.0722	0.1762	0.1821
	BF	2549	0.3901	0.4410	0.2817	0.4043	N/A[b]	0.3154	0.3980	0.3381	0.3255	0.3470	0.2816	0.2724	**0.4484**	0.3934
	LMD	2549	0.3491	0.4103	0.2560	0.3760	N/A	0.3041	0.3412	0.2903	0.3029	0.2831	0.2363	0.2588	**0.4559**	0.3815
	SW	7256	0.3031	0.3760	0.1317	0.1445	0.1212	0.0520	0.1091	0.1109	0.1035	0.1660	0.1153	0.0938	**0.7688**	0.7343
	BW	7256	0.2880	0.3751	0.1263	0.1780	0.1250	0.0570	0.1039	0.1105	0.1243	0.1620	0.1146	0.0912	**0.7533**	0.7530
	DP	7256	0.2761	0.2968	0.0765	0.0886	N/A	0.0481	0.0462	0.0565	0.0543	0.0486	0.0558	0.0421	0.7294	**0.7343**
	AGG	4511	0.3462	0.3802	0.1522	0.2457	0.1272	0.1670	0.2082	0.1968	0.1692	0.1896	0.1395	0.1457	0.3647	**0.4022**
III	ADFI	2610	0.2577	0.3154	0.1398	0.2097	N/A	0.1124	0.1976	0.1455	0.1377	0.1750	0.1167	0.1023	0.2874	**0.3106**
	FPV	2610	0.2833	**0.3304**	0.1449	0.2452	0.2246	0.1017	0.1621	0.0816	0.0938	0.1272	0.0700	0.0922	0.1299	0.1637
	AGE	2549	0.2928	0.3620	0.2672	0.3648	0.3432	0.3671	0.3223	0.4039	0.3400	0.3648	0.2385	0.3128	**0.4538**	0.3863
	NVD	2610	0.3247	**0.3521**	0.1728	0.2752	N/A	0.1181	0.2533	0.1568	0.1733	0.1911	0.1268	0.1152	0.2215	0.2630
	FR	2610	0.4568	**0.4671**	0.2447	0.3878	0.1764	0.2520	0.3584	0.2674	0.2650	0.3223	0.1747	0.2294	0.2747	0.3372
	LMA	2549	0.3816	**0.4003**	0.2936	0.3763	N/A	0.2486	0.3365	0.2947	0.2881	0.3090	0.2069	0.2262	0.3873	0.3679
	TPD	2610	0.4594	**0.4756**	0.2703	0.4448	0.3680	0.2675	0.3596	0.2758	0.2667	0.3554	0.2510	0.2862	0.3731	0.4326
	TPV	2610	0.4240	**0.4460**	0.2081	0.3587	N/A	0.2275	0.3456	0.2113	0.1924	0.2578	0.1637	0.1818	0.2612	0.3299
	NGG	4511	0.3065	**0.3408**	0.1276	0.2403	0.2187	0.1715	0.2374	0.2050	0.2072	0.2014	0.1449	0.1191	0.2147	0.2266

[a] not applicable; [b] fails to fit; [c] optimal result. The standard deviation ranges from 0.014 to 0.058.

Table S3. The impact of different parameters on the results using simulated data

Single Variable	Other parameters	LightGBM	CatBoost	BayesR	GBLUP
$h^2=0.1$	QTL=50	0.1033	0.1235	0.1649	0.5413
$h^2=0.3$	normal distribution	0.3741	0.3457	0.4886	0.7155
$h^2=0.7$	additive	0.7230	0.7608	0.8189	0.9226
QTL=50	$h^2=0.3$	0.3741	0.3457	0.4886	0.7155
QTL=2000	normal distribution	0.2840	0.3121	0.3956	0.7529
QTL=100000	additive	0.2812	0.3210	0.3941	0.7582
normal distribution	QTL=50, $h^2=0.3$	0.3741	0.3457	0.4886	0.7155
gamma distribution	additive	0.4569	0.4994	0.4972	0.7031
A ($h^2=0.7$)	QTL=10, SNP=10k	0.7809	0.7982	0.8224	0.7969
A ($h^2=0.7$)+A×A ($h^2=0.1$)	normal distribution	0.8625	0.8841	0.8507	0.8201

Table S4 Comparison of machine learning models for genomic prediction using dimensionality reduction (PCA = 100)

