Group kernels for Gaussian process metamodels with categorical inputs

O. Roustant$^a,b$

Joint work with E. Padonou$^b$, Y. Deville$^c$, A. Clément$^d$, G. Perrin$^d$, J. Giorla$^d$ and H. Wynn$^e$

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$^d$ CEA – $^e$ London School of Economics

Updated slide show, following talks in the OQUAIDO Chair (funding the project), Isaac Newton Institute (Cambridge, UK), IMT Toulouse and Univ. of Montpellier. Thanks to all the participants for their feedback!
Outline

1. Context and motivation
2. Background on GPs with categorical inputs
3. Group covariance functions
4. Examples and application
5. Conclusion and perspectives
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1. Context and motivation
2. Background on GPs with categorical inputs
3. Group covariance functions
4. Examples and application
5. Conclusion and perspectives
Chair in Applied Mathematics OQUAIDO (2016 - 2020)

- **Domain**: Computer experiments
- **Position**: Upstream research guided by case-studies

- 6 technological research partners from:
  - Energy: CEA, IFPEN, IRSN, Storengy
  - Transport: Safran
  - Natural risks: BRGM

- 5 academics:
  - EMSE, EC Lyon, Univ. of Grenoble, Nice, Toulouse

- 3 experts: J. Garnier (Ecole Polytechnique), D. Ginsbourger (Idiap), Y. Deville (AlpeStat)

- **Chair life**: PhD supervision, training sessions (maths, software), research invitations (J. Hensmann, T. Santner, H. Wynn), ...
Metamodelling – Computer experiments

\[ \text{design} \]
Metamodelling – Computer experiments
Metamodelling – Computer experiments

- **Design** → **Experiment + Measurements** → **Meas. Output**

- **Simulator Inputs**: $x^1, x^2, \ldots, x^n$

- **Simulator**
  - Physical model, numerical methods

- **Simulator Output**: $f_{\text{sim}}(x^1), f_{\text{sim}}(x^2), \ldots, f_{\text{sim}}(x^n)$

- **Metamodel Inputs**: $x^1, x^2, \ldots, x^n$

- **Metamodel Output**: $y = g(x^T \beta + z(x))$
Context and motivation

Metamodeling – Computer experiments

- **design** → **experiment + measurements** → **meas. output**
- **simulator inputs** \( x^1, x^2, \ldots, x^n \) → **simulator**
  - **physical model, numerical methods**
  - **simulator output** \( f_{\text{sim}}(x^1), f_{\text{sim}}(x^2), \ldots, f_{\text{sim}}(x^n) \)
- **metamodel inputs** \( x^1, x^2, \ldots, x^n \) → **metamodel**
  - **metamodel** \( y = g(x)^T \beta + Z(x) \)
  - **metamodel output** \( \hat{y}(x), \ldots \)
Metamodelling – Computer experiments

design → experiment + measurements → meas. output

simulator inputs
\( x^1, x^2, \ldots, x^n \)

simulator
physical model, numerical methods

simulator output
\( f_{\text{sim}}(x^1), f_{\text{sim}}(x^2), \ldots, f_{\text{sim}}(x^n) \)

param.

design

metamodel inputs
\( x^1, x^2, \ldots, x^n \)

metamodelling
\[ y = g(x)^T \beta + Z(x) \]

metamodel output
\( \tilde{y}(x), \ldots \)
Metamodelling with Gaussian processes (GP)

Interpolation of a 1-dimensional function in the context of small data...

Thanks to N. Durrande for the slide!
Metamodelling with Gaussian processes (GP)

Interpolation with GPs: conditional mean and prevision intervals
Gaussian processes

Gaussian processes are stochastic processes (or random fields) s.t. every finite dimensional distribution is Gaussian. \( \rightarrow \) Parameterized by two functions

\[ Z_x \sim GP(m(x), k(x, x')) \]

- The trend can be any function.
- The kernel is positive semidefinite:

\[ \forall n, \alpha_1, \ldots, \alpha_n, x^{(1)}, \ldots, x^{(n)}, \quad \sum_{i=1}^{n} \alpha_i \alpha_j k(x^{(i)}, x^{(j)}) \geq 0. \]

It contains the spatial dependence.
Playing with kernels

A lot of flexibility can be obtained with kernels!

