论文

以多肽组分特异性和 GC 含量分类细菌的有效性分析

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摘要 本文研究了细菌的蛋白质多肽组分统计特征与基因组 GC(Guanine+Cytosine)含量的相关性, 发现当多肽长度较小时多肽组分特异性和 GC 含量存在着很强的关联; 随着多肽长度增加, 上述关联发生突变, 关联迅速丧失. 这一结果表明, 基于组分特异性确定细菌亲缘关系的方法的确给出了不同于 GC 含量的信息, 从而能实现有效分类.

关键词 种系基因组学, 非序列比对, 多肽组分矢量, GC 含量

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1 引言

传统生物亲缘关系的确定主要基于表型特征(如生存环境、外部形态、解剖生理和代谢途径等), 这对微生物来说就显得无能为力^[1]. 分子生物学的发展, 特别是测序技术的不断完善, 使基于核苷酸或氨基酸序列确定生物亲缘关系成为可能. 其中, 最具代表性和影响力的是沃斯(Carl Richard Woese)及其合作者利用核糖体小亚基序列(SSU rRNA)发现了古细菌是介于真核生物和细菌的独立“域”这一事实^[2-4]. 然而, 这种单基因序列比对的方法因其判定结果的不稳定性而备受质疑^[5]. 随着不同物种全基因组测序的相继完成, 利用全基因组的序列特征(如共享基因数

目^[6]或其在染色体上的排序^[7]、基因含量^[8,9]及保守基因对^[10]等)来确定生物亲缘关系的方法不断发展, 逐渐形成了所谓的种系基因组学^[11]. 但是这些方法本质上仍然需要序列比对, 与单基因序列比对方法一样易受基因组大小^[12]、横向基因迁移(Horizontal Gene Transfer)^[13]、平行基因缺失(Parallel Gene Loss)^[14,15]及基因进化速度^[16]等因素的影响, 导致判定指标特异性差、分辨率低而不能正确区分已测序物种的亲缘关系^[17,18]. 另一方面, GC 含量特征是目前确定微生物亲缘关系的重要判据之一. 简单来说, GC 含量越接近的生物, 其亲缘关系也越近. GC 含量与基因识别标志有一定的关联, 有关基因识别标志(Genomic Signature)的研究发现, 四核苷酸(Tetranu-

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$$e_i(\alpha_1\alpha_2\ldots\alpha_n) = \frac{p_i(\alpha_1\alpha_2\ldots\alpha_n)}{b_i(\alpha_1\alpha_2\ldots\alpha_n)} - 1, \quad (2)$$

其中

$$b_i(\alpha_1\alpha_2\ldots\alpha_n) = \frac{p_i(\alpha_2\alpha_3\ldots\alpha_n) \cdot p_i(\alpha_1\alpha_2\ldots\alpha_{n-1})}{p_i(\alpha_2\alpha_3\ldots\alpha_{n-1})}, \quad (3)$$

当 $b_i(\alpha_1\alpha_2\ldots\alpha_n)=0$ 时, 我们同样令 $e_i(\alpha_1\alpha_2\ldots\alpha_n)=0$. 这里 $p_i(\alpha_2\alpha_3\ldots\alpha_{n-1})$ 是长度为 $n-2$ 多肽 $\alpha_2\alpha_3\ldots\alpha_{n-1}$ 的观察概率, 而 $p_i(\alpha_2\alpha_3\ldots\alpha_n)$ 和 $p_i(\alpha_1\alpha_2\ldots\alpha_{n-1})$ 是长度为 $n-1$ 的多肽 $\alpha_2\alpha_3\ldots\alpha_n$ 和 $\alpha_1\alpha_2\ldots\alpha_{n-1}$ 的观察概率. 对每种细菌 i , 把 20^n 个 $e_i(\alpha_1\alpha_2\ldots\alpha_n)$ 按照相同的多肽组合顺序排成一行得到进化信息矢量 E_i , 由此计算出细菌间亲缘关系距离

$$d_{ij} = \frac{(E_i)^T \cdot E_j}{\|E_i\| \cdot \|E_j\|}, \quad (4)$$

d_{ij} 越接近 1 说明细菌 i 和 j 的亲缘关系越近.

