

Comparison of hotspots identified by GCB with a curated dataset.

Genome complexity estimating method was assessed as the way for genomic islands (GI) detection. We assumed that regions with high complexity values (hotspots) may represent genomic islands. To detect hotspot regions we used common outlier detection method proposed by Tukey:

$$complexity_i \geq Q3 + 1.5 * (Q3 - Q1),$$

where $Q1$ and $Q3$ are 0.25 and 0.75 percentiles of complexity profile. Hotspots regions were regarded as GIs.

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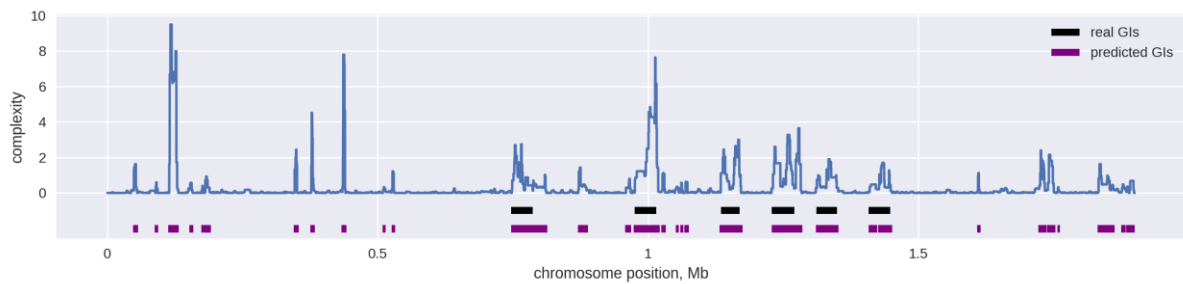


Fig 1. Example of complexity based approach for prediction genomic islands in *Streptococcus pyogenes* MGAS315, NC_004070.1 chromosome.

To get a confusion matrix trueness of the prediction was checked for each nucleotide separately. MCC, F1 score and precision metrics were used to estimate quality of GI prediction:

$$MCC = \frac{TP * TN - FP * FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

$$F1\ score = \frac{2TP}{2TP + FP + FN}$$

$$precision = \frac{TP}{TP + FP}$$

From the genomes available in curated literature-based dataset [Bertelli et al., 2019] only 4 chromosomes were also present in our precalculated set.

Results:

| chromosome | MCC score | F1 score | precision |
|-------------|--------------------|--------------------|--------------------|
| NC_004431.1 | 0.6398974787389852 | 0.6942167816826945 | 0.6039911283491597 |
| NC_004070.1 | 0.655472809862469 | 0.6844523104895646 | 0.5494813503524955 |
| NC_003923.1 | 0.5952671253837918 | 0.5892016756020617 | 0.4286045699930403 |

| | | | |
|-------------|--------------------|-------------------|--------------------|
| NC_002695.1 | 0.5469882821186525 | 0.622686519552352 | 0.5896994002603333 |
| mean | 0.609406424025975 | 0.647639321831668 | 0.542944112238757 |

By MCC and F1-score this approach is comparable to existing tools such as IslandPath-DIMOB, GIIHunter and IslandViewer 4. But there is a huge number of false positive detected GIs, so, the precision score is very low compared to other methods.

References dataset obtained by using the comparative genomics approach of IslandPick [Bertelli et al., 2019], also was used to validate complexity based approach.

| chromosome | MCC score | F1 score | precision |
|-------------|----------------------|---------------------|----------------------|
| NC_009708.1 | 0.38487104690031365 | 0.3734107527432849 | 0.2451605459656494 |
| NC_007005.1 | 0.2054826380489073 | 0.25008881198628097 | 0.17050550994785096 |
| NC_010501.1 | 0.1656805277399133 | 0.2497633887301143 | 0.22984014707278763 |
| NC_008253.1 | 0.31920178349975015 | 0.3263252331260368 | 0.21389808518495657 |
| NC_009076.1 | 0.238251125314444 | 0.2786501010119271 | 0.18458251701690434 |
| NC_009487.1 | 0.0903831957409384 | 0.05332905771389135 | 0.02803553366462905 |
| NC_004578.1 | 0.25403435531999186 | 0.34446613497841755 | 0.286251319388785 |
| NC_008463.1 | 0.30182788811643274 | 0.2992938488723532 | 0.19363758817684576 |
| NC_003485.1 | 0.2579527628894837 | 0.1740849990936506 | 0.09638635877810856 |
| NC_009512.1 | 0.27820951615033646 | 0.3445637427241827 | 0.3388378919734103 |
| NC_004606.1 | 0.15200885258105978 | 0.10312124791584637 | 0.05589103172094004 |
| NC_010167.1 | 0.000466314090059021 | 0.12570593895109675 | 0.33321936163527827 |
| NC_007530.2 | 0.06398331158846338 | 0.04689342484723675 | 0.024840549813711664 |
| NC_010410.1 | 0.3766808133470356 | 0.2920455742723105 | 0.17116491420042124 |
| NC_005139.1 | 0.19703389818572514 | 0.150013006485706 | 0.08424900608332814 |
| NC_008061.1 | 0.19022392344977773 | 0.3225759083357807 | 0.33217554977792224 |
| NC_010084.1 | 0.253070606088803 | 0.26344416769198453 | 0.16848999568158918 |
| NC_003997.3 | 0.08390639743001588 | 0.05575501749959223 | 0.029555952338787134 |
| NC_009080.1 | 0.12260548261530846 | 0.14317482232583406 | 0.0870655839240245 |
| NC_010515.1 | 0.04983208533937494 | 0.2227876295579963 | 0.24346152492483925 |

