

Machine learning using intrinsic genomic signatures for rapid classification of novel pathogens: COVID-19 case study

Supplementary Material

Gurjit S. Randhawa, Maximillian P.M. Soltysiak, Hadi El Roz,
Camila P.E. de Souza, Kathleen A. Hill, and Lila Kari

1) Software availability

MLDSP-GUI is an open-source alignment-free tool with Graphical User Interface is publicly available for download at the following link (No license is required to download and use the tool):

<https://sourceforge.net/projects/mldsp-gui/>

MLDSP is an open-source alignment-free tool (MATLAB license required to run this program) available at the following link:

<https://github.com/grandhawa/MLDSP>

2) Spearman's rank correlation coefficient test results

The ρ values from the Spearman's correlation coefficient test for k=1 to k=7 are given in Supplementary Table S1. The P-value is <1e-5 for k=2 to k=6, 0.0833 for k=1 with an exception of 0.3333 in case of *Deltacorovavirus*.

2019-nCoV vs.	k=1	k=2	k=3	k=4	k=5	k=6	k=7
<i>Alphacoronavirus</i>	1	0.97	0.96	0.96	0.94	0.88	0.7
<i>Betacoronavirus</i>	1	0.95	0.95	0.95	0.94	0.89	0.74
<i>Gammacoronavirus</i>	1	0.93	0.91	0.92	0.90	0.83	0.63
<i>Deltacoronavirus</i>	0.8	0.98	0.94	0.92	0.90	0.81	0.60
<i>Embecovirus</i>	1	0.85	0.88	0.88	0.86	0.79	0.59
<i>Merbecovirus</i>	1	0.96	0.95	0.94	0.92	0.84	0.64
<i>Nobecovirus</i>	1	0.89	0.83	0.83	0.8	0.73	0.54
<i>Sarbecovirus</i>	1	0.98	0.97	0.97	0.95	0.88	0.72

Supplementary Table S1: Spearman's rank correlation coefficient (ρ) value for k=1 to k=7.

3) Dataset availability

All sequences downloaded from NCBI and Virus-Host-DB are uploaded to the SourceForge as fasta files. Accession numbers of 29 sequences downloaded from GISAID (28 COVID19 and a bat betacoronavirus RaTG13) are provided in 'GISAIDsequences.txt'.

<https://sourceforge.net/projects/mldsp-gui/files/COVID19Dataset/>

The sequences are downloaded from three databases: Virus-Host-DB, NCBI, and GISAID.

Virus-Host-DB:

All the viral sequences (apart from the ones downloaded from NCBI and GISAID) used in this study are obtained from the Virus-Host-DB available at:

<https://www.genome.jp/virushostdb/>

NCBI

Wuhan-Hu-1 complete genome (Accession: NC_045512.2), bat-SL-CoVZC45 (Accession: MG772933.1), and bat-SL-CoVZXC21 (Accession: MG772934.1) are obtained from the Virus-Host-DB available at:

<https://www.ncbi.nlm.nih.gov/>

GISAID

28 2019-nCoV sequences and Beta-CoV-RaTG13 sequence (from Bat) are downloaded from the GISAID. We gratefully acknowledge the Authors, the Originating and Submitting Laboratories for their sequence and metadata shared through GISAID, which is used in this research. All submitters of 28 2019-nCoV sequences and 1 BetaCoV/Bat/RaTG13 sequence may be contacted directly via www.gisaid.org

