

Supplementary Materials

Practical selection of representative sets of RNA-seq samples using a hierarchical approach

Laura H. Tung¹ and Carl Kingsford^{1*}

¹Computational Biology Department, School of Computer Science, Carnegie Mellon University, Pittsburgh, PA 15213, USA

*To whom correspondence should be addressed: carlk@cs.cmu.edu

Table S1 – Partial Hausdorff distance, classical Hausdorff distance, runtime, and memory usage of direct apricot, hierarchical selection, and random selection, using the most recent 1000, 2000, 5000, 8000, 10000 samples in the SRA as the full sets.

Set of samples	Method	Hausdorff d_H	Partial Hausdorff d_{HK}	Runtime (seconds)			Memory (GB)
				Real	User	Sys	
Recent 1000 (select 100, $l = 5$)	direct apricot	0.688321022	0.685257115	174.58	11070.16	111.42	17.131
	hierarchical (seeded)	0.578381536	0.569809642	118.91	3449.28	292.08	up to 8.061
	random selection	0.837951394	0.826812255	—	—	—	—
Recent 2000 (select 200, $l = 10$)	direct apricot	0.664517495	0.662815581	655.18	42882.64	286.79	29.223
	hierarchical (seeded)	0.650712434	0.637185175	240.77	6906.76	586.80	up to 10.077
	random selection	0.894947772	0.848467165	—	—	—	—
Recent 5000 (select 500, $l = 10$)	direct apricot	0.624796548	0.62353618	4334.92	306588.88	1323.23	67.515
	hierarchical (seeded)	0.696114667	0.675768259	717.42	35803.41	1164.84	up to 15.115
	random selection	0.973292492	0.896965855	—	—	—	—
Recent 8000 (select 800, $l = 10$)	direct apricot	0.610919893	0.610735987	10095.85	701276.54	1513.85	101.776
	hierarchical (seeded)	0.760030601	0.679049314	1545.26	84481.00	1588.09	up to 22.169
	random selection	0.991018754	0.904692245	—	—	—	—
Recent 10000 (select 1000, $l = 10$)	direct apricot	0.607682609	0.607369442	14768.33	1047257.38	2273.86	118.906
	hierarchical (seeded)	0.70951932	0.665272021	2103.18	123182.85	1749.27	up to 26.200
	random selection	0.994547626	0.986377775	—	—	—	—

In Tables S1, S2, and S3, for $N=1000, 2000, 5000$, d_{HK} is the 3rd largest distance; for $N=8000, 10000$, d_{HK} is the 4th largest distance.

Table S2 – Partial Hausdorff distance, classical Hausdorff distance, runtime, and memory usage of direct apricot, hierarchical selection, and random selection, using the early-time 1000, 2000, 5000, 8000, 10000 samples in the SRA as the full sets.

Set of samples	Method	Hausdorff d_H	Partial Hausdorff d_{HK}	Runtime (seconds)			Memory (GB)
				Real	User	Sys	
Early 1000	direct apricot	0.725003411	0.723976221	153.22	7701.56	125.76	11.084
(select 100, $l = 5$)	hierarchical (seeded)	0.745518016	0.725044029	100.12	2351.73	215.52	up to 5.038
	random selection	0.950139546	0.938242439	—	—	—	—
Early 2000	direct apricot	0.67307199	0.672427473	401.49	22979.13	218.19	17.131
(select 200, $l = 10$)	hierarchical (seeded)	0.760020571	0.706453874	187.64	4360.50	383.16	up to 6.046
	random selection	0.872261407	0.838447692	—	—	—	—
Early 5000	direct apricot	0.61634404	0.615099659	2298.45	133723.63	565.12	39.300
(select 500, $l = 10$)	hierarchical (seeded)	0.666160711	0.659981919	497.60	21561.05	1262.98	up to 9.069
	random selection	0.938632619	0.935902009	—	—	—	—
Early 8000	direct apricot	0.630098995	0.628989605	5719.26	382221.70	874.59	70.538
(select 800, $l = 10$)	hierarchical (seeded)	0.834517734	0.71208656	1145.94	60263.98	1509.99	up to 16.123
	random selection	0.9916713	0.908157434	—	—	—	—
Early 10000	direct apricot	0.639209628	0.6383828	12315.44	800933.84	1446.46	89.684
(select 1000, $l = 10$)	hierarchical (seeded)	0.837916798	0.713645489	1648.26	95117.21	1381.86	up to 19.146
	random selection	0.99772421	0.990244824	—	—	—	—