<table>
<thead>
<tr>
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<td>$k(x, x') = k_1(f(x), f(x'))$</td>
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Example : $k_1(x, x'; \sigma^2, \ell) = \sigma^2 \exp \left(-\frac{(x-x')^2}{\ell^2}\right)$

$\rightarrow k_d(x, x') = \sigma^2 \prod_{j=1}^d k_1(x_j, x'_j; 1, \ell_j) = \sigma^2 \exp \left(-\sum_{j=1}^d \frac{(x_j-x'_j)^2}{\ell_j^2}\right)$

See other examples in *Rasmussen and Williams (2006)*... and in this talk!
A guiding case-study in nuclear engineering

A particle transport simulator MCNP (Clément, 2016)

1. Computation using Monte Carlo
2. 4 continuous inputs: \( L \), density, mean width, lateral surface
3. 3 categorical inputs: energy, form, chemical element.

Specific problem: a categorical input with a large number of levels

(a) Form (3 levels)
(b) Atomic number: 94 levels!
(c) Energy (6 levels)
A guiding case-study in nuclear engineering

A 2-stage approach

1. GP metamodeling of the computer code
   ▶ This talk!
   ▶ A challenge is the large number of levels (> 90) of one categorical input
   ▶ More details on the preprint, to appear in SIAM/ASA Journal on Uncertainty Quantification

2. Metamodell-based inversion
   ▶ See Clement et al. (2018) on a similar application (continuous inputs)
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**GP interpretation when no distance is available**

A GP for \((x, u) \in [0, 1] \times \{"red", "yellow", "blue"\}\) can be defined with:

- a kernel on \([0, 1]\), i.e. a covariance function
- a kernel on \(\{"red", "yellow", "blue"\}\), i.e. a covariance matrix
- a valid operation between them, such as *, +, ...

Example: \[\text{Cov}(Y(x, "blue"), Y(x', "red")) = k(x, x') \times 0.8\]
A formulation - Combination of 1-dimensional kernels

What is a kernel for $u_j$ on $\{1, \ldots, m_j\}$?

A positive semidefinite matrix $T_j$ of size $m_j$
A formulation - Combination of 1-dimensional kernels

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**Combining 1D kernels for** $w = (x, u)$

Examples of valid operations:

- **(Product)** $k(w, w') = k_{\text{cont}}(x, x')k_{\text{cat}}(u, u')$
- **(Sum)** $k(w, w') = k_{\text{cont}}(x, x') + k_{\text{cat}}(u, u')$
- **(ANOVA)** $k(w, w') = (1 + k_{\text{cont}}(x, x'))(1 + k_{\text{cat}}(u, u'))$
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(ANOVA) \[ k(w, w') = (1 + k_{\text{cont}}(x, x'))(1 + k_{\text{cat}}(u, u')) \]

Notice $\ast$ one of them. Examples of valid kernels for $w$:

\[ k(w, w') = k_{\text{cont}}^1(x_1, x'_1) \ast \cdots \ast k_{\text{cont}}^l(x_l, x'_l) \ast [T_1]_{u_l, u'_l} \ast \cdots \ast [T_J]_{u_J, u'_J} \]
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Combining 1D kernels for $w = (x, u)$

Examples of valid operations:

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Notice $\star$ one of them. Examples of valid kernels for $w$:

$$k(w, w') = k_{\text{cont}}^1(x_1, x'_1) \star \cdots \star k_{\text{cont}}^I(x_I, x'_I) \star [T_1]_{u_1, u'_1} \star \cdots \star [T_J]_{u_J, u'_J}$$

Not the most general way, but recovers the usual models of the literature.