由文献[21]知, 上述扣除随机背景方法得到的多肽组分特异性对确定细菌亲缘关系效果最好, 并且 n 越大, E_i 的特异性越强, d_{ij} 分辨率也越高, 当 $n=5$ 或 6 时就可以完全重建如图 1 所示的亲缘关系. 需要说明的是, 我们还计算了 $n=2$ 时的 d_{ij} , 此时由最强马尔科

夫过程来估计随机变异信息, 即 $b_i(\alpha_1\alpha_2)=p_i(\alpha_1) \cdot p_i(\alpha_2)$.

下面, 我们给出不同 n 值下多肽组分特异性(即进化信息矢量 E_i)与基因组 GC 含量关联性计算的结果(图 2).

首先, 统计氨基酸序列所对应的核苷酸序列的 GC 含量 a_i , 并用

$$r_{ij} = \min \left\{ \frac{a_i}{a_j}, \frac{a_j}{a_i} \right\}, \quad (5)$$

即取 $\frac{a_i}{a_j}$ 和 $\frac{a_j}{a_i}$ 中较小的一个来度量细菌 i 和细菌 j 的

亲缘关系. 由 GC 含量判据可知, r_{ij} 越接近 1 表明两种细菌的亲缘关系越近. 即 r_{ij} 和 d_{ij} 具有相同含义, 都给出了细菌亲缘关系的相对距离. 这样, 我们就可以定义

$$c_i = \frac{\sum_{j=1}^m d_{ij} r_{ij}}{\sqrt{\sum_{j=1}^m d_{ij}^2} \cdot \sqrt{\sum_{j=1}^m r_{ij}^2}}, \quad (6)$$

来度量多肽组份特异性与 GC 含量的相关性. 显然, c_i 越接近 1, 说明矢量 $d_i=(d_{i1}, d_{i2}, \ldots, d_{im})$ 和矢量 $r_i=(r_{i1}, r_{i2}, \ldots, r_{im})$ 的方向越趋于一致, 表明由这两种距离预

图 2 (网络版彩图) n 取不同值时 99 种细菌的 c_i

Figure 2 (Color online) The c_i of selected bacteria with different n .

测的细菌亲缘关系越趋于等价, 表明同种细菌的多肽组分特异性与其基因组 GC 含量的关联性越强.

3 结果与讨论

图 2 给出了上述 99 种细菌在 n 取不同数值时的 c_i . 可以发现, 当 $n=2, 3, 4$ 时绝大多数的 c_i 都明显大于 0.5, 特别是当 $n=2$ 或 3 时几乎所有的 c_i 都大于 0.8. 当 $n=5$ 或 6 时所有的 c_i 都急剧减小到 0.3 以下.

图 3 n 取不同值时的 $\langle c_i \rangle$, 其中误差棒表示 c_i 的均方差
Figure 3 $\langle c_i \rangle$ for different n and error bar for standard deviation of c_i .

为了研究上述结果的普遍性, 同时为了能更清楚地显示 c_i 随 n 的变化规律, 我们计算了不同 n 值下所有 1564 种细菌的 c_i 平均值 $\langle c_i \rangle$, 结果如图 3 所示. 可以看到, 在 $n=4$ 和 5 时 $\langle c_i \rangle$ 发生了一次突变.

以上结果表明: (1) 当多肽长度小于 4 时多肽组分特异性与 GC 含量之间具有很强的正关联. 意味着在这种情况下多肽组分统计所得到的信息等价于基因组 GC 含量的特异性信息. 由于郝柏林等人以前的研究表明在这一长度上 GC 含量和小 n 值下多肽组分特异性都能对“属”以上级别的亲缘关系做出准确且一致的判定, 表明 GC 含量和小 n 值多肽组分只能区分这个层次上的特异性. 由于和 GC 含量的等价性, 短多肽组分统计不能正确判定更精细层次上的细菌亲缘关系. 这一结果也暗示基因识别标志无法准确重构微生物亲缘关系, 因为它只等价于 GC 含量特异性. (2) 当多肽长度大于 4 时, 多肽组分特异性与 GC 含量之间的关联发生突变, 急剧降低到几乎无关联的程度. 在 $n=5$ 或 6 的情况下, 多肽组分特异性能准确给出细菌到种株的分类树的事实表明, 这种新方法的确超越了 GC 含量分析方法和基因识别标志方法, 挖掘出了物种特异性特征. 我们还直接计算了寡核苷酸的组分特异性与相应基因组 GC 含量的关联, 得到一致的结论.

