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In[*]:= (* P(G1) and P(G1a), under the IM model for 3 sequences (a1, a2, b) for heuristic species delimitation.
The notation is from Kornai et al. (2024).
PG1a works if M>0 only. PG1aInt works if M is specified with high precision,
such as M = 10`100.
*)
(* theta = 2 is fixed so that 2*tau/theta is branch length in coalescent units *)
theta = 2;
Q[M_] := Block[{theta1, theta2, M12, M21, w12, w21},
theta1 = theta; theta2 = theta; M12 = M; M21 = M;
c1 = 2 / theta1; c2 = 2 / theta2; w12 = 4 M12 / theta2; w21 = 4 M21 / theta1;

{{-3 (c1 + w21), w21, w21, 0, w21, 0, 0, 0, c1, c1, c1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{w12, -(c1 + w12 + 2 w21), 0, w21, 0, w21, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, c1, 0},
{w12, 0, -(c1 + w12 + 2 w21), w21, 0, 0, w21, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, c1, 0},
{0, w12, w12, -(c2 + 2 w12 + w21), 0, 0, 0, w21, 0, 0, 0, 0, 0, 0, 0, c2, 0, 0, 0, 0, 0},
{w12, 0, 0, 0, -(c1 + w12 + 2 w21), w21, w21, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, c1, 0, 0, 0},
{0, w12, 0, 0, w12, -(c2 + 2 w12 + w21), 0, w21, 0, 0, 0, 0, 0, 0, 0, c2, 0, 0, 0, 0, 0},
{0, 0, w12, 0, w12, 0, -(c2 + 2 w12 + w21), w21, 0, 0, 0, 0, 0, 0, 0, c2, 0, 0, 0, 0, 0},
{0, 0, 0, w12, 0, w12, w12, -3 (c2 + w12), 0, 0, 0, c2, c2, c2, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, -2 w21 - c1, 0, 0, 0, 0, 0, 0, w21, 0, 0, w21, 0, 0, c1},
{0, 0, 0, 0, 0, 0, 0, 0, -2 w21 - c1, 0, 0, 0, 0, 0, 0, w21, 0, 0, w21, 0, 0, c1},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2 w21 - c1, 0, 0, 0, 0, 0, 0, w21, 0, 0, w21, c1},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2 w12 - c2, 0, 0, 0, w12, 0, 0, w12, 0, 0, c2},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2 w12 - c2, 0, 0, 0, w12, 0, 0, w12, 0, 0, c2},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2 w12 - c2, 0, 0, 0, w12, 0, 0, w12, 0, 0, c2},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, w12, 0, 0, 0, w21, 0, 0, -w12 - w21, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}}
];

In[*]:= PG1a[tau_, M_] := Block[{Esys, U, Evalues, P, theta1, theta2},
theta1 = theta; theta2 = theta;
Esys = Eigensystem[Q[M]];
Evalues = Esys[[1]];
If[Abs[Evalues[[21]]] > 10^(-20), Print["eigenvalue 21 is not 0?"]];
Evalues[[21]] = -1; (* eigenvalues are ordered increasingly, last one is 0. *)
Evalues = (Exp[Evalues * tau] - 1) / Evalues;
Evalues[[21]] = tau;
U = Transpose[Esys[[2]]];
P = Chop[U . DiagonalMatrix[Evalues] . Inverse[U]];
(P[[2, 1]] + P[[2, 2]]) * 2 / theta1 + (P[[2, 7]] + P[[2, 8]]) * 2 / theta2
];

PG1b[tau_, M_] := Block[{P},
P = MatrixExp[Q[M] * tau];
(P[[2, 1]] + P[[2, 2]] + P[[2, 3]] + P[[2, 4]] + P[[2, 5]] + P[[2, 6]] + P[[2, 7]] + P[[2, 8]]) / 3
];

PG1[tau_, M_] := PG1a[tau, M] + PG1b[tau, M];