Accession ID	Originating lab	Submitting lab	Authors
EPI_ISL_404227	Zhejiang Provincial Center for Disease Control and Prevention	Department of Microbiology, Zhejiang Provincial Center for Disease Control and Prevention	Yin Chen, Yanjun Zhang, Haiyan Mao, Junhang Pan, Xiuyu Lou, Yiyu Lu, Juying Yan, Hanping Zhu, Jian Gao, Yan Feng, Yi Sun, Hao Yan, Zhen Li, Yisheng Sun, Liming Gong, Qiong Ge, Wen Shi, Xinying Wang, Wenwu Yao, Zhangnv Yang, Fang Xu, Chen Chen, Enfu Chen, Zhen Wang, Zhiping Chen, Jianmin Jiang, Chonggao Hu
EPI_ISL_404228	Zhejiang Provincial Center for Disease Control and Prevention	Department of Microbiology, Zhejiang Provincial Center for Disease Control and Prevention	Yanjun Zhang, Yin Chen, Haiyan Mao, Junhang Pan, Xiuyu Lou, Yiyu Lu, Juying Yan, Hanping Zhu, Jian Gao, Yan Feng, Yi Sun, Hao Yan, Zhen Li, Yisheng Sun, Liming Gong, Qiong Ge, Wen Shi, Xinying Wang, Wenwu Yao, Zhangnv Yang, Fang Xu, Chen Chen, Enfu Chen, Zhen Wang, Zhiping Chen, Jianmin Jiang, Chonggao Hu
EPI_ISL_402132	Wuhan Jinyintan Hospital	Hubei Provincial Center for Disease Control and Prevention	Bin Fang, Xiang Li, Xiao Yu, Linlin Liu, Bo Yang, Faxian Zhan, Guojun Ye, Xixiang Huo, Junqiang Xu, Bo Yu, Kun Cai, Jing Li, Yongzhong Jiang.
EPI_ISL_402127 EPI_ISL_402128 EPI_ISL_402129 EPI_ISL_402130 EPI_ISL_402124	Wuhan Jinyintan Hospital	Wuhan Institute of Virology, Chinese Academy of Sciences	Peng Zhou, Xing-Lou Yang, Ding-Yu Zhang, Lei Zhang, Yan Zhu, Hao-Rui Si, Zhengli Shi
EPI_ISL_403963 EPI_ISL_403962	Bamrasnaradura Hospital	1. Department of Medical Sciences, Ministry of Public Health, Thailand 2. Thai Red Cross	Pilailuk, Okada; Siripaporn, Phuygun; Thanutsapa, Thanadachakul; Supaporn, Wacharapluesadee; Sittiporn, Parnmen; Warawan, Wongboot; Sunthareeyea,

		Emerging Infectious Diseases - Health Science Centre 3. Department of Disease Control, Ministry of Public Health, Thailand	Waicharoen; Rome, Buathong; Malinee, Chittaganpitch; Nanthawan, Mekha
EPI_ISL_402120 EPI_ISL_402119 EPI_ISL_402121	National Institute for Viral Disease Control and Prevention, China CDC	National Institute for Viral Disease Control and Prevention, China CDC	Wenjie Tan, Xiang Zhao, Wenling Wang, Xuejun Ma, Yongzhong Jiang, Roujian Lu, Ji Wang, Weimin Zhou, Peihua Niu, Peipei Liu, Faxian Zhan, Weifeng Shi, Baoying Huang, Jun Liu, Li Zhao, Yao Meng, Xiaozhou He, Fei Ye, Na Zhu, Yang Li, Jing Chen, Wenbo Xu, George F. Gao, Guizhen Wu
EPI_ISL_402123	Institute of Pathogen Biology, Chinese Academy of Medical Sciences & Peking Union Medical College	Institute of Pathogen Biology, Chinese Academy of Medical Sciences & Peking Union Medical College	Lili Ren, Jianwei Wang, Qi Jin, Zichun Xiang, Zhiqiang Wu, Chao Wu, Yiwei Liu
EPI_ISL_402125	unknown	National Institute for Communicable Disease Control and Prevention (ICDC) Chinese Center for Disease Control and Prevention (China CDC)	Zhang,Y.-Z., Wu,F., Chen,Y.-M., Pei,Y.-Y., Xu,L., Wang,W., Zhao,S., Yu,B., Hu,Y., Tao,Z.-W., Song,Z.-G., Tian,J.-H., Zhang,Y.-L., Liu,Y., Zheng,J.-J., Dai,F.-H., Wang,Q.-M., She,J.-L. and Zhu,T.-Y.
EPI_ISL_403931 EPI_ISL_403928 EPI_ISL_403930 EPI_ISL_403929	Institute of Pathogen Biology, Chinese Academy of Medical Sciences & Peking Union Medical College	Institute of Pathogen Biology, Chinese Academy of Medical Sciences & Peking Union Medical College	Lili Ren, Jianwei Wang, Qi Jin, Zichun Xiang, Zhiqiang Wu, Chao Wu, Yiwei Liu
EPI_ISL_403937 EPI_ISL_403936 EPI_ISL_403935 EPI_ISL_403934 EPI_ISL_403933 EPI_ISL_403932	Guangdong Provincial Center for Diseases Control and Prevention; Guangdong Provincial Public Health	Department of Microbiology, Guangdong Provincial Center for Diseases Control and Prevention	Min Kang, Jie Wu, Jing Lu, Tao Liu, Baisheng Li, Shuijiang Mei, Feng Ruan, Lifeng Lin, Changwen Ke, Haojie Zhong, Yingtao Zhang, Lirong Zou, Xuguang Chen, Qi Zhu, Jianpeng Xiao, Jianxiang Geng, Zhe Liu, Jianxiong Hu, Weilin Zeng, Xing Li, Yuhuang Liao, Xiujuan Tang, Songjian Xiao, Ying Wang, Yingchao Song, Xue Zhuang, Lijun Liang, Guanhao He, Huihong Deng, Tie Song, Jianfeng He, Wenjun Ma
EPI_ISL_404895	Providence Regional Medical Center	Division of Viral Diseases, Centers for Disease Control and Prevention	Queen,K., Tao,Y., Li,Y., Paden,C.R., Lu,X., Zhang,J., Gerber,S.I., Lindstrom,S.

