
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 $\{v_{i,1}, \dots, v_{i,m_i}\}$.

Associated with \mathcal{X} , there is a DAG structure \mathcal{D} , whose vertices are the dimensions $\{1, \dots, D\}$. \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 $\delta_i: \mathcal{X} \rightarrow \mathcal{B}$, for $i \in \{1, \dots, D\}$, and where $\mathcal{B} = \{\text{true}, \text{false}\}$. We take

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

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

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

product,

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

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 $\delta_i(\underline{x})$,

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

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

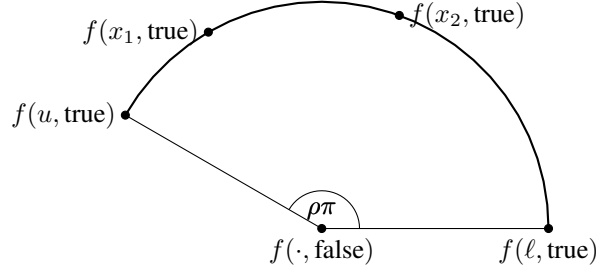


Figure 1: A demonstration of the embedding giving rise to the pseudo-metric: All points for which $\delta_i(x) = \text{false}$ are mapped to the same point. Points for which $\delta_i(x) = \text{true}$ are mapped to a semicircle. This embedding gives a constant distance between pairs of points which 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

$$d_i(\underline{x}, \underline{x}') = d_E(f_i(\underline{x}), f_i(\underline{x}')) \quad (5)$$

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 $\kappa: \mathbb{R}^+ \rightarrow \mathbb{R}$ is a positive semi-definite covariance function over Euclidean space if $K \in \mathbb{R}^{N \times N}$, defined by

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

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, $k_i: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$, defined by

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

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

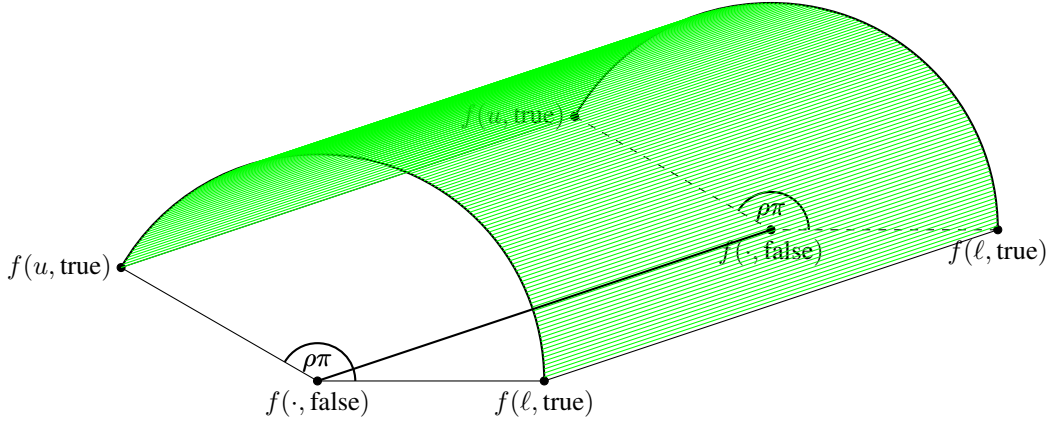
$$K_{m,n} = \kappa(d_i(\underline{x}_m, \underline{x}_n)), \quad \text{for } \underline{x}_m, \underline{x}_n \in \mathcal{X}, \quad m, n = 1, \dots, N,$$

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

$$K_{m,n} = \kappa(d_E(f_i(\underline{x}_m), f_i(\underline{x}_n))) = \kappa(d_E(\underline{y}_m, \underline{y}_n))$$

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. \square

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_E as f_i^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} .

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

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

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

$$\omega_i = \prod_{j \in \text{anc}_i \cup \{i\}} \gamma_j, \quad (6)$$

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^r can be plugged into a positive semi-definite kernel over Euclidean space to define a valid kernel over space \mathcal{X} .

¹Note 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, $k_i: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$, defined by

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

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 $d_E(f_i^r(\underline{x}), f_i^r(\underline{x}')) = d_i^r(\underline{x}, \underline{x}')$ 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: $\delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{false}$. In this case, we trivially have

$$d_E(f_i^r(\underline{x}), f_i^r(\underline{x}')) = d_E([0, 0]^\top, [0, 0]^\top) = 0 = d_i^r(\underline{x}, \underline{x}').$$

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

$$d_E(f_i^r(\underline{x}), f_i^r(\underline{x}')) = d_E([\sin \alpha, \cos \alpha]^\top, [0, 0]^\top) = \sqrt{\omega_i^2 (\sin^2 \alpha + \cos^2 \alpha)} = \omega_i = d_i^r(\underline{x}, \underline{x}'),$$

and symmetrically for $d_E([0, 0]^\top, [\sin \alpha, \cos \alpha]^\top)$.

