A Kernel for Hierarchical Parameter Spaces

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Abstract

We define kernels for mixed continuous/discrete spaces and conditional spaces and show that they are positive definite.

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 whether 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 $\delta_i \colon \mathcal{X} \mapsto \mathcal{B}$, 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 g, *i.e.*, a positive semi-definite function $k \colon \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$. We will first specify an individual kernel for each input dimension, *i.e.*, a positive semi-definite function $k_i \colon \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$. 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 will depend on an input vector $\underline{x}$ only through dependence on both 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 $d_i \colon \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}^+$: that is, d_i satisfies the requirements of a metric aside from the identity of indiscernibles. As for k_i, these pseudometrics will depend 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 the following Proposition.

Define $\kappa \colon \mathbb{R}^+ \to \mathbb{R}$ as a semi-positive definite function over Euclidean space. By the latter, we mean that $K \in \mathbb{R}^{N\times N}$, defined by

$$K_{m,n} = \kappa\big(d_{\mathrm{E}}(\underline{y}_m, \underline{y}_n)\big), \quad \text{for } \underline{y}_m, \underline{y}_n \in \mathbb{R}^P, \quad m, n = 1, \ldots, N, \tag{6}$$

is positive semi-definite. 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 1. $\kappa\big(d_i(\cdot,\cdot)\big)$ *is a positive semi-definite covariance function over input space* $\mathcal{X}$.

Proof. We require that $K \in \mathbb{R}^{N\times N}$ defined by

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

is positive semi-definite. Now, from above,

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

where $\underline{y}_m = f_i(\underline{x}_m)$ and similar for $\underline{x}_m$. Then, by assumption that κ is a positive semi-definite 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.

1 Bounded Real Dimensions

Let's first define f_i^{br} and d_i^{br} for the case that the input $\mathcal{X}_i = [L_i, U_i]$ is bounded real. We first define a 'difference' function d_i^{br} on $\mathcal{X}$,

$$d_i^{\text{br}}(\underline{x}, \underline{x}') = \begin{cases} 0 & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{false} \\ w_i & \text{if } \delta_i(\underline{x}) \neq \delta_i(\underline{x}') \\ w_i\sqrt{2}\sqrt{1-\cos(\pi\frac{x_i - x_i'}{U_i - L_i})} & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{true}. \end{cases}$$

As desired, if i is inactive for both $\underline{x}$ and $\underline{x}'$, d_i^{br} specifies that $g(\underline{x})$ and $g(\underline{x}')$ should not differ owing to differences between x_i and x_i'. 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 x_i and x_i'. 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 $|x_i - x_i'|$.

Proposition 2. *d_i^{br} is a pseudometric on $\mathcal{X}$.*

Proof. The non-negativity and symmetry of d_i^{br} 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 $d_i^{\text{br}}(\underline{x}, \underline{x}') = 0$. Here, from non-negativity, clearly $d_i^{\text{br}}(\underline{x}, \underline{x}') = 0 \leq d_i^{\text{br}}(\underline{x}, \underline{x}'') + d_i^{\text{br}}(\underline{x}', \underline{x}'')$.

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

$$d_i^{\text{br}}(\underline{x}, \underline{x}'') + d_i^{\text{br}}(\underline{x}', \underline{x}'') = d_i^{\text{br}}(\underline{x}, \underline{x}'') + w_i \tag{7}$$

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

Case 3: $\delta_i(\underline{x}) = \delta_i(\underline{x}') = $ true, such that $d_i^{\text{br}}(\underline{x}, \underline{x}') = w_i\sqrt{2}\sqrt{1-\cos(\pi\frac{x_i - x_i'}{U_i - L_i})}$. If $\delta_i(\underline{x}'') = $ false,

$$d_i^{\text{br}}(\underline{x}, \underline{x}'') + d_i^{\text{br}}(\underline{x}', \underline{x}'') = 2w_i \geq w_i\sqrt{2}\sqrt{1-\cos(\pi\frac{x_i - x_i'}{U_i - L_i})} = d_i^{\text{br}}(\underline{x}, \underline{x}'). \tag{8}$$