Table S3 – Partial Hausdorff distance, classical Hausdorff distance, runtime, and memory usage of direct apricot, hierarchical selection, and random selection, using the mid-time 1000, 2000, 5000, 8000, 10000 samples in the SRA as the full sets.

Set of samples	Method	Hausdorff d_H	Partial Hausdorff d_{HK}	Runtime (seconds)			Memory (GB)
				Real	User	Sys	
Mid 1000	direct apricot	0.666185918	0.664052819	150.21	9130.84	126.60	14.108
(select 100, $l = 5$)	hierarchical (seeded)	0.685598613	0.648069325	160.45	2705.68	252.78	up to 6.046
	random selection	0.968587397	0.753610206	—	—	—	—
Mid 2000	direct apricot	0.651423605	0.648054888	545.46	34587.00	248.80	25.192
(select 200, $l = 10$)	hierarchical (seeded)	0.732927883	0.676261249	243.70	5827.03	508.06	up to 9.069
	random selection	0.967519071	0.923284417	—	—	—	—
Mid 5000	direct apricot	0.646540816	0.646398158	3084.32	209037.81	892.53	55.422
(select 500, $l = 10$)	hierarchical (seeded)	0.719052575	0.676710291	626.75	28509.77	983.47	up to 12.092
	random selection	0.961274547	0.867699133	—	—	—	—
Mid 8000	direct apricot	0.636313583	0.635731787	7142.40	464515.34	865.10	81.622
(select 800, $l = 10$)	hierarchical (seeded)	0.943464491	0.686230795	1262.73	64248.73	1301.38	up to 18.138
	random selection	0.998728362	0.989508253	—	—	—	—
Mid 10000	direct apricot	0.654537313	0.653742747	12582.81	780770.97	1574.01	100.768
(select 1000, $l = 10$)	hierarchical (seeded)	0.807148615	0.734005	1818.98	98855.02	1548.71	up to 22.169
	random selection	0.999886845	0.997812734	—	—	—	—

Table S4 – Selecting different sizes of representative sets from the SRA entire set ($N=196523$ human RNA-seq samples): partial Hausdorff distance and classical Hausdorff distance of hierarchical selection and random selection.

Metric	Select 3000		Select 4000		Select 5000		Select 7000	
	hierarchical (seeded)	random selection						
Hausdorff d_H	0.945978504	0.998763361	0.945978504	0.998763361	0.945978504	0.998763361	0.875009817	0.998763361
Partial Hausdorff d_{HK}	0.844519904	0.997721045	0.844274154	0.997718649	0.844274154	0.997718649	0.753391502	0.997718289
Representative -set-size/ Full-set-size	0.0153		0.0204		0.0254		0.0356	

Table S5 – Performance comparison of hierarchical selection using seeded-chunking method vs. using sequential chunking method: partial Hausdorff distance and classical Hausdorff distance, using the most recent 1000, 2000, 5000, 8000, 10000 samples in the SRA as the full sets.