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

$$\begin{aligned} d_E(f_i^r(\underline{x}), f_i^r(\underline{x}')) &= d_E(\omega_i [\sin \alpha, \cos \alpha]^\top, \omega_i [\sin \alpha', \cos \alpha']^\top) \\ &= \omega_i \sqrt{(\sin \alpha - \sin \alpha')^2 + (\cos \alpha - \cos \alpha')^2} \\ &= \omega_i \sqrt{\sin^2 \alpha - 2 \sin \alpha \sin \alpha' + \sin^2 \alpha' + \cos^2 \alpha - 2 \cos \alpha \cos \alpha' + \cos^2 \alpha'} \\ &= \omega_i \sqrt{(\sin^2 \alpha + \cos^2 \alpha) + (\sin^2 \alpha' + \cos^2 \alpha') - 2(\sin \alpha \sin \alpha' + \cos \alpha \cos \alpha')} \\ &= \omega_i \sqrt{1 + 1 - 2 \cos(\alpha - \alpha')} \\ &= \omega_i \sqrt{2} \sqrt{1 - \cos(\pi \rho_i \frac{x_i - x'_i}{u_i - l_i})} = d_i^r(\underline{x}, \underline{x}'), \end{aligned} \tag{7}$$

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 $\mathcal{X}_i = \{v_{i,1}, \dots, v_{i,m_i}\}$ 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^c) to $(\mathbb{R}^{m_i}, d_E^{m_i})$, and show that we can combine these with a kernel over Euclidean space to construct a valid kernel over space \mathcal{X} .

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

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

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

$$\sqrt{1 + (m_i - 1)(1 - \rho)^2} = \left\| \underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l \right\|. \quad (8)$$

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

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

$\rho_i < \rho_i^*$ 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, $k_i: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$, defined by*

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

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 $d_E^{m_i}(f_i^c(\underline{x}), f_i^c(\underline{x}')) = d_i^c(\underline{x}, \underline{x}')$ holds.

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

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

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

$$d_E^{m_i}(f_i^c(\underline{x}), f_i^c(\underline{x}')) = d_E^{m_i}\left(\omega_i \frac{\underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l}{\|\underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l\|}, \underline{0}\right) = \omega_i = d_i(\underline{x}, \underline{x}'),$$

and symmetrically for $d_E\left(\underline{0}, \omega_i \frac{\underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l}{\|\underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l\|}\right)$.

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

$$d_E^{m_i}(f_i^c(\underline{x}), f_i^c(\underline{x}')) = d_E^{m_i}(f_i^c(\underline{x}), f_i^c(\underline{x})) = 0 = d_i^c(\underline{x}, \underline{x}').$$

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

$$\begin{aligned} d_E(f_i^c(\underline{x}), f_i^c(\underline{x}')) &= d_E^{m_i}\left(\omega_i \frac{\underline{e}_j + (1 - \rho) \sum_{l \neq j} \underline{e}_l}{\sqrt{1 + (m_i - 1)(1 - \rho)^2}}, \omega_i \frac{\underline{e}_{j'} + (1 - \rho) \sum_{l \neq j'} \underline{e}_l}{\sqrt{1 + (m_i - 1)(1 - \rho)^2}}\right) \\ &= \omega_i \frac{\sqrt{(1 - (1 - \rho))^2 + (1 - (1 - \rho))^2}}{1 + (m_i - 1)(1 - \rho)^2} \\ &= \omega_i \frac{\sqrt{2}\rho}{1 + (m_i - 1)(1 - \rho)^2} \\ &= d_i^c(\underline{x}, \underline{x}'). \end{aligned} \quad (10)$$

□

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 nan	NN nan log	NN nan half	NN nan log half
Separate Linear	0.997	0.881	1.074	2.200
Separate GP	0.917	0.632	0.876	0.877
Poor Man's embedding Linear	0.947	0.740	1.054	0.814
Poor Man's embedding GP	0.934	0.512	1.221	0.747
Separate Hierarchical GP	0.812	0.617	1.004	0.988
Hierarchical GP	0.820	0.429	1.041	0.688

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

\square

[1]

References

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