→ Alternatives: Use a $d$-dim. continuous kernel, use $\star_i, \star_j$, and so on...
Kernels for ordinal variables

Warping

- When the levels of $u$ are ordered: $1 \leq 2 \leq \cdots \leq L$, define:

$$[T]_{\ell, \ell'} = k_c(F(\ell), F(\ell')),$$  \quad $\ell, \ell' = 1, \ldots, L.$

where $k_c(x, x')$ is a continuous kernel, and $F$ is $\uparrow$.

It is the covariance kernel of $Y_{F(\ell)}$ if $Y \sim GP(0, k_c)$.

**Figure** – An example of warping as a spline of degree 2, now available on kergp.
Kernels for nominal variables

- **General**
  - Spectral param. $T = PDP^T$
  - Spherical param. $T = LL^T$

- **Compound symmetry** $[T]_{\ell, \ell'} = \begin{cases} v & \text{if } \ell = \ell' \\ c & \text{if } \ell \neq \ell' \end{cases}$

- **Group kernels**, such as $[T]_{\ell, \ell'} = \begin{cases} v_g & \text{if } \ell = \ell' \\ c_{g(\ell), g(\ell')} & \text{if } \ell \neq \ell' \end{cases}$

- **Low “rank” approaches** (Rapisarda et al. (2007), Zhang et al. (+2020))

- **Low-rank** $T = UU^T$, with $U : L \times q$
- **Latent-variable** $[T]_{\ell, \ell'} = k_c(F(\ell), F(\ell'))$, with $F : \{1, \ldots, L\} \rightarrow \mathbb{R}^q$
Details on low-rank approaches

Interpretation of latent variable kernels (Zhang et al. (+2020))

The underlying Gaussian process for a latent variable kernel is

\[ Z(u) = Y(F_1(u), \ldots, F_q(u)) \]

where \( F_1, \ldots, F_q \) are mapping from \( \{1, \ldots, L\} \rightarrow \mathbb{R} \), called “latent variables”.

- Example: \( u \) : type of lubricant, \( \phi_1 \) : viscosity, \( \phi_2 \) : boiling point, ...
- Only the values of the \( F_i \)'s at 1, \ldots, \( L \) are used: the kernel is parameterized by (a subset of) \( F_i(\ell), \ell = 1, \ldots, L, \ i = 1, \ldots, q \).
Background on GPs with categorical inputs

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Links with low-rank kernels

If \( k_c(x, x') = \langle x, x' \rangle \) the dot product on \( \mathbb{R}^q \), then the latent variable kernel is a low-rank kernel \( T = U U^\top \), with \( U_{\ell,i} = F_i(\ell) \), for \( \ell = 1, \ldots, L, \quad i = 1, \ldots, q \).

→ Latent variables kernels are extending low-rank kernels for general \( k_c \).
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Block covariance matrices

- Form considered, “Generalized compound symmetry” (GCS):

$$T = \begin{pmatrix}
W_1 & B_{1,2} & \cdots & B_{1,G} \\
B_{2,1} & W_2 & \cdots & \cdots \\
\vdots & \vdots & \ddots & \vdots \\
B_{G,1} & \cdots & B_{G,G-1} & W_G \\
\end{pmatrix}$$  \hspace{1cm} (1)

- $W_g$ within-group covariances, s.t. $W_g - \overline{W}_g \mathbf{J}_{ng,ng} \succeq 0$
- $B_{g,g'}$ between-group covariances, with $B_{g,g'} \equiv c_{g,g'}$

- Particular case: $W_g$ is compound symmetry (CS)

$$W_g = \begin{pmatrix}
V_g & c_g & \cdots & c_g \\
c_g & \ddots & \cdots & \cdots \\
\vdots & \vdots & \ddots & c_g \\
c_g & \cdots & c_g & V_g \\
\end{pmatrix}$$
Theorem 1

For all GCS block matrices $T$,

$$