Set of samples	Method	Hausdorff d_H	Partial Hausdorff d_{HK}
Recent 1000	hierarchical (seeded)	0.578381536	0.569809642
(select 100, $l = 5$)	hierarchical (sequential)	0.612622717	0.578381536
Recent 2000	hierarchical (seeded)	0.650712434	0.637185175
(select 200, $l = 10$)	hierarchical (sequential)	0.656343899	0.643755957
Recent 5000	hierarchical (seeded)	0.696114667	0.675768259
(select 500, $l = 10$)	hierarchical (sequential)	0.72711968	0.708127649
Recent 8000	hierarchical (seeded)	0.760030601	0.679049314
(select 800, $l = 10$)	hierarchical (sequential)	0.770009257	0.754661415
Recent 10000	hierarchical (seeded)	0.70951932	0.665272021
(select 1000, $l = 10$)	hierarchical (sequential)	0.790246213	0.752879052

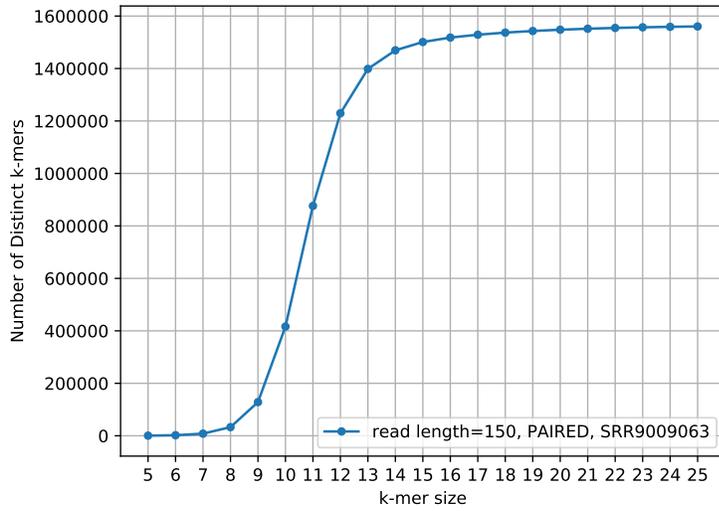


Figure S1 – The number of distinct k -mers vs. k -mer size: read-length=150, paired-end reads, from SRR9009063 (10000 random reads).

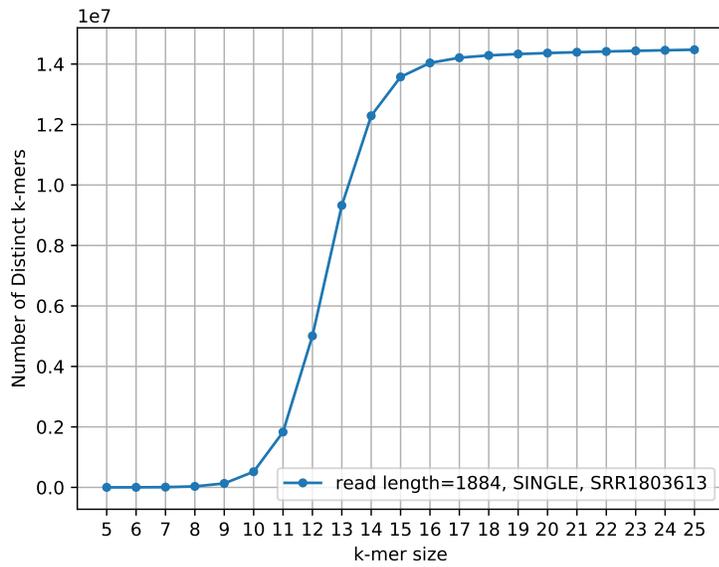


Figure S2 – The number of distinct k -mers vs. k -mer size: read-length=1884, single-end reads, from SRR1803613 (10000 random reads).