EPI_ISL_404253	IL Department of Public Health Chicago Laboratory	Pathogen Discovery, Respiratory Viruses Branch, Division of Viral Diseases, Centers for Diseases Control and Prevention	Ying Tao, Krista Queen, Clinton R. Paden, Jing Zhang, Yan Li, Anna Uehara, Xiaoyan Lu, Brian Lynch, Senthil Kumar K. Sakthivel, Brett L. Whitaker, Shifaq Kamili, Lijuan Wang, Janna' R. Murray, Susan I. Gerber, Stephen Lindstrom, Suxiang Tong
EPI_ISL_405839	The University of Hong Kong - Shenzhen Hospital	Li Ka Shing Faculty of Medicine, The University of Hong Kong	Chan,J.F.-W., Yuan,S., Kok,K.H., To,K.K.-W., Chu,H., Yang,J., Xing,F., Liu,J., Yip,C.C.-Y., Poon,R.W.-S., Tsai,H.W., Lo,S.K.-F., Chan,K.H., Poon,V.K.-M., Chan,W.M., Ip,J.D., Cai,J.P., Cheng,V.C.-C., Chen,H., Hui,C.K.-M. and Yuen,K.Y.
EPI_ISL_402131 (Bat RaTG13)	Wuhan Institute of Virology, Chinese Academy of Sciences	Wuhan Institute of Virology, Chinese Academy of Sciences	Yan Zhu, Ping Yu, Bei Li, Ben Hu, Hao-Rui Si, Xing-Lou Yang, Peng Zhou, Zheng-Li Shi

Supplementary Table S2: Accession IDs of the Sequences downloaded from the GISAID.

The accession numbers and the sources for all the used sequences are given below:

Test-1; Source: Virus-Host-DB	
Adenoviridae	
AB448767,AC_000007,JN880453,JN880454,JN880455,JN880456,JN935766,JQ326209,JQ776547,KC 529648,KC693021,KF268207,AC_000008,KF279629,KF528688,KF802426,KF906413,KM591901,KM59 1902,KM591903,NC_000899,NC_000942,NC_001405,AC_000009,NC_001454,NC_001460,NC_00172 0,NC_001734,NC_001813,NC_001876,NC_001958,NC_002501,NC_002513,NC_002685,AC_000010, NC_002702,NC_003266,NC_004037,NC_006144,NC_006879,NC_009989,NC_010956,NC_011202,NC _011203,NC_012584,AC_000011,NC_012959,NC_014564,NC_014899,NC_014969,NC_015225,NC_0 15323,NC_015455,NC_015932,NC_016437,NC_016895,AC_000012,NC_017825,NC_017979,NC_020 074,NC_020485,NC_020487,NC_021168,NC_021221,NC_022266,NC_022612,NC_022613,AC_00001 3,NC_024150,NC_024474,NC_024486,NC_024684,NC_025678,NC_025962,NC_027705,NC_027708, NC_028103,NC_028105,AC_000014,NC_028107,NC_028113,NC_029898,NC_029899,NC_029902,NC _030116,NC_030792,NC_030860,NC_030874,NC_031503,AC_000016,NC_031948,NC_032105,NC_0 34382,NC_034626,NC_034834,NC_035072,NC_035207,NC_035619,NC_038332,NC_038333,AC_000 017,NC_038334,NC_039032,NC_040811,NC_043094,NC_043405,NC_043696,U46933,X73487,Y0959 8,AB724351,AC_000018,AC_000019,AC_000020,AC_000189,AC_000190,AC_000191,AF036092,AF0 83975,AF108105,AM749299,AB765926,AP012285,AP012302,AY458656,AY737797,AY737798,AY8032 94,AY849321,AY875648,DQ086466,DQ315364,AC_000001,DQ393829,DQ792570,DQ900900,DQ9231 22,EF121005,EF564601,FJ025899,FJ025900,FJ025901,FJ025902,AC_000002,FJ025903,FJ025904,FJ 025905,FJ025906,FJ025907,FJ025908,FJ025909,FJ025910,FJ025911,FJ025912,AC_000003,FJ02591 3,FJ025914,FJ025915,FJ025916,FJ025917,FJ025918,FJ025919,FJ025920,FJ025921,FJ025922,AC_0 00004,FJ025923,FJ025924,FJ025925,FJ025926,FJ025927,FJ025928,FJ025929,FJ025930,FJ349096,F J404771,AC_000005,FJ597732,FJ643676,FJ824826,GQ384080,GU191019,HM770721,HQ241818,HQ 241820,HQ883276,JF964962,AC_000006,JN860676,JN860677,JN860678,JN860679,JN860680,JN880 448,JN880449,JN880450,JN880451,JN880452	
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Caudovirales

