multidistribute の使い方: mtREV + F + Γ モデルを用いたアミノ酸配列解析
～各パラメーターの設定方法～

“aga2aa.mlc” ファイル – codeml の output

Gamma category → 0 1 2 3 4 5 6 7

relative rate

```
alpha (gamma) =  1.25590
r ( 8):   0.10050  0.26957  0.44367  0.64063  0.87777  1.18658  1.64892  2.83237
f:        0.12500  0.12500  0.12500  0.12500  0.12500  0.12500  0.12500  0.12500


Root, U, V, freq
          A         R         N         D         C         Q         E
   1.000000  0.998912  0.998320  0.998099  0.997573  0.996449  0.996094

   1.000000 -0.188510  0.182838  0.011741 -0.235152 -0.407133  0.058994
   1.000000 -0.105989 -8.877536 -0.341450 -1.106593 -0.704911 -0.177025
   1.000000 -0.179571  0.006838  0.107767  0.296757  0.546165  0.689090
   1.000000 -0.189455 -0.087309 -0.149606  3.140859  1.814943 11.481157
   1.000000 -0.123494 -0.022817  0.148193 -0.180232  0.622782 -0.181623
   1.000000 -0.218079 -0.511173  0.267554  0.956677  1.073080  0.377902
   1.000000 -0.302048 -0.510044  0.061191  8.076613 -1.973469 -2.491839
   1.000000 -0.248597  0.299951 -4.851414 -0.095465  0.204243 -0.202494
   1.000000 -0.200803 -0.436715  0.318227  0.627433  3.158573  0.169548
   1.000000 -0.173031  0.210390  0.277543 -0.317961 -0.453267 -0.172263
   1.000000 -0.136980  0.204169  0.318606 -0.344729 -0.403495 -0.281518
   1.000000 -0.169016 -0.263360  0.174107  0.756575  0.478794  0.335749
   1.000000 -0.156390  0.194774  0.267122 -0.283804 -0.388437 -0.146216
   1.000000 -0.166596  0.215694  0.453958 -0.390279  1.248053 -1.433962
   1.000000 -0.213748  0.071228  0.296300 -0.061922 -0.205956  1.114004
   1.000000 -0.155948  0.150679  0.050213 -0.111534 -0.179785  0.146313
   1.000000 -0.172502  0.168240  0.184934 -0.193360 -0.303918  0.034566
   1.000000  5.782142  0.028841 -0.091764  0.102947 -0.003557  0.016885
   1.000000 -0.134614  0.004296  0.457219  0.136089  5.120856 -1.747132
   1.000000 -0.178601  0.216305  0.277324 -0.328350 -0.538546 -0.171348

   0.082317  0.012089  0.036927  0.005275  0.002308  0.033630  0.012529
  -0.015518 -0.001281 -0.006631 -0.000999 -0.000285 -0.007334 -0.003784
   0.015051 -0.107323  0.000253 -0.000461 -0.000053 -0.017191 -0.006390
   0.000966 -0.004128  0.003980 -0.000789  0.000342  0.008998  0.000767
  -0.019357 -0.013378  0.010958  0.016569 -0.000416  0.032173  0.101191
  -0.033514 -0.008522  0.020168  0.009574  0.001437  0.036088 -0.024725
   0.004856 -0.002140  0.025446  0.060567 -0.000419  0.012709 -0.031220
   0.004022  0.008380 -0.008966  0.032235  0.000046 -0.058800  0.008220
  -0.012321  0.007964 -0.026803  0.008737 -0.000268 -0.075840  0.017143
  -0.050311 -0.003425 -0.007088  0.002561 -0.010285  0.065015 -0.007737
  -0.005112 -0.001182 -0.001236  0.000330  0.046648  0.010293 -0.000811
   0.009201  0.000126  0.028961 -0.001425 -0.000522 -0.005518 -0.007643
   0.040887  0.001322  0.052500 -0.005675 -0.001798 -0.118166  0.002720
   0.150707  0.000574  0.013030 -0.001905 -0.003647  0.044637  0.000782
  -0.101410  0.000969  0.157437 -0.006973 -0.000256  0.004948  0.001316
   0.078538 -0.000369 -0.026371  0.000846 -0.000131 -0.001573 -0.000099
  -0.167121  0.000317 -0.064191  0.001359 -0.001058 -0.002492 -0.000405
  -0.010960  0.000171  0.010407 -0.000089  0.000127 -0.000971  0.000470
  -0.032379  0.000093  0.001146  0.000034  0.000103 -0.002294  0.000192
  -0.028401  0.000016 -0.001435  0.000005 -0.000207 -0.001514  0.000074

   0.082317  0.012089  0.036927  0.005275  0.002308  0.033630  0.012529
          A         R         N         D         C         Q         E
```