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In[ ]:= b = 10; Mmin = 0.001; Mmax = 10;  $\tau$ min = 0.01;  $\tau$ max = 10;
newStyle[x_] := x /. 1_Line  $\Rightarrow$  Sequence[Opacity[.4], Thick, Red, 1]
ContourPlot[(PG1[b $\tau$ , bM] - 1/3) * 3/2,
  { $\tau$ , Log[b,  $\tau$ min], Log[b,  $\tau$ max]}, {M, Log[b, Mmin], Log[b, Mmax]},
  Contours  $\rightarrow$  {0.025, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95},
  (* ContourStyle  $\rightarrow$  {{Red, Thin}}, *)
  BaseStyle  $\rightarrow$  {FontFamily  $\rightarrow$  "Arial", FontSize  $\rightarrow$  9}, PlotPoints  $\rightarrow$  30, ContourLabels  $\rightarrow$  All,
  ColorFunction  $\rightarrow$  (ColorData[{"BeachColors", "Reverse"}]), ContourStyle  $\rightarrow$  Thin, AspectRatio  $\rightarrow$  1,
  (* Frame  $\rightarrow$  False, *)
  FrameTicks  $\rightarrow$  {Table[{ $\tau$ , ToString[Round[b $\tau$ ,  $\tau$ min]}], { $\tau$ , Log[b,  $\tau$ min], Log[b,  $\tau$ max]}],
    Table[{M, ToString[Round[bM, Mmin]}], {M, Log[b, Mmin], Log[b, Mmax]}}}
] /. Tooltip[x_, 0.2]  $\Rightarrow$  Tooltip[newStyle[x], 0.2] /.
Tooltip[x_, 0.7]  $\Rightarrow$  Tooltip[newStyle[x], 0.7]

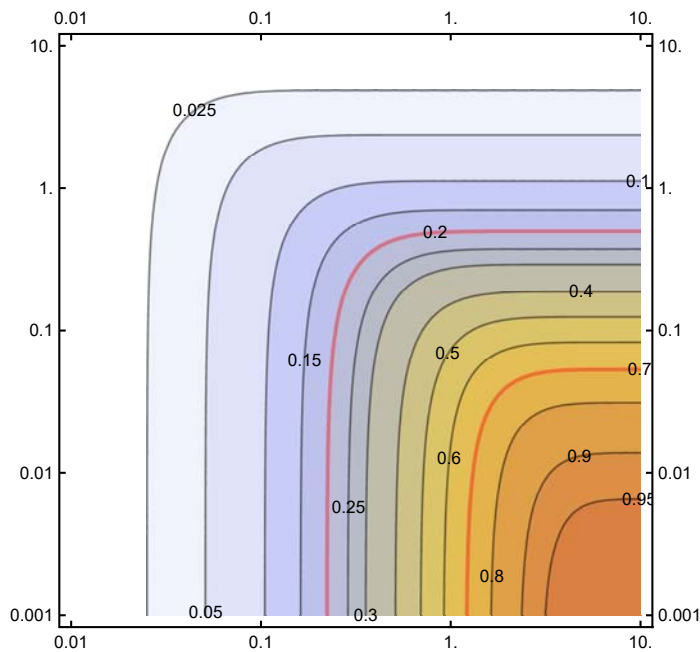
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ContourPlot[PG1a[b $\tau$ , bM], { $\tau$ , Log[b,  $\tau$ min], Log[b,  $\tau$ max]}, {M, Log[b, Mmin], Log[b, Mmax]},
  Contours  $\rightarrow$  {0.025, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95},
  BaseStyle  $\rightarrow$  {FontFamily  $\rightarrow$  "Arial", FontSize  $\rightarrow$  9}, PlotPoints  $\rightarrow$  30, ContourLabels  $\rightarrow$  All,
  ColorFunction  $\rightarrow$  (ColorData[{"BeachColors", "Reverse"}]), ContourStyle  $\rightarrow$  Thin, AspectRatio  $\rightarrow$  1,
  (* Frame  $\rightarrow$  False, *)
  FrameTicks  $\rightarrow$  {Table[{ $\tau$ , ToString[Round[b $\tau$ ,  $\tau$ min]}], { $\tau$ , Log[b,  $\tau$ min], Log[b,  $\tau$ max]}],
    Table[{M, ToString[Round[bM, Mmin]}], {M, Log[b, Mmin], Log[b, Mmax]}}}
] /. Tooltip[x_, 0.2]  $\Rightarrow$  Tooltip[newStyle[x], 0.2] /.
Tooltip[x_, 0.7]  $\Rightarrow$  Tooltip[newStyle[x], 0.7]

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Out[ ]:=



Out[ ]=