AB626963,AB746912,AB757801,AF527608,AP011956,AY526908,AY526909,CP000711,CP008753,DQ113772,DQ121662,DQ222851,DQ289556,DQ394806,DQ394807,DQ394808,DQ394809,DQ394810,DQ426905,DQ838728,EU056923,EU568876,EU622808,FQ482084,GQ303261,GQ478082,GQ478083,GQ478085,GQ478087,GU196281,HE614282,HE956707,HE983844,HG428758,HG793132,HG796219,HG796220,HG796221,HM152765,HQ110083,HQ634152,HQ641341,HQ641343,HQ641344,HQ641346,JF314845,JF767210,JF773396,JN175269,JN254801,JN255163,JN699002,JN811560,JQ067085,JQ267518,JQ691610,JQ740790,JQ740791,JQ740792,JQ740793,JQ740794,JQ740795,JQ740796,JQ740797,JQ740798,JQ740799,JQ740800,JQ740801,JQ740802,JQ740803,JQ740805,JQ740806,JQ740807,JQ740808,JQ740809,JQ740810,JQ740811,JQ740812,JQ740814,JQ780163,JQ957925,JQ965700,JQ965701,JQ965702,JQ965703,JX000007,JX174275,JX274646,JX274647,JX403939,JX409894,JX409895,JX421753,JX483873,JX483874,JX483875,JX483879,JX483880,JX564242,JX570703,JX570707,JX570708,JX570711,JX681814,KC182543,KC182544,KC182545,KC182548,KC182549,KC182550,KC330681,KC333879,KC348598,KC348599,KC348600,KC348601,KC348602,KC348603,KC348604,KC413987,KC413988,KC522412,KC542353,KC556893,KC556894,KC556895,KC556896,KC556898,KC787107,KC787108,KC821615,KC821627,KC911856,KC911857,KC969441,KF030445,KF302032,KF302033,KF302035,KF302036,KF302037,KF591601,KF669657,KF676640,KF751793,KF751794,KF751795,KF751796,KF751797,KF771236,KF800937,KJ018210,KJ021043,KJ417497,KJ502657,KJ545483,KJ572844,KJ578763,KJ578764,KJ578766,KJ578769,KJ578771,KJ578775,KJ578777,KJ617393,KJ725374,KM058087,KM091442,KM091443,KM091444,KM233455,KM591905,KM612260,KM612261,KM612262,KM612263,KM612265,KM923970,KP017310,KP209285,KP296794,KP791807,KP869108,KR131710,LK985321,LN610580,LN681534,M11813,NC_000871,NC_000872,NC_000896,NC_000929,NC_000935,NC_001271,NC_001317,NC_001416,NC_001604,NC_001609,NC_001629,NC_001697,NC_001706,NC_001825,NC_001835,NC_001895,NC_001900,NC_001901,NC_001902,NC_001909,NC_001978,NC_002072,NC_002166,NC_002167,NC_002185,NC_002214,NC_002321,NC_002371,NC_002486,NC_002515,NC_002519,NC_002628,NC_002649,NC_002661,NC_002666,NC_002667,NC_002668,NC_002669,NC_002670,NC_002671,NC_002703,NC_002730,NC_002747,NC_002796,NC_003050,NC_003085,NC_003157,NC_003216,NC_003278,NC_003288,NC_003291,NC_003298,NC_003313,NC_003315,NC_003356,NC_003390,NC_003444,NC_003524,NC_003907,NC_004066,NC_004112,NC_004165,NC_004166,NC_004167,NC_004302,NC_004303,NC_004305,NC_004313,NC_004333,NC_004348,NC_004456,NC_004466,NC_004584,NC_004585,NC_004586,NC_004587,NC_004588,NC_004589,NC_004615,NC_004616,NC_004617,NC_004664,NC_004665,NC_004678,NC_004679,NC_004740,NC_004745,NC_004746,NC_004775,NC_004777,NC_004814,NC_004821,NC_004827,NC_004831,NC_004902,NC_004996,NC_005045,NC_005056,NC_005069,NC_005178,NC_005263,NC_005294,NC_005340,NC_005342,NC_005344,NC_005345,NC_005354,NC_005355,NC_005356,NC_005357,NC_005822,NC_005833,NC_005841,NC_005879,NC_005882,NC_005884,NC_005886,NC_005887,NC_005891,NC_005893,NC_006356,NC_006548,NC_006557,NC_006882,NC_006936,NC_006940,NC_006949,NC_006953,NC_007019,NC_007046,NC_007047,NC_007048,NC_007049,NC_007050,NC_007051,NC_007052,NC_007053,NC_007054,NC_007055,NC_007056,NC_007057,NC_007058,NC_007059,NC_007060,NC_007061,NC_007062,NC_007063,NC_007064,NC_007065,NC_007145,NC_007149,NC_007291,NC_007456,NC_007458,NC_007497,NC_007501,NC_007603,NC_007637,NC_007709,NC_007710,NC_007734,NC_007804,NC_007805,NC_007806,NC_007807,NC_007808,NC_007814,NC_007924,NC_007967,NC_008152,NC_008193,NC_008201,NC_008202,NC_008265,NC_008363,NC_008364,NC_008367,NC_008370,NC_008371,NC_008376,NC_008583,NC_008617,NC_008689,NC_008694,NC_008695,NC_008717,NC_008721,NC_008722,NC_008723,NC_008798,NC_008799,NC_009014,NC_009016,NC_009018,NC_009232,NC_009234,NC_009235,NC_009236,NC_009237,NC_009382,NC_009514,NC_009526,NC_009531,NC_009540,NC_009541,NC_009542,NC_009543,NC_009551,NC_009552,NC_009554,NC_009603,NC_009604,