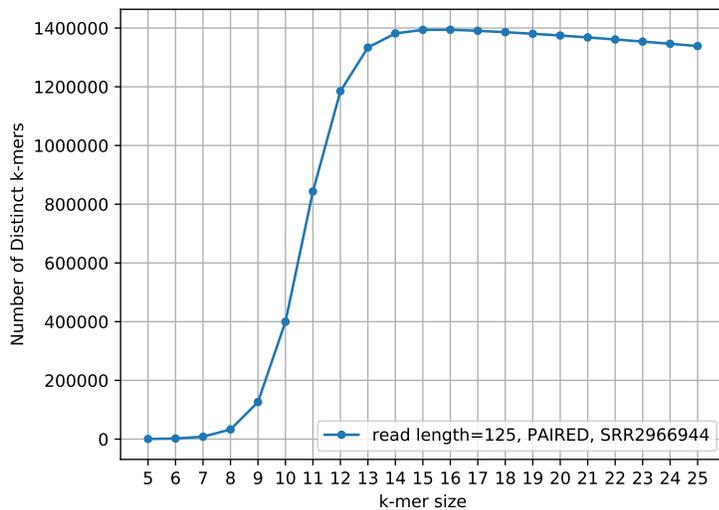


Figure S3 – The number of distinct k -mers vs. k -mer size: read-length=125, paired-end reads, from SRR2966944 (10000 random reads).

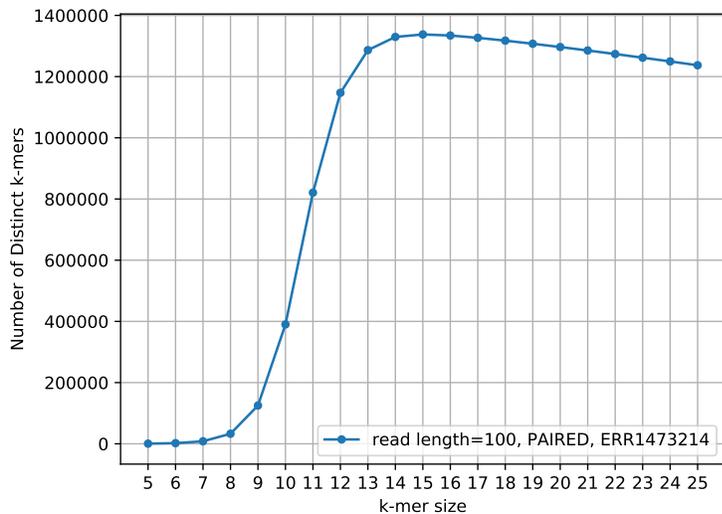


Figure S4 – The number of distinct k-mers vs. k-mer size: read-length=100, paired-end reads, from ERR1473214 (10000 random reads).

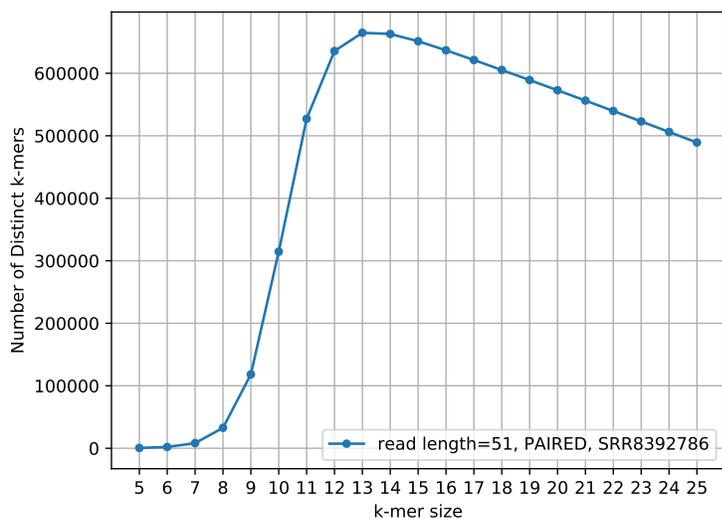


Figure S5 – The number of distinct k-mers vs. k-mer size: read-length=51, paired-end reads, from SRR8392786 (10000 random reads).

In Figs. S3, S4, and S5, the horizontal part of the curve bends down as k-mer size further increases, especially for shorter read-lengths, since when read-lengths are short, using larger k-mers would reduce the number of distinct k-mers.