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 $d_i^{\text{br}}(\underline{x}, \underline{x}') = 2w_i^2$. We define the abbreviation $\beta'' = \frac{x_i'' - L_i}{U_i - L_i}$, giving

$$\begin{aligned}
\left(d_i^{\text{br}}(\underline{x}, \underline{x}'') + d_i^{\text{br}}(\underline{x}', \underline{x}'')\right)^2 &= 2w_i^2\Big(\sqrt{1-\cos(\pi\beta'')} + \sqrt{1-\cos\big(\pi(1-\beta'')\big)}\Big)^2 \\
&= 2w_i^2\Bigg(2 - \cos(\pi\beta'') - \cos\big(\pi(1-\beta'')\big) \\
&\qquad + 2\sqrt{\Big(1-\cos(\pi\beta'')\Big)\Big(1-\cos\big(\pi(1-\beta'')\big)\Big)}\Bigg) \\
&= 2w_i^2\Big(2 + 2\sqrt{1+\cos(\pi\beta'')\cos\big(\pi(1-\beta'')\big)}\Big) \\
&= 4w_i^2\big(1 + |\sin\pi\beta''|\big) \\
&\geq 4w_i^2 = d_i^{\text{br}}(\underline{x}, \underline{x}')^2.
\end{aligned} \tag{9}$$

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

Now we define an isometric embedding f_i^{br} of $(\mathcal{X}, d_i^{\text{br}})$ into $(\mathbb{R}^2, d_{\text{E}})$:

$$f_i^{\text{br}}(\underline{x}) \quad = \quad \begin{cases} [0,0]^\intercal & \text{if } \delta_i(\underline{x}) = \text{ false} \\ w_i[\sin \pi \frac{x_i}{U_i - L_i}, \cos \pi \frac{x_i}{U_i - L_i}]^\intercal & \text{otherwise.} \end{cases} .$$

Proposition 3. *f_i^{br} is an isometry from $(\mathcal{X}, d_i^{\text{br}})$ to $(\mathbb{R}^2, d_{\text{E}})$.*

Proof. Consider two inputs $\underline{x}, \underline{x}' \in \mathcal{X}$. We need to show that $d_i^{\text{br}}(\underline{x}, \underline{x}') = d_{\text{E}}\big(f_i^{\text{br}}(\underline{x}), f_i^{\text{br}}(\underline{x}')\big)$. We use the abbreviation $\alpha = \pi \frac{x_i}{U_i - L_i}$ and $\alpha' = \pi \frac{x_i'}{U_i - L_i}$ 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

$$d_{\text{E}}(f_i^{\text{br}}(\underline{x}), f_i^{\text{br}}(\underline{x}')) = d_{\text{E}}([0,0]^\intercal, [0,0]^\intercal) = 0 = d_i^{\text{br}}(\underline{x}, \underline{x}').$$

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

$$d_{\text{E}}(f_i^{\text{br}}(\underline{x}), f_i^{\text{br}}(\underline{x}')) = d_{\text{E}}([\sin\alpha, \cos\alpha]^\intercal, [0,0]^\intercal) = \sqrt{w_i^2(\sin^2\alpha + \cos^2\alpha)} = w_i = d_i^{\text{br}}(\underline{x}, \underline{x}'),$$