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Geminiviridae

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Test-2; Source: Virus-Host-DB

Betaflexiviridae

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Bromoviridae

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Coronaviridae

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Flaviviridae

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Peribunyaviridae

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Potyviridae	
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Test-3a; Source: Virus-Host-DB; NCBI; GISAID
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Betacoronavirus
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Gammacoronavirus
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Test-3b; Source: Virus-Host-DB; GISAID
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Betacoronavirus
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Deltacoronavirus
FJ376620,KJ481931,KJ567050,KJ601777,KJ601778,KJ601779,KJ601780,KJ769231,KM820765,KP981395,NC_011547,NC_011549,NC_011550,NC_016991,NC_016992,NC_016993,NC_016994,NC_016995,NC_016996,NC_039208
Test-4; Source: Virus-Host-DB; NCBI; GISAID
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Merbecovirus
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Nobecovirus
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Sarbecovirus
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Test-5; Source: Virus-Host-DB; NCBI; GISAID
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same as Test-4
2019-nCoV
EPI_ISL_402119,EPI_ISL_402130,EPI_ISL_402132,EPI_ISL_403928,EPI_ISL_403929,EPI_ISL_403930,EPI_ISL_403931,EPI_ISL_403932,EPI_ISL_403933,EPI_ISL_403934,EPI_ISL_403935,EPI_ISL_402120,EPI_ISL_403936,EPI_ISL_403937,EPI_ISL_403962,EPI_ISL_403963,EPI_ISL_404227,EPI_ISL_404228, MN908947.3 ,EPI_ISL_402121,EPI_ISL_402123,EPI_ISL_402124,EPI_ISL_402125,EPI_ISL_402127,EPI_ISL_402128,EPI_ISL_402129,EPI_ISL_404253,EPI_ISL_404895,EPI_ISL_405839
Test-6; Source: Virus-Host-DB; NCBI; GISAID
Sarbecovirus; 2019-nCoV
same as Test-5

Supplementary Table S3: Accession IDs of sequences used in Test-1 to Test-6.