Raiders of the Lost Architecture: A Kernel for Hierarchical Parameter Spaces

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Abstract

We define a family of kernels for mixed continuous/discrete hierarchical parameter spaces and show that they are positive definite.

1 Introduction

We aim to do inference about some function g with domain (input space) $\mathcal{X}$. $\mathcal{X} = \prod_{i=1}^{D} \mathcal{X}_i$ is a D-dimensional input space, where each individual dimension is either bounded real or categorical, that is, $\mathcal{X}_i$ is either $[l_i, u_i] \subset \mathbb{R}$ (with lower and upper bounds l_i and u_i, respectively) or $\{v_{i,1}, \ldots, v_{i,m_i}\}$.

Associated with $\mathcal{X}$, there is a DAG structure $\mathcal{D}$, whose vertices are the dimensions $\{1, \ldots, D\}$. $\mathcal{X}$ will be restricted by $\mathcal{D}$: if vertex i has children under $\mathcal{D}$, $\mathcal{X}_i$ must be categorical. $\mathcal{D}$ is also used to specify when each input is *active* (that is, relevant to inference about g). In particular, we assume each input dimension is only active under some instantiations of its ancestor dimensions in $\mathcal{D}$. More precisely, we define D functions $\delta_i \colon \mathcal{X} \to \mathcal{B}$, for $i \in \{1, \ldots, D\}$, and where $\mathcal{B} = \{\text{true}, \text{false}\}$. We take

$$\delta_i(\underline{x}) = \delta_i\big(\underline{x}(\text{anc}_i)\big), \tag{1}$$

where anc_i are the ancestor vertices of i in $\mathcal{D}$, such that $\delta_i(\underline{x})$ is true only for appropriate values of those entries of $\underline{x}$ corresponding to ancestors of i in $\mathcal{D}$. We say i is active for $\underline{x}$ iff $\delta_i(\underline{x})$.

Our aim is to specify a kernel for $\mathcal{X}$, *i.e.*, a positive semi-definite function $k \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. We will first specify an individual kernel for each input dimension, *i.e.*, a positive semi-definite function $k_i \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. k can then be taken as either a sum,

$$k(\underline{x}, \underline{x}') = \sum_{i=1}^{D} k_i(\underline{x}, \underline{x}'), \tag{2}$$

product,

$$k(\underline{x}, \underline{x}') = \prod_{i=1}^{D} k_i(\underline{x}, \underline{x}'), \tag{3}$$

or any other permitted combination, of these individual kernels. Note that each individual kernel k_i will depend on an input vector $\underline{x}$ only through dependence on x_i and $\delta_i(\underline{x})$,

$$k_i(\underline{x}, \underline{x}') = \tilde{k}_i\big(x_i, \delta_i(\underline{x}), x_i', \delta_i(\underline{x}')\big). \tag{4}$$

That is, x_j for $j \neq i$ will influence $k_i(\underline{x}, \underline{x}')$ only if $j \in \text{anc}_i$, and only by affecting whether i is active.

Below we will construct pseudometrics $d_i \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$: that is, d_i satisfies the requirements of a metric aside from the identity of indiscernibles. As for k_i, these pseudometrics will depend

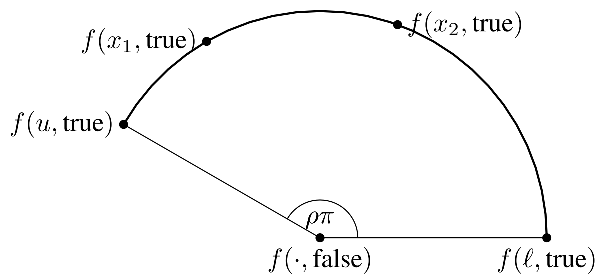


Figure 1: A demonstration of the embedding giving rise to the pseduo-metric: All points for which $\delta_i(x) = \text{false}$ are mapped to the same point. Points for which $\delta_i(x) = \text{true}$ are mapped to a semicircle. This embedding gives a constant distance between pairs of points which have differing values of δ. The parameter ρ determines how much distance there is along the arc.

on an input vector $\underline{x}$ only through dependence on both x_i and $\delta_i(\underline{x})$. $d_i(\underline{x}, \underline{x}')$ will be designed to provide an intuitive measure of how different $g(\underline{x})$ is from $g(\underline{x}')$. For each i, we will then construct a (pseudo-)isometry f_i from $\mathcal{X}$ to a Euclidean space ($\mathbb{R}^2$ for bounded real parameters, and $\mathbb{R}^m$ for categorical-valued parameters with m choices). That is, denoting the Euclidean metric on the appropriate space as d_E, f_i will be such that

$$d_i(\underline{x}, \underline{x}') = d_{\mathrm{E}}\big(f_i(\underline{x}), f_i(\underline{x}')\big) \tag{5}$$

for all $\underline{x}, \underline{x}' \in \mathcal{X}$. We can then use our transformed inputs, $f_i(\underline{x})$, within any standard Euclidean kernel κ. We'll make this explicit in Proposition 2.