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

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

$$\begin{aligned} d_{\text{E}}(f_i^{\text{br}}(\underline{x}), f_i^{\text{br}}(\underline{x}')) &= d_{\text{E}}(w_i[\sin\alpha, \cos\alpha]^\intercal, w_i[\sin\alpha', \cos\alpha']^\intercal) \\ &= w_i\sqrt{(\sin\alpha - \sin\alpha')^2 + (\cos\alpha - \cos\alpha')^2} \\ &= w_i\sqrt{\sin^2\alpha - 2\sin\alpha\sin\alpha' + \sin^2\alpha' + \cos^2\alpha - 2\cos\alpha\cos\alpha' + \cos^2\alpha'} \\ &= w_i\sqrt{(\sin^2\alpha + \cos^2\alpha) + (\sin^2\alpha' + \cos^2\alpha') - 2(\sin\alpha\sin\alpha' + \cos\alpha\cos\alpha')} \\ &= w_i\sqrt{1 + 1 - 2\cos(\alpha - \alpha')} \\ &= w_i\sqrt{2}\sqrt{1 - \cos(\pi\frac{x_i - x_i'}{U_i - L_i})} = d_i^{\text{br}}(\underline{x}, \underline{x}'), \end{aligned} \tag{10}$$

where (10) follows from the previous line by using the identity

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

$\square$

2 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 $(\mathcal{X}, d_i^{\text{c}})$ to $(\mathbb{R}^{m_i}, d_{\text{E}}^{m_i})$.

Firstly,

$$d_i^{\text{c}}(\underline{x}, \underline{x}') \quad = \quad \begin{cases} 0 & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{false} \\ w_i & \text{if } \delta_i(\underline{x}) \neq \delta_i(\underline{x}') \\ w_i\sqrt{2}\mathbb{I}_{x_i \neq x_i'} & \text{if } \delta_i(\underline{x}) = \delta_i(\underline{x}') = \text{true.} \end{cases}$$

Proposition 4. *d_i^{c} is a pseudometric on $\mathcal{X}$.*

Proof. A trivial modification of the proof to Proposition 2. □

Secondly,

$$f_i^{\text{c}}(\underline{x}) \quad = \quad \begin{cases} \underline{0} \in \mathbb{R}^{m_i} & \text{if } \delta_i(\underline{x}) = \text{ false} \\ w_i\, \underline{e_j} & \delta_i(\underline{x}) = \text{ true and } x_i = v_{i,j}, \end{cases}$$

where $\underline{e_j} \in \mathbb{R}^{m_i}$ is zero in all dimensions except j, where it it 1.

Proposition 5. *Embedding f_i^{c} is an isometric embedding of $(\mathcal{X}, d_i^{\text{c}})$ into $(\mathbb{R}^{m_i}, d_E^{m_i})$.*

Proof. Consider two inputs $\underline{x}, \underline{x}' \in \mathcal{X}$. As in the proof of Proposition 3, we need to show that $d_i^{\text{c}}(\underline{x}, \underline{x}') = d_{\text{E}}^{m_i}(f_i^{\text{c}}(\underline{x}), f_i^{\text{c}}(\underline{x}'))$ and consider the following cases.

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

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

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

$$d_{\text{E}}^{m_i}(f_i^{\text{c}}(\underline{x}), f_i^{\text{c}}(\underline{x}')) = d_{\text{E}}^{m_i}(w_i\, \underline{e_j}, \underline{0}) = w_i = d_i(\underline{x}, \underline{x}'),$$

and symmetrically for $d_{\text{E}}(\underline{0}, w_i\, \underline{e_j})$.

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

$$d_{\text{E}}^{m_i}(f_i^{\text{c}}(\underline{x}), f_i^{\text{c}}(\underline{x}')) \quad = \quad d_{\text{E}}^{m_i}(w_i\, \underline{e_j}, w_i\, \underline{e_j}) = 0 = d_i^{\text{c}}(\underline{x}, \underline{x}')$$

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

$$d_{\text{E}}(f_i^{\text{c}}(\underline{x}), f_i^{\text{c}}(\underline{x}')) \quad = \quad d_{\text{E}}^{m_i}(w_i\, \underline{e_j}, w_i \underline{e_{j'}}) = w_i\sqrt{2} = d_i^{\text{c}}(\underline{x}, \underline{x}')$$

□