Traits		OLS Regression			Nonlinear		Bagging		Boosting				
Category	Abbr.	Linear (Logistic)	Ridge	ElasticNet	KNN	SVM	Random Forest	Decision Tree	GBDT	XgBoost	AdaBoost	LightGBM	CatBoost
I	SSK	0.9412	-	-	0.9374	0.9412	0.9374	0.9013	0.9317	0.9374	0.9355	0.9431	0.9393
	YKW	0.7994	-	-	0.7931	0.8025	0.7962	0.6708	0.7649	0.7868	0.8025	0.7900	0.7994
	GDD	0.8840	0.8856	0.8842	0.8669	0.7287	0.8885	0.8315	0.8839	0.8695	0.8521	0.8864	0.8920
	HC	0.5167	-	-	0.6312	0.6458	0.6438	0.4771	0.5896	0.6333	0.6438	0.6708	0.6808
II	TW	0.1508	0.1530	-	0.0490	0.0879	0.0760	0.0622	0.0648	0.0542	0.0737	0.2288	0.2389
	BF	0.3689	0.3718	0.3590	0.3044	0.4073	0.3131	0.3304	0.2977	0.2732	0.2207	0.4220	0.4346
	LMD	0.3326	0.3361	0.3332	0.2979	0.3533	0.2857	0.2913	0.2700	0.2180	0.2207	0.4334	0.4425
	SW	0.1256	0.1272	0.1257	0.0476	0.1045	0.1005	0.0864	0.0781	0.0536	0.0715	0.7548	0.7634
	BW	0.1235	0.1248	0.1236	0.0599	0.1000	0.0806	0.1031	0.0772	0.0685	0.0550	0.7274	0.7383
	DP	0.0763	0.0767	0.0000	0.0342	0.0352	0.0436	0.0677	0.0518	0.0342	0.0268	0.5253	0.5434
	AGG	0.1877	0.2048	0.1867	0.1699	0.1924	0.1728	0.1684	0.1583	0.1256	0.1379	0.3731	0.3850
III	ADFI	0.1764	0.1730	-	0.1421	0.1623	0.1182	0.1205	0.1384	0.1173	0.1140	0.2745	0.3094
	FPV	0.1838	0.1813	0.1838	0.0764	0.1430	0.1015	0.0648	0.0931	0.0751	0.0887	0.1455	0.1834
	AGE	0.3180	0.3241	0.3194	0.3391	0.3406	0.3462	0.3157	0.2916	0.2674	0.2028	0.4863	0.5149
	NVD	0.2340	0.2321	0.2097	0.1031	0.1869	0.1359	0.1218	0.1263	0.1078	0.1367	0.1763	0.2216
	FR	0.3363	0.3413	0.3379	0.2102	0.3278	0.2592	0.2425	0.2778	0.2296	0.2199	0.2428	0.2887
	LMA	0.3024	0.3034	0.3093	0.2737	0.3180	0.2805	0.2731	0.2376	0.1930	0.2003	0.3572	0.3557
	TPD	0.3828	0.3855	0.3846	0.2451	0.3503	0.2930	0.3002	0.2972	0.2213	0.2766	0.3717	0.3660
	TPV	0.3096	0.3127	0.3030	0.2066	0.3043	0.2076	0.2147	0.2291	0.1680	0.2157	0.2513	0.3146
	NGG	0.2033	0.2160	0.2085	0.1185	0.2059	0.1760	0.1923	0.1507	0.2398	0.1457	0.1823	0.2398

Table S5 Comparison of machine learning models for genomic prediction using dimensionality reduction (PHATE = 100)