Definition 1. *A function* $\kappa \colon \mathbb{R}^+ \to \mathbb{R}$ *is* a positive semi-definite covariance function over Euclidean space *if* $K \in \mathbb{R}^{N\times N}$*, defined by*

$$K_{m,n} = \kappa\big(d_E(\underline{y}_m, \underline{y}_n)\big), \quad \textit{for } \underline{y}_m, \underline{y}_n \in \mathbb{R}^P, \quad m, n = 1, \dots, N,$$

is positive semi-definite for any $\underline{y}_1, \dots, \underline{y}_N \in \mathbb{R}^P$.

A popular example of such a κ is the exponentiated quadratic, for which $\kappa(\delta) = \sigma^2 \exp(-\frac{1}{2}\frac{\delta^2}{\lambda^2})$; another popular choice is the rational quadratic, for which $\kappa(\delta) = \sigma^2(1 + \frac{1}{2\alpha}\frac{\delta^2}{\lambda^2})^{-\alpha}$.

Proposition 2. *Let* κ *be a positive semi-definite covariance function over Euclidean space and let* d_i *satisfy Equation 5. Then,* $k_i \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$*, defined by*

$$k_i(\underline{x}, \underline{x}') = \kappa\big(d_i(\underline{x}, \underline{x}')\big)$$

is a positive semi-definite covariance function over input space $\mathcal{X}$.

Proof. We need to show that for any $\underline{x}_1, \dots, \underline{x}_N \in \mathcal{X}$, $K \in \mathbb{R}^{N\times N}$ defined by

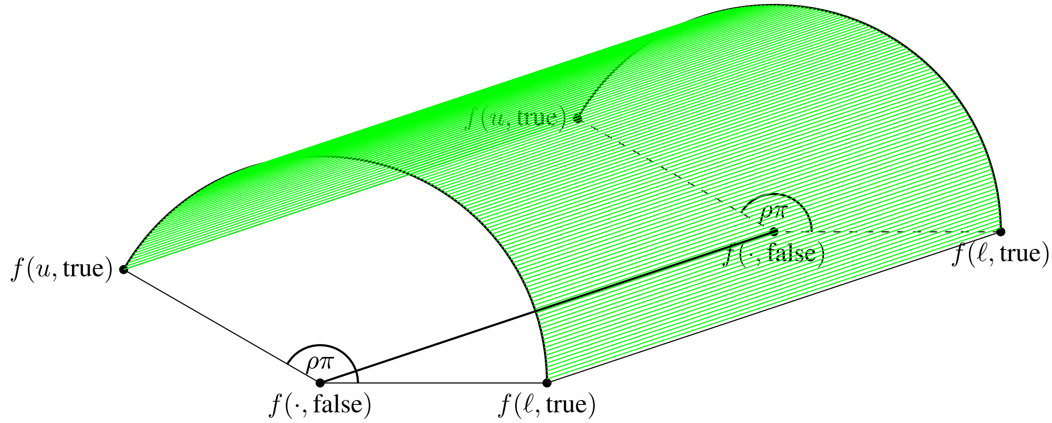
$$K_{m,n} = \kappa\big(d_i(\underline{x}_m, \underline{x}_n)\big), \quad \text{for } \underline{x}_m, \underline{x}_n \in \mathcal{X}, \quad m, n = 1, \dots, N,$$

is positive semi-definite. Now, by the definition of d_i,

$$K_{m,n} = \kappa\Big(d_{\mathrm{E}}\big(f_i(\underline{x}_m), f_i(\underline{x}_n)\big)\Big) = \kappa\big(d_{\mathrm{E}}(\underline{y}_m, \underline{y}_n)\big)$$

where $\underline{y}_m = f_i(\underline{x}_m)$ and $\underline{y}_n = f_i(\underline{x}_n)$ are elements of $\mathbb{R}^P$. Then, by assumption that κ is a positive semi-definite covariance function over Euclidean space, K is positive semi-definite. □

We'll now define pseudometrics d_i and associated isometries f_i for both the bounded real and categorical cases.