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|-------------|----------------------|----------------------|----------------------|
| NC_000907.1 | 0.09296002068782915 | 0.034584556473813956 | 0.017713963421374095 |
| NC_008563.1 | 0.3935844374822941 | 0.38242186952979623 | 0.2515840311452063 |
| NC_009800.1 | 0.19061720695979295 | 0.09702586444736065 | 0.051312273685759746 |
| NC_010498.1 | 0.327133637346465 | 0.2597803467991166 | 0.15236272552588775 |
| NC_004088.1 | 0.05911317631934262 | 0.052376147229830375 | 0.02926301686490688 |
| NC_004116.1 | 0.2495949994749722 | 0.17778414841262602 | 0.09951760827068401 |
| NC_008060.1 | 0.3415246066690782 | 0.44232779482012574 | 0.37481743033385473 |
| NC_002944.2 | 0.07018640090967038 | 0.07504233105244104 | 0.042077179321005555 |
| NC_010582.1 | 0.13071463422847124 | 0.12897879089527856 | 0.07521532748386954 |
| NC_004368.1 | 0.28484822356765815 | 0.31553935338230515 | 0.21422814331310497 |
| NC_007146.2 | 0.36024382180513154 | 0.3149167421444994 | 0.193772219653427 |
| NC_010380.1 | 0.2336884661910294 | 0.23388640964119076 | 0.14489939693845189 |
| NC_007434.1 | 0.3833920912799913 | 0.45966224818025575 | 0.35400710325841206 |
| NC_004431.1 | 0.47005108656504924 | 0.5091760136438895 | 0.37988349456852866 |
| NC_010465.1 | 0.37337575395475303 | 0.36600955692191756 | 0.23925061631367175 |
| NC_006350.1 | 0.3458290477930752 | 0.39563460781220766 | 0.28059620614261555 |
| NC_010473.1 | 0.06707619633431747 | 0.044255182787441144 | 0.023417902855171528 |
| NC_002695.1 | 0.3903822256193024 | 0.46597765476482533 | 0.38414359689708727 |
| NC_004070.1 | 0.2367698334411089 | 0.131330169255604 | 0.07032568299222543 |
| NC_010102.1 | 0.2814133285495277 | 0.22346937518731244 | 0.12993039443155452 |
| NC_008543.1 | 0.2128452820810379 | 0.2672648562640155 | 0.1898330414767529 |
| NC_010184.1 | 0.1008380525664982 | 0.05916659388971843 | 0.03125161731648099 |
| NC_008600.1 | 0.03806952653775363 | 0.022079794650779565 | 0.01136477165453867 |
| NC_006155.1 | 0.3077655936920609 | 0.29831291471034593 | 0.18815448858629918 |
| NC_008595.1 | 0.2322583123376348 | 0.29932392244640826 | 0.21834619883281148 |
| NC_003909.8 | 0.18936903106619443 | 0.13706508158499245 | 0.076058265611407 |
| NC_010159.1 | -0.03414126616396267 | 0.003108575879328839 | 0.001715206630597444 |
| NC_008022.1 | 0.19154922127994686 | 0.17830576368746082 | 0.10471699362854835 |
| NC_002516.2 | 0.08692207405991095 | 0.08808184125921077 | 0.04971620468391139 |
| NC_007946.1 | 0.46096590075508376 | 0.5136607961327568 | 0.40380701925813894 |

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| NC_003923.1 | 0.18794417019300338 | 0.09020057602747758 | 0.04742209004136109 |
| NC_010322.1 | 0.2321622659018411 | 0.3050790907253817 | 0.3218192076660855 |
| NC_008024.1 | 0.31654162612791337 | 0.21890083701594967 | 0.12290210537699855 |
| NC_007432.1 | 0.33099343383472785 | 0.2967752098476495 | 0.18335437371046587 |
| NC_009801.1 | 0.4078800664945426 | 0.3496928952424733 | 0.2142028994220997 |
| NC_004722.1 | 0.16287408707503673 | 0.08902883035739562 | 0.04719050652395732 |
| NC_005945.1 | 0.07993009039643954 | 0.055643426639708664 | 0.029571384905213122 |
| mean | 0.22408724890966067 | 0.2245853154141476 | 0.16257883607040766 |

Literature

Bertelli, C., Tilley, K. E., & Brinkman, F. S. (2019). Microbial genomic island discovery, visualization and analysis. *Briefings in bioinformatics*, 20(5), 1685-1698.