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附录

表 a1 细菌的名字、缩写、索取号和 Berger's 代码

Table a1 Bacterium name, abbreviation, NCBI accession numbers and Berger's code

Species/strain	Abbrev	Accession No.	Bergey code
Aquifex aeolicus	Aquae	NC_000918	B1.1.1.1.1
Thermotoga lettingae TMO	Thele	NC_009828	B2.1.1.1.1
Thermotoga maritima	Thema	NC_000853	B2.1.1.1.1
Deinococcus proteolyticus MRP	Deipr	NC_015161	B4.1.1.1.1
Deinococcus radiodurans R1	Deira	NC_001263	B4.1.1.1.1
Chloroflexus aggregans DSM	Chlag	NC_011831	B6.1.1.1.1
Chloroflexus aurantiacus J	Chlau	NC_010175	B6.1.1.1.1
Leptospirillum ferriphilum ML	LepfM	NC_018649	B8.1.1.1.2
Leptospirillum ferrooxidans C2	LepfC	NC_017094	B8.1.1.1.2
Deferribacter desulfuricans SSM1	Defde	NC_013939	B9.1.1.1.1
Denitrovibrio acetiphilus DSM	Denac	NC_013943	B9.1.1.1.2
Thermosynechococcus elongatus BP	Theel	NC_004113	B10.1.1.1.13
synechocystis PCC6803	Synpc	NC_000911	B10.1.1.1.14
nostoc PCC7120	Anasp	NC_003272	B10.1.4.1.8
Chlorobium tepidum TLS	Chlte	NC_002932	B11.1.1.1.1
Rickettsia conorii	Riccn	NC_003103	B12.1.2.1.1
Rickettsia prowazekii	Ricpr	NC_000963	B12.1.2.1.1
Caulobacter crescentus CB15	Caucr	NC_002696	B12.1.5.1.1
Agrobacterium fabrum C58	Agrt5	NC_003062	B12.1.6.1.2
Sinorhizobium meliloti 1021	Rhime	NC_003047	B12.1.6.1.7
Brucella melitensis bv	Brume	NC_003317	B12.1.6.4.1

表 1(续)