2 Bounded Real Dimensions

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Let's first focus on a bounded real input dimension i, i.e., $\mathcal{X}_i = [l_i, u_i]$. To emphasize that we're in this real case, we explicitly denote the pseudometric as d_i^{r} and the (pseudo-)isometry from $(\mathcal{X}, d_i)$ to $\mathbb{R}^2, d_{\mathrm{E}}$ as $f_i{}^{\mathrm{r}}$. For the definitions, recall that $\delta_i(\underline{x})$ is true iff dimension i is active given the instantiation of i's ancestors in $\underline{x}$.

$$d_i^{\mathrm{r}}(\underline{x}, \underline{x}') \quad = \quad \begin{cases} 0 & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{false} \\ \omega_i & \text{if } \delta_i(\underline{x}) \neq \delta_i(\underline{x}') \\ \omega_i \sqrt{2}\sqrt{1 - \cos(\pi \rho_i \frac{x_i - x_i'}{u_i - l_i})} & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{true}. \end{cases}$$

$$f_i{}^{\mathrm{r}}(\underline{x}) \quad = \quad \begin{cases} [0, 0]^{\mathsf{T}} & \text{if } \delta_i(\underline{x}) = \text{ false} \\ \omega_i [\sin \pi \rho_i \frac{x_i}{u_i - l_i}, \cos \pi \rho_i \frac{x_i}{u_i - l_i}]^{\mathsf{T}} & \text{otherwise.} \end{cases} \qquad .$$

Although our formal arguments do not rely on this, Proposition 5 in the appendix shows that d_i^{r} is a pseudometric. This pseudometric is defined by two parameters: $\omega_i \in [0, 1]$ and $\rho_i \in [0, 1]$. We firstly define

$$\omega_i = \prod_{j \in \mathrm{anc}_i \cup \{i\}} \gamma_j, \tag{6}$$

where $\gamma_j \in [0, 1]$. This encodes the intuitive notion that differences on lower levels of the hierarchy count less than differences in their ancestors.

Also note that, as desired, if i is inactive for both $\underline{x}$ and $\underline{x}'$, d_i^{r} specifies that $g(\underline{x})$ and $g(\underline{x}')$ should not differ owing to differences between x_i and x_i'. Secondly, if i is active for both $\underline{x}$ and $\underline{x}'$, the difference between $g(\underline{x})$ and $g(\underline{x}')$ due to x_i and x_i' increases monotonically with increasing $|x_i - x_i'|$. Parameter ρ_i controls whether differing in the activity of i contributes more or less to the distance than differing in x_i should i be active. If $\rho = 1/3$, and if i is inactive for exactly one of $\underline{x}$ and $\underline{x}'$, $g(\underline{x})$ and $g(\underline{x}')$ are as different as is possible due to dimension i; that is, $g(\underline{x})$ and $g(\underline{x}')$ are exactly as different in that case as if $x_i = l_i$ and $x_i' = u_i$. For $\rho > 1/3$, i being active for both $\underline{x}$ and $\underline{x}'$ means that $g(\underline{x})$ and $g(\underline{x}')$ could potentially be more different than if i was active in only one of them. For $\rho < 1/3$, the converse is true.[1]

We now show that d_i^{r} and $f_i{}^{\mathrm{r}}$ can be plugged into a positive semi-definite kernel over Euclidean space to define a valid kernel over space $\mathcal{X}$.

[1]Note that $\underline{x}$ and $\underline{x}'$ must differ in at least one ancestor dimension of i in order for $\delta_i(\underline{x}) \neq \delta_i(\underline{x}')$ to hold, such that in the final kernel combining kernels k_i due to each dimension i, differences in the activity of dimension i are penalized both in kernel k_i and in the distance for the kernel of the ancestor dimension causing the difference in i's activity.

Proposition 3. *Let κ be a positive semi-definite covariance function over Euclidean space. Then, $k_i\colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$, defined by*

$$k_i(\underline{x}, \underline{x}') = \kappa\big(d_i^{\mathrm{r}}(\underline{x}, \underline{x}')\big)$$

is a positive semi-definite covariance function over input space $\mathcal{X}$.

