

Details about the kernels in GP.

Radial Basis Function

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In[1]:= k[x_, y_, l_, A_] = A^2 E^(-(x-y)^2/(2 l^2));
AtoK = Solve[k[x, y, l, A] == K[x, y], A][[2]];

(* needed GP relations *)
K[x, y] == k[x, y, l, A]
DxK[x, y] == (Dxk[x, y, l, A]) /. AtoK // Simplify
DyK[x, y] == (Dyk[x, y, l, A]) /. AtoK // Simplify
Dx,yK[x, y] == (Dx,yk[x, y, l, A]) /. AtoK // Simplify
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$$\text{Out[3]}= K[x, y] == A^2 e^{-\frac{(x-y)^2}{2 l^2}}$$

$$\text{Out[4]}= K^{(1,0)}[x, y] == -\frac{(x-y) K[x, y]}{l^2}$$

$$\text{Out[5]}= K^{(0,1)}[x, y] == \frac{(x-y) K[x, y]}{l^2}$$

$$\text{Out[6]}= K^{(1,1)}[x, y] == \frac{(l^2 - (x-y)^2) K[x, y]}{l^4}$$

Cauchy function

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In[7]:= k[x_, y_, l_, A_] = A^2 \frac{1^2}{(x-y)^2 + 1^2};
AtoK = Solve[k[x, y, l, A] == K[x, y], A][[2]];

(* needed GP relations *)
K[x, y] == k[x, y, l, A]
DxK[x, y] == (Dxk[x, y, l, A]) /. AtoK // Simplify
DyK[x, y] == (Dyk[x, y, l, A]) /. AtoK // Simplify
Dx,yK[x, y] == (Dx,yk[x, y, l, A]) /. AtoK // Simplify
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$$\text{Out[9]}= K[x, y] == \frac{A^2 l^2}{l^2 + (x-y)^2}$$

$$\text{Out[10]}= K^{(1,0)}[x, y] == -\frac{2(x-y) K[x, y]}{l^2 + (x-y)^2}$$

$$\text{Out[11]}= K^{(0,1)}[x, y] == \frac{2(x-y) K[x, y]}{l^2 + (x-y)^2}$$

$$\text{Out[12]}= K^{(1,1)}[x, y] == \frac{2(l^2 - 3(x-y)^2) K[x, y]}{(l^2 + (x-y)^2)^2}$$

Matern 5/2 function

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In[100]:= d[x_, y_] = x - y;
r[x_, y_] = Abs[d[x, y]];
X[x_, y_, l_] =  $\sqrt{5} \frac{r[x, y]}{l}$ ;

B[Y_] = 1 + Y +  $\frac{Y^2}{3}$ ;
k[x_, y_, l_, A_] = A2 B[X[x, y, l]] E-X[x, y, l];
AtoK = Solve[k[x, y, l, A] == K[x, y], A][[2]];

(* needed GP relations *)
K[x, y] == k[x, y, l, A] /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /. Abs[x_] => r[x]
∂xK[x, y] == ((∂xk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
Abs[x_] => r[x] // Simplify)
∂yK[x, y] == ((∂yk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
Abs[x_] => r[x] // Simplify)
∂x,yK[x, y] == ((∂x,yk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
Abs[x_] => r[x] // Simplify)

Out[106]= K[x, y] == A2 e $-\frac{\sqrt{5} r[x-y]}{l}$   $\left(1 + \frac{\sqrt{5} r[x-y]}{l} + \frac{5 r[x-y]^2}{3 l^2}\right)$ 

Out[107]= K(1,0)[x, y] == -  $\frac{5 H[x-y] \times r[x-y] \left(1 + \sqrt{5} r[x-y]\right) K[x, y]}{l \left(3 l^2 + 3 \sqrt{5} l r[x-y] + 5 r[x-y]^2\right)}$ 

Out[108]= K(0,1)[x, y] ==  $\frac{5 H[x-y] \times r[x-y] \left(1 + \sqrt{5} r[x-y]\right) K[x, y]}{l \left(3 l^2 + 3 \sqrt{5} l r[x-y] + 5 r[x-y]^2\right)}$ 

Out[109]= K(1,1)[x, y] ==  $\frac{5 H[x-y]^2 \left(l^2 + \sqrt{5} l r[x-y] - 5 r[x-y]^2\right) K[x, y]}{l^2 \left(3 l^2 + 3 \sqrt{5} l r[x-y] + 5 r[x-y]^2\right)}$ 

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Matern 7/2 function

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In[111]:= d[x_, y_] = x - y;
r[x_, y_] = Abs[d[x, y]];
R[x_, y_, l_] =  $\frac{r[x, y]}{1}$ ;
X[x_, y_, l_] =  $\sqrt{7} R[x, y, l]$ ;
B[Y_] =  $1 + \sqrt{7} Y + \frac{14 Y^2}{5} + \frac{7 \sqrt{7} Y^3}{15}$ ;
k[x_, y_, l_, A_] = A2 B[R[x, y, l]] E-X[x, y, l];
AtoK = Solve[k[x, y, l, A] == K[x, y], A][[2]];

(* needed GP relations *)
K[x, y] == k[x, y, l, A] /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /. Abs[x_] => r[x]
∂xK[x, y] == ((∂xk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
  Abs[x_] => r[x] // FullSimplify)
∂yK[x, y] == ((∂yk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
  Abs[x_] => r[x] // FullSimplify)
∂x,yK[x, y] == ((∂x,yk[x, y, l, A]) /. AtoK /. Abs'[x - y] → 0 /. Abs'[x - y] → H[x - y] /.
  Abs[x_] => r[x] // FullSimplify)

Out[118]= K[x, y] == A2 e $-\frac{\sqrt{7} r[x-y]}{1}$   $\left(1 + \frac{\sqrt{7} r[x-y]}{1} + \frac{14 r[x-y]^2}{5 l^2} + \frac{7 \sqrt{7} r[x-y]^3}{15 l^3}\right)$ 

Out[119]= K(1,0)[x, y] ==  $-\frac{7 H[x-y] \times r[x-y] \left(3 l^2 + 3 \sqrt{7} l r[x-y] + 7 r[x-y]^2\right) K[x, y]}{15 l^4 + l r[x-y] \left(15 \sqrt{7} l^2 + 7 r[x-y] \left(6 l + \sqrt{7} r[x-y]\right)\right)}$ 

Out[120]= K(0,1)[x, y] ==  $\frac{7 H[x-y] \times r[x-y] \left(3 l^2 + 3 \sqrt{7} l r[x-y] + 7 r[x-y]^2\right) K[x, y]}{15 l^4 + l r[x-y] \left(15 \sqrt{7} l^2 + 7 r[x-y] \left(6 l + \sqrt{7} r[x-y]\right)\right)}$ 

Out[121]= K(1,1)[x, y] ==  $\frac{7 H[x-y]^2 \left(3 l^3 + \sqrt{7} r[x-y] \left(3 l^2 - 7 r[x-y]^2\right)\right) K[x, y]}{15 l^5 + l^2 r[x-y] \left(15 \sqrt{7} l^2 + 7 r[x-y] \left(6 l + \sqrt{7} r[x-y]\right)\right)}$ 

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