right eigen vector

evecfl.aga2aa

left eigen vector

ievecfl.aga2aa

横の行を縦に並べる

各アミノ酸のオリジナルの Eigen value (固有値). A の値を 1 としている.

“aga2aa.xls” ファイル – codeml の推定値を Excel で変換

aga2aa.xls

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	A	1	A	1	A	1	A	1	A	1	A	1	A	1
2	R	0.998912	R	0.999890602	R	0.999706591	R	0.999517141	R	0.999302858	R	0.999044923	R	0.998709132
3	N	0.99832	N	0.999831032	N	0.999546844	N	0.999254286	N	0.998923416	N	0.998525195	N	0.998006858
4	D	0.998099	D	0.999808786	D	0.999487191	D	0.999156137	D	0.998781746	D	0.998331165	D	0.997744712
5	C	0.997573	C	0.99975582	C	0.999345173	C	0.998922485	C	0.998444512	C	0.997869336	C	0.997120823
6	Q	0.996449	Q	0.999642553	Q	0.999041513	Q	0.998422969	Q	0.997723669	Q	0.996882361	Q	0.995787852
7	E	0.996094	E	0.999606756	E	0.998945554	E	0.998265138	E	0.99749594	E	0.996570611	E	0.995366909
8	G	0.995966	G	0.999593846	G	0.998910949	G	0.998208223	G	0.997413822	G	0.996458202	G	0.99521514
9	H	0.995328	H	0.999529474	H	0.998738414	H	0.997924473	H	0.997004459	H	0.995897886	H	0.994458718
10	I	0.994456	I	0.999441434	I	0.998502468	I	0.997536489	I	0.9964448	I	0.995131991	I	0.993425008
11	L	0.99409	L	0.99940446	L	0.998403391	L	0.997373586	L	0.996209845	L	0.994810501	L	0.992991185
12	K	0.993631	K	0.999358075	K	0.9982791	K	0.997169243	K	0.995915145	K	0.994407302	K	0.99244717
13	M	0.993114	M	0.999305804	M	0.998139054	M	0.996939015	M	0.995583146	M	0.993953126	M	0.991834469
14	F	0.992234	F	0.999216777	F	0.997900555	F	0.996546985	F	0.9950179	F	0.993179993	F	0.99079171
15	P	0.989668	P	0.998956777	P	0.99720423	P	0.995402756	P	0.993368665	P	0.990925131	P	0.987752106
16	S	0.988368	S	0.998824823	S	0.996850951	S	0.994822431	S	0.992532534	S	0.989782489	S	0.986212726
17	T	0.985819	T	0.998565637	T	0.996157266	T	0.993683313	T	0.990891927	T	0.987541498	T	0.983195456
18	W	0.983013	W	0.998279622	W	0.995392124	W	0.992427448	W	0.989084144	W	0.985073742	W	0.979875656
19	Y	0.981048	Y	0.998078892	Y	0.994855356	Y	0.991546798	Y	0.987817076	Y	0.983345097	Y	0.977551902
20	V	0.978249	V	0.997792341	V	0.994089412	V	0.990290678	V	0.986010653	V	0.980882036	V	0.974243381
21			0	0.1005	1	0.26957	2	0.44367	3	0.64063	4	0.87777	5	1.18658

Gamma category → 0 1 2 3 4 5

各固有値 (B 列) を rate (21 行) で累乗し, category 0 の固有値 (D 列) を得る.

Category 0, R の例)

$0.998912^{0.1005} = 0.999890602$

evalfl.aga2aa_0

Category 0 の固有値 (D 列) を保存.

reveqps.aga2aa

アミノ酸組成