Proof. Due to Proposition 2, we only need to show that, for any two inputs $\underline{x}, \underline{x}' \in \mathcal{X}$, the isometry condition $d_{\mathrm{E}}\big(f_i^{\mathrm{r}}(\underline{x}), f_i^{\mathrm{r}}(\underline{x}')\big) = d_i^{\mathrm{r}}(\underline{x}, \underline{x}')$ holds.

We use the abbreviation $\alpha = \pi\rho_i \frac{x_i}{u_i - l_i}$ and $\alpha' = \pi\rho_i \frac{x_i'}{u_i - l_i}$ and consider the following three possible cases of dimension i being active or inactive in $\underline{x}$ and $\underline{x}'$.

Case 1: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ false. In this case, we trivially have

$$d_{\mathrm{E}}(f_i^{\mathrm{r}}(\underline{x}), f_i^{\mathrm{r}}(\underline{x}')) = d_{\mathrm{E}}([0,0]^{\mathsf{T}}, [0,0]^{\mathsf{T}}) = 0 = d_i^{\mathrm{r}}(\underline{x}, \underline{x}').$$

Case 2: $\delta_i(\underline{x}) \neq \delta_i(\underline{x}')$. In this case, we have

$$d_{\mathrm{E}}(f_i^{\mathrm{r}}(\underline{x}), f_i^{\mathrm{r}}(\underline{x}')) = d_{\mathrm{E}}([\sin\alpha, \cos\alpha]^{\mathsf{T}}, [0,0]^{\mathsf{T}}) = \sqrt{\omega_i^2(\sin^2\alpha + \cos^2\alpha)} = \omega_i = d_i^{\mathrm{r}}(\underline{x}, \underline{x}'),$$

and symmetrically for $d_{\mathrm{E}}([0,0]^{\mathsf{T}}, [\sin\alpha, \cos\alpha]^{\mathsf{T}})$.

Case 3: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ true. We have:

$$\begin{aligned}
d_{\mathrm{E}}(f_i^{\mathrm{r}}(\underline{x}), f_i^{\mathrm{r}}(\underline{x}')) &= d_{\mathrm{E}}(\omega_i[\sin\alpha, \cos\alpha]^{\mathsf{T}}, \omega_i[\sin\alpha', \cos\alpha']^{\mathsf{T}}) \\
&= \omega_i\sqrt{(\sin\alpha - \sin\alpha')^2 + (\cos\alpha - \cos\alpha')^2} \\
&= \omega_i\sqrt{\sin^2\alpha - 2\sin\alpha\sin\alpha' + \sin^2\alpha' + \cos^2\alpha - 2\cos\alpha\cos\alpha' + \cos^2\alpha'} \\
&= \omega_i\sqrt{(\sin^2\alpha + \cos^2\alpha) + (\sin^2\alpha' + \cos^2\alpha') - 2(\sin\alpha\sin\alpha' + \cos\alpha\cos\alpha')} \\
&= \omega_i\sqrt{1 + 1 - 2\cos(\alpha - \alpha')} \qquad (7) \\
&= \omega_i\sqrt{2}\sqrt{1 - \cos(\pi\rho_i\frac{x_i - x_i'}{u_i - l_i})} = d_i^{\mathrm{r}}(\underline{x}, \underline{x}'),
\end{aligned}$$

where (7) follows from the previous line by using the identity

$$\cos(a - b) = \cos a \cos b + \sin a \sin b.$$

□

3 Categorical Dimensions

Now let's define f_i^{c} and d_i^{c} for the case that the input $\mathcal{X}_i = \{v_{i,1}, \ldots, v_{i,m_i}\}$ is categorical with m_i possible values. Proceeding as above, we define a pseudometric d_i^{c} on $\mathcal{X}$ and an isometry from $(\mathcal{X}, d_i^{\mathrm{c}})$ to $(\mathbb{R}^{m_i}, d_{\mathrm{E}}^{m_i})$, and show that we can combine these with a kernel over Euclidean space to construct a valid kernel over space $\mathcal{X}$.