| Traits | | OLS Regression | | | Nonlinear | | Bagging | | Boosting | | | | |
Category	Abbr.	Linear (Logistic)	Ridge	ElasticNet	KNN	SVM	Random Forest	Decision Tree	GBDT	XgBoost	AdaBoost	LightGBM	CatBoost
I	SSK	0.9355	-	-	0.9412	0.9412	0.9317	0.9032	0.9051	0.9317	0.9355	0.9298	0.9374
	YKW	0.7962	-	-	0.7618	0.8025	0.7868	0.7429	0.7649	0.8056	0.7994	0.7900	0.7931
	GDD	0.8562	0.8524	0.7327	0.8681	0.7787	0.8713	0.8232	0.8744	0.8541	0.8316	0.8864	0.8920
	HC	0.6042	-	-	0.5875	0.6167	0.6083	0.4688	0.5416	0.5729	0.6000	0.5688	0.6021
II	TW	0.1468	0.1556	-	0.0461	0.0892	0.0737	0.0641	0.0673	0.0562	0.0692	0.2152	0.2448
	BF	0.3167	0.2252	-	0.2760	0.2868	0.2884	0.2916	0.3120	0.2613	0.2264	0.4110	0.4151
	LMD	0.2922	0.2479	-	0.2991	0.2822	0.3142	0.2645	0.3091	0.2604	0.2705	0.4410	0.4324
	SW	0.1178	0.1267	0.1178	0.0569	0.1052	0.0793	0.0801	0.0747	0.0560	0.0731	0.6865	0.7109
	BW	0.1208	0.1130	0.1222	0.0539	0.1031	0.0930	0.0765	0.0885	0.0673	0.0517	0.6907	0.7031
	DP	0.0732	0.0701	-	0.0389	0.0317	0.0450	0.0533	0.0527	0.0189	0.0287	0.5160	0.5392
	AGG	0.1746	0.1959	-	0.1972	0.2030	0.1915	0.1462	0.1920	0.1769	0.1594	0.2353	0.3664
III	ADFI	0.1265	0.0810	-	0.1143	0.1298	0.1197	0.1125	0.1139	0.1009	0.1124	0.2484	0.3020
	FPV	0.0678	0.0955	-	0.0744	0.0480	0.0517	0.0612	0.0540	0.0648	0.0748	0.0976	0.1193
	AGE	0.3777	0.2939	-	0.3351	0.3131	0.3788	0.3489	0.3816	0.3498	0.3388	0.4942	0.5082
	NVD	0.0857	0.1054	-	0.0944	0.1522	0.0855	0.1001	0.1315	0.0514	0.1209	0.1408	0.1811
	FR	0.2164	0.2091	-	0.1626	0.2380	0.1764	0.1661	0.1663	0.1265	0.1975	0.1792	0.2387
	LMA	0.2355	0.2181	-	0.2533	0.2325	0.3032	0.2742	0.2737	0.2468	0.2156	0.3804	0.3417
	TPD	0.2195	0.2529	-	0.2079	0.2605	0.2123	0.2390	0.2429	0.1748	0.2097	0.2303	0.3323
	TPV	0.1661	0.2126	-	0.1651	0.2392	0.1610	0.1239	0.1901	0.1626	0.1640	0.1391	0.2529
	NGG	0.1622	0.1733	0.0000	0.1274	0.1587	0.1045	0.0952	0.1363	0.0939	0.1050	0.1100	0.1829

Table S6. Predictive performance of WheatGP and Cropformer models across different traits

Traits		WheatGP	Cropformer	LightGBM	Catboost
I	SSK	0.8956	0.9108	0.9374	0.9412
	YKW	0.6740	0.7649	0.7868	0.7962
	GDD	0.7920	0.8740	0.8858	0.9001
	HC	0.7503	0.8583	0.8604	0.8667
II	TW	0.1212	0.2689	0.1762	0.1821
	BF	0.1292	0.4208	0.4484	0.3934
	LMD	0.1368	0.4056	0.4559	0.3815
	SW	0.1203	0.3360	0.7688	0.7343
	BW	0.0713	0.3116	0.7533	0.7530
	DP	0.0987	0.2958	0.7294	0.7343
	AGG	0.0988	0.3293	0.3647	0.4022
III	ADFI	0.1013	0.1220	0.2874	0.3106
	FPV	0.1524	0.3388	0.1299	0.1637
	AGE	0.1076	0.3855	0.4538	0.3863
	NVD	0.1143	0.3730	0.2215	0.2630
	FR	0.1462	0.3961	0.2747	0.3372
	LMA	0.1319	0.3581	0.3873	0.3679
	TPD	0.1250	0.5039	0.3731	0.4326
	TPV	0.1060	0.4397	0.2612	0.3299
	NGG	0.0677	0.2191	0.2147	0.2266

Table S7. Prediction accuracy between 5-fold and 10-fold cross-validation

Traits	BayesR (5-fold)/(10fold)	Lightgbm (5-fold)/(10-fold)	Catboost (5-fold)/(10-fold)
HC	0.8125/0.8307	0.8604/0.8583	0.8667/0.8445
SSK	0.7945/ 0.7980	0.9374 / 0.9393	0.9412/0.9374
AGE	0.3620/0.3646	0.4538/0.4612	0.3863/0.3940
TW	0.2584/0.2613	0.1762/0.1820	0.1821/0.1895
AGG	0.3802/0.3821	0.3647/0.3704	0.4022/0.4113

Table S8. Comparison of prediction accuracy in different number of iterations

Traits		50,000 Iterations	300,000 Iterations
I	SSK	0.2863	0.7945
	YKW	0.3031	0.7620
	GDD	0.8672	0.8862
	HC	0.7502	0.8125
II	TW	0.2306	0.2584
	BF	0.4265	0.4410
	LMD	0.3901	0.4103
	SW	0.3504	0.3760
	BW	0.3427	0.3751
	DP	0.3023	0.2968
	AGG	0.3713	0.3802
III	ADFI	0.3023	0.3154
	FPV	0.3228	0.3304
	AGE	0.3296	0.3620
	NVD	0.3403	0.3521
	FR	0.4675	0.4671
	LMA	0.3998	0.4003
	TPD	0.4712	0.4756
	TPV	0.4377	0.4460
	NGG	0.3352	0.3408