Species/strain	Abbrev	Accession No.	Bergey code
<i>Brucella suis</i> 1330	Brusu	NC_004310	B12.1.6.4.1
<i>Mesorhizobium loti</i>	Rhilo	NC_002678	B12.1.6.5.6
<i>Ralstonia solanacearum</i> GMI1000	Ralso	NC_003295	B12.2.1.1.8
<i>Neisseria meningitidis</i> MC58	NeimeM	NC_003112	B12.2.4.1.1
<i>Xanthomonas axonopodis citri</i> 306	Xanax	NC_003919	B12.3.3.1.1
<i>Xanthomonas campestris</i> ATCC 33913	Xanca	NC_003902	B12.3.3.1.1
<i>Xylella fastidiosa</i> 9a5c	Xylfa	NC_002488	B12.3.3.1.12
<i>Pseudomonas aeruginosa</i> PA01	Pseae	NC_002516	B12.3.9.1.1
<i>Pseudomonas putida</i> KT2440	Psepu	NC_002947	B12.3.9.1.1
<i>Shewanella oneidensis</i> MR-1	Sheon	NC_004347	B12.3.10.1.14
<i>Vibrio cholerae</i> O1 biovar	Vibch	NC_002505	B12.3.11.1.1
<i>Vibrio vulnificus</i> CMCP6	Vibvu	NC_004459	B12.3.11.1.1
<i>Buchnera aphidicola</i> Sg	Bucap	NC_004061	B12.3.13.1.5
<i>Buchnera</i> sp. APS	Bucai	NC_002528	B12.3.13.1.5
<i>Escherichia coli</i> CFT073	EcoliC	NC_004431	B12.3.13.1.1
<i>Salmonella enterica</i> serovar Typhi CT18	Salti	NC_003198	B12.3.13.1.34
<i>Salmonella enterica</i> serovar Typhimurium	Salty	NC_003197	B12.3.13.1.34
<i>Shigella flexneri</i> 2a strain 301	Shifl	NC_004337	B12.3.13.1.37
<i>Wigglesworthia brevipalpis</i>	Wigbr	NC_004344	B12.3.13.1.41
<i>Yersinia pestis</i> strain C092	YerpeC	NC_003143	B12.3.13.1.43
<i>Pasteurella multocida</i> PM70	Pasmu	NC_002663	B12.3.14.1.1
<i>Haemophilus influenzae</i> Rd	Haein	NC_000907	B12.3.14.1.4
<i>Campylobacter jejuni</i> NCTC 11168 ATCC	Camje	NC_002163	B12.5.1.1.1
<i>Helicobacter pylori</i> 26695	Helpy	NC_000915	B12.5.1.2.1
<i>Clostridium acetobutylicum</i> ATCC824	Cloab	NC_003030	B13.1.1.1.1
<i>Clostridium perfringens</i>	Clope	NC_003366	B13.1.1.1.1
<i>Thermoanaerobacter tengcongensis</i>	Thete	NC_003869	B13.1.2.1.11
<i>Mycoplasma genitalium</i> G37	Mycge	NC_000908	B13.2.1.1.1
<i>Mycoplasma penetrans</i>	Mycpe	NC_004432	B13.2.1.1.1
<i>Mycoplasma pneumoniae</i> M129	Mycpn	NC_000912	B13.2.1.1.1
<i>Mycoplasma pulmonis</i> UAB CTIP	Mycpu	NC_002771	B13.2.1.1.1
<i>Ureaplasma urealyticum</i>	Urepa	NC_002162	B13.2.1.1.4
<i>Oceanobacillus iheyensis</i>	Oceih	NC_004193	B13.3.1.1.12
<i>Bacillus halodurans</i>	Bachd	NC_002570	B13.3.1.1.1
<i>Bacillus subtilis</i> 168	Bacsu	NC_000964	B13.3.1.1.1
<i>Listeria innocua</i>	Lisin	NC_003212	B13.3.1.4.1
<i>Listeria monocytogenes</i> EGD-e	Lismo	NC_003210	B13.3.1.4.1
<i>Staphylococcus aureus</i> Mu50	Staaum	NC_002758	B13.3.1.8.1
<i>Staphylococcus epidermidis</i> ATCC	Staep	NC_004461	B13.3.1.8.1
<i>Streptococcus agalactiae</i> 2603 V/R	StragV	NC_004116	B13.3.2.6.1
<i>Streptococcus mutans</i> UA159	Strmu	NC_004350	B13.3.2.6.1
<i>Streptococcus pneumoniae</i> R6	StrpnR	NC_003098	B13.3.2.6.1
<i>Streptococcus pyogenes</i> MGAS8232	Strpy8	NC_003485	B13.3.2.6.1
<i>Lactococcus lactis</i> sp. IL1403	Lacla	NC_002662	B13.3.2.6.2
<i>Corynebacterium efficiens</i> YS-314	Coref	NC_004369	B14.(1.5).(1.10).1.1
<i>Corynebacterium glutamicum</i>	Corgl	NC_003450	B14.(1.5).(1.10).1.1
<i>Mycobacterium leprae</i> TN	Mytle	NC_002677	B14.(1.5).(1.10).4.1
<i>Mycobacterium tuberculosis</i> CDC1551	MyctuC	NC_002755	B14.(1.5).(1.10).4.1
<i>Streptomyces coelicolor</i> A3	Strco	NC_003888	B14.(1.5).(1.14).1.1
<i>Bifidobacterium longum</i> NCC2705	Biflo	NC_004307	B14.(1.5).2.1.1
<i>Chlamydia muridarum</i>	Chlmu	NC_002620	B16.1.1.1.1
<i>Chlamydia trachomatis</i>	Chltr	NC_000117	B16.1.1.1.1

表 1(续)

Species/strain	Abbrev	Accession No.	Bergey code
<i>Chlamydomonas reinhardtii</i> AR39	ChlpaA	NC_002179	B16.1.1.1.2
<i>Borrelia burgdorferi</i> B31	Borbu	NC_001318	B17.1.1.1.2
<i>Treponema pallidum</i> Nichols	Trepa	NC_000919	B17.1.1.1.9
<i>Leptospira interrogans</i> serovar lai	Lepin	NC_004342	B17.1.1.3.1
<i>Bacteroides fragilis</i> 638R	Bacfr6	NC_016776	B20.1.1.1.1
<i>Bacteroides helcogenes</i> P	Bache	NC_014933	B20.1.1.1.1
<i>Bacteroides thetaiotaomicron</i> VPI	Bacth	NC_004663	B20.1.1.1.1
<i>Flavobacterium branchiophilum</i> FL	Flabr	NC_016001	B20.2.1.1.1
<i>Flavobacterium columnare</i> ATCC	Flaco	NC_016510	B20.2.1.1.1
<i>Fusobacterium nucleatum</i> ATCC	Fusnu	NC_003454	B21.1.1.1.1

表 a2 古细菌的名字、缩写、索取号和 Berger's 代码

Table a2 Archaea name, abbreviation, NCBI accession numbers and Berger's code

Species/strain	Abbrev	Accession No.	Bergey code
<i>Pyrobaculum aerophilum</i>	Pyrae	NC_003364	A1.1.1.1.3
<i>Aeropyrum pernix</i> K1	Aerpe	NC_000854	A1.1.3.1.3
<i>Sulfolobus solfataricus</i>	Sulso	NC_002754	A1.1.3.1.1
<i>Sulfolobus tokodaii</i>	Sulto	NC_003106	A1.1.3.1.1
<i>Methanothermobacter</i> <i>thermautotrophicus</i>	Metth	NC_000916	A2.1.1.1.4
<i>Methanocaldococcus jannaschii</i>	Metja	NC_000909	A2.2.1.2.1
<i>Methanosarcina acetivorans</i> C2A	Metac	NC_003552	A2.3.2.1.1
<i>Methanosarcina mazei</i> Goel	MetmG	NC_003901	A2.3.2.1.1
<i>Halobacterium</i> sp. NRC-1	Halsp	NC_002607	A2.4.1.1.1
<i>Thermoplasma acidophilum</i>	Theac	NC_002578	A2.5.1.1.1
<i>Thermoplasma volcanium</i>	Thevo	NC_002689	A2.5.1.1.1
<i>Pyrococcus abyssi</i> GE5	Pyrab	NC_000868	A2.6.1.1.3
<i>Pyrococcus furiosus</i>	Pyrfu	NC_003413	A2.6.1.1.3
<i>Pyrococcus horikoshii</i>	Pyrho	NC_000961	A2.6.1.1.3
<i>Archaeoglobus fulgidus</i>	Arcfu	NC_000917	A2.7.1.1.1
<i>Methanopyrus kandleri</i> AV19	Metka	NC_003551	A2.8.1.1.1

Validity of peptide composition and GC-content for classifying bacteria

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In the past decades, a lot of methods have been proposed to construct Genome Tree. Among them, K-String Composition Approach which is Alignment-Free shows nonnegligible superiority. On the other hand, the species specificity of GC (Guanine+Cytosine)-content which actually is the lowest-order version of K-String Composition has been discovered for a long time, especially in bacteria. Unfortunately, its resolution is too poor to be applied to reconstruct phylogeny. Motivated by those facts, in this paper, relationship between composition vector of peptides and GC-content of corresponding DNA sequence is studied for bacteria. A strong correlation is uncovered for short peptides, and with the increase of peptide length the correlation exhibits an abrupt change, that is, tends to vanish quickly. These results indicate that the composition vector of longer peptide do contains more precise information of species specificity than that of GC-content, and therefore can effectively measure the genetic relationship of bacteria. Short peptides are obviously not competent.

phylogenomics, alignment-free phylogeny, composition vector, GC-content

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