$$d_i^{\mathrm{c}}(\underline{x}, \underline{x}') = \begin{cases} 0 & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{false} \\ \omega_i & \text{if } \delta_i(\underline{x}) \neq \delta_i(\underline{x}') \\ \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1-\rho)^2} \mathbb{I}_{x_i \neq x_i'} & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{true.} \end{cases}$$

$$f_i^{\mathrm{c}}(\underline{x}) = \begin{cases} \underline{0} \in \mathbb{R}^{m_i} & \text{if } \delta_i(\underline{x}) = \text{ false} \\ \omega_i \frac{e_j + (1-\rho)\sum_{l \neq j} e_l}{\sqrt{1 + (m_i - 1)(1-\rho)^2}} & \text{if } \delta_i(\underline{x}) = \text{ true and } x_i = v_{i,j}, \end{cases}$$

where $\underline{e_j} \in \mathbb{R}^{m_i}$ is the jth unit vector: zero in all dimensions except j, where it is 1. Note that

$$\sqrt{1 + (m_i - 1)(1-\rho)^2} = \left\| \underline{e_j} + (1-\rho) \sum_{l \neq j} \underline{e_l} \right\|. \tag{8}$$

Again, although our analysis does not require it, we prove in Proposition 6 (see appendix) that d_i^{c} is a pseudometric. Our pseudometric is again defined by two hyperparameters. Firstly, $\omega_i \in [0, 1]$ is exactly as defined in (6), and similarly allows higher-level inputs to attain greater importance. Similarly, $\rho_i \in [0, 1]$ allows control of to what extent differing in the activity of i affects the distance relative to the influence of differing in x_i should i be active. In particular, for

$$\rho_i^* = \frac{\sqrt{2} - 2 + 2m_i - \sqrt{6 - 4\sqrt{2} + 4(\sqrt{2}-1)m_i}}{2(m_i - 1)}, \tag{9}$$

$\rho_i < \rho_i^*$ implies that differing in the activity of i is more significant, whereas $\rho_i > \rho_i^*$ implies the converse. The special case $\rho = 0$ dictates that differing in x_i has no influence on the distance; $\rho = 1$ assigns maximal importance to differing in x_i.

Proposition 4. *Let κ be a positive semi-definite covariance function over Euclidean space. Then, $k_i \colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$, defined by*

$$k_i(\underline{x}, \underline{x}') = \kappa\big(d_i^{\mathrm{c}}(\underline{x}, \underline{x}')\big)$$

is a positive semi-definite covariance function over input space $\mathcal{X}$.

Proof. We proceed as in the proof of Proposition 3 to show that, for any two inputs $\underline{x}, \underline{x}' \in \mathcal{X}$, the isometry condition $d_{\mathrm{E}}^{m_i}(f_i^{\mathrm{c}}(\underline{x}), f_i^{\mathrm{c}}(\underline{x}')) = d_i^{\mathrm{c}}(\underline{x}, \underline{x}')$ holds.

Case 1: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ false. In this case, we trivially have

$$d_{\mathrm{E}}^{m_i}(f_i^{\mathrm{r}}(\underline{x}), f_i^{\mathrm{r}}(\underline{x}')) = d_{\mathrm{E}}^{m_i}(\underline{0}, \underline{0}) = 0 = d_i^{\mathrm{r}}(\underline{x}, \underline{x}').$$

Case 2: $\delta_i(\underline{x}) \neq \delta_i(\underline{x}')$. In this case, we have

$$d_{\mathrm{E}}^{m_i}(f_i^{\mathrm{c}}(\underline{x}), f_i^{\mathrm{c}}(\underline{x}')) = d_{\mathrm{E}}^{m_i}\left(\omega_i \, \frac{\underline{e_j} + (1-\rho)\sum_{l \neq j} \underline{e_l}}{\|\underline{e_j} + (1-\rho)\sum_{l\neq j} \underline{e_l}\|}, \underline{0}\right) = \omega_i = d_i(\underline{x}, \underline{x}'),$$

and symmetrically for $d_{\mathrm{E}}\left(\underline{0}, \omega_i \, \frac{\underline{e_j} + (1-\rho)\sum_{l \neq j} \underline{e_l}}{\|\underline{e_j} + (1-\rho)\sum_{l\neq j} \underline{e_l}\|}\right)$.

Case 3: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ true. If $x_i = x_i' = v_{i,j}$, we have

$$d_{\mathrm{E}}^{m_i}(f_i^{\mathrm{c}}(\underline{x}), f_i^{\mathrm{c}}(\underline{x}')) \quad = \quad d_{\mathrm{E}}^{m_i}\big(f_i^{\mathrm{c}}(\underline{x}), f_i^{\mathrm{c}}(\underline{x})\big) = 0 = d_i^{\mathrm{c}}(\underline{x}, \underline{x}').$$

If $x_i = v_{i,j} \neq v_{i,j'} = x_i'$, we have

$$\begin{aligned}
d_{\mathrm{E}}(f_i^{\mathrm{c}}(\underline{x}), f_i^{\mathrm{c}}(\underline{x}')) &= d_{\mathrm{E}}^{m_i}\left(\omega_i \, \frac{\underline{e_j} + (1-\rho)\sum_{l\neq j} \underline{e_l}}{\sqrt{1 + (m_i - 1)(1-\rho)^2}}, \, \omega_i \, \frac{\underline{e_j}' + (1-\rho)\sum_{l\neq j'} \underline{e_l}}{\sqrt{1 + (m_i - 1)(1-\rho)^2}}\right) \\
&= \omega_i \frac{\sqrt{\big(1 - (1-\rho)\big)^2 + \big(1 - (1-\rho)\big)^2}}{1 + (m_i - 1)(1-\rho)^2} \\
&= \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1-\rho)^2} \\
&= d_i^{\mathrm{c}}(\underline{x}, \underline{x}').
\end{aligned} \tag{10}$$

□

4 Experiments

All the separate models split the data into 6 different datasets, one for each level, and build a separate model for each level. The gp-hierarchical model gets all the data together because it can handle it.

However, The gp-hierarchical model changes two things at once compared to the separate-gp-ard model: besides embedding the missing data in a different spot, it also has embeds the fully-observed data on semi-circles, and has a different parameterization. So, it could be the case that even when the data are fully observed, embedding the data on a semi-circle and using a different parameterization might cause better or worse performance than a standard squared-exp. To find out if this is the case, we compare separate-gp-ard and separate-hierarchical to find out if these two models have different performance even in the standard fully-observed case.

Table 1: Normalized Mean Squared Error

Method	NN	NN log	NN half	NN log half
Separate Linear	$\mathbf{0.968}$	0.886	$\mathbf{1.039}$	2.120
Separate GP	$\mathbf{0.925}$	0.641	$\mathbf{0.860}$	0.848
Poor Man's embedding Linear	$\mathbf{0.905}$	0.763	0.996	0.851
Poor Man's embedding GP	$\mathbf{0.907}$	0.518	$\mathbf{1.178}$	$\mathbf{0.752}$
Separate Hierarchical GP	$\mathbf{0.801}$	0.627	$\mathbf{0.956}$	0.950
Hierarchical GP	$\mathbf{0.801}$	$\mathbf{0.441}$	$\mathbf{0.993}$	$\mathbf{0.674}$

A Proof of pseudometric properties

Proposition 5. *d_i^{r} is a pseudometric on $\mathcal{X}$.*

Proof. The non-negativity and symmetry of d_i^{r} are trivially proven. To prove the triangle inequality, consider $\underline{x}, \underline{x}', \underline{x}'' \in \mathcal{X}$.

Case 1: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ false, such that $d_i^{\mathrm{r}}(\underline{x}, \underline{x}') = 0$. Here, from non-negativity, clearly $d_i^{\mathrm{r}}(\underline{x}, \underline{x}') = 0 \leq d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'')$.

Case 2: $\delta_i(\underline{x}) \neq \delta_i(\underline{x}')$, such that such that $d_i^{\mathrm{r}}(\underline{x}, \underline{x}') = \omega_i$. Without loss of generality, assume $\delta_i(\underline{x}) =$ true, $\delta_i(\underline{x}') =$ false and $\delta_i(\underline{x}'') =$ true.

$$d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'') = d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + \omega_i \tag{11}$$

Hence $d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'') \geq \omega_i = d_i^{\mathrm{r}}(\underline{x}, \underline{x}')$ by non-negativity.

Case 3: $\delta_i(\underline{x}) = \delta_i(\underline{x}') =$ true, such that $d_i^{\mathrm{r}}(\underline{x}, \underline{x}') = \omega_i \sqrt{2}\sqrt{1 - \cos(\pi \rho_i \frac{x_i - x_i'}{u_i - l_i})}$. If $\delta_i(\underline{x}'') =$ false,

$$d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'') = 2\omega_i \geq \omega_i \sqrt{2}\sqrt{1 - \cos(\pi \rho_i \frac{x_i - x_i'}{u_i - l_i})} = d_i^{\mathrm{r}}(\underline{x}, \underline{x}'). \tag{12}$$

If $\delta_i(\underline{x}'') = $ true, consider the 'worst' possible case in which, without loss of generality, $x_i = l_i$ and $x'_i = u_i$, such that $d_i^{\mathrm{r}}(\underline{x}, \underline{x}') = 2\omega_i^2$. We define the abbreviation $\beta'' = \frac{x''_i - l_i}{u_i - l_i}$, giving

$$
\begin{aligned}
\big(d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'')\big)^2 &= 2\omega_i^2 \Big(\sqrt{1 - \cos(\pi\rho_i\beta'')} + \sqrt{1 - \cos\big(\pi\rho_i(1 - \beta'')\big)}\Big)^2 \\
&= 2\omega_i^2 \bigg(2 - \cos(\pi\rho_i\beta'') - \cos\big(\pi\rho_i(1 - \beta'')\big) \\
&\qquad + 2\sqrt{\Big(1 - \cos(\pi\rho_i\beta'')\Big)\Big(1 - \cos\big(\pi\rho_i(1 - \beta'')\big)\Big)}\bigg) \\
&= 2\omega_i^2 \bigg(2 + 2\sqrt{1 + \cos(\pi\rho_i\beta'')\cos\big(\pi\rho_i(1 - \beta'')\big)}\bigg) \\
&= 4\omega_i^2 \big(1 + |\sin \pi\rho_i\beta''|\big) \\
&\geq 4\omega_i^2 = d_i^{\mathrm{r}}(\underline{x}, \underline{x}')^2.
\end{aligned} \tag{13}
$$

Hence, from non-negativity, we have $d_i^{\mathrm{r}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{r}}(\underline{x}', \underline{x}'') \geq d_i^{\mathrm{r}}(\underline{x}, \underline{x}')$. □

Proposition 6. *d_i^{c} is a pseudometric on $\mathcal{X}$.*

Proof. The non-negativity and symmetry of d_i^{c} are trivially proven. To prove the triangle inequality, consider $\underline{x}, \underline{x}', \underline{x}'' \in \mathcal{X}$.

Case 1: $\delta_i(\underline{x}) = \delta_i(\underline{x}') = $ false, such that $d_i^{\mathrm{c}}(\underline{x}, \underline{x}') = 0$. Here, from non-negativity, clearly $d_i^{\mathrm{c}}(\underline{x}, \underline{x}') = 0 \leq d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{c}}(\underline{x}', \underline{x}'')$.

Case 2: $\delta_i(\underline{x}) \neq \delta_i(\underline{x}')$, such that such that $d_i^{\mathrm{c}}(\underline{x}, \underline{x}') = \omega_i$. Without loss of generality, assume $\delta_i(\underline{x}) = $ true, $\delta_i(\underline{x}') = $ false and $\delta_i(\underline{x}'') = $ true.

$$
d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{c}}(\underline{x}', \underline{x}'') = d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + \omega_i \tag{14}
$$

Hence $d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{c}}(\underline{x}', \underline{x}'') \geq \omega_i = d_i^{\mathrm{c}}(\underline{x}, \underline{x}')$ by non-negativity.

Case 3: $\delta_i(\underline{x}) = \delta_i(\underline{x}') = $ true, such that $d_i^{\mathrm{c}}(\underline{x}, \underline{x}') = \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1 - \rho)^2} \mathbb{I}_{x_i \neq x'_i}$. If $\delta_i(\underline{x}'') = $ false,

$$
d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{c}}(\underline{x}', \underline{x}'') = 2\omega_i \geq \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1 - \rho)^2} \mathbb{I}_{x_i \neq x'_i} = d_i^{\mathrm{c}}(\underline{x}, \underline{x}'). \tag{15}
$$

If $\delta_i(\underline{x}'') = $ true,

$$
\begin{aligned}
d_i^{\mathrm{c}}(\underline{x}, \underline{x}'') + d_i^{\mathrm{c}}(\underline{x}', \underline{x}'') &= \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1 - \rho)^2} \big(\mathbb{I}_{x_i \neq x''_i} + \mathbb{I}_{x'_i \neq x''_i}\big) \\
&\geq \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1 - \rho)^2} \mathbb{I}_{x_i \neq x'_i} = d_i^{\mathrm{c}}(\underline{x}, \underline{x}').
\end{aligned} \tag{16}
$$

□

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References

[1] C.E. Rasmussen and CKI Williams. Gaussian Processes for Machine Learning. *The MIT Press, Cambridge, MA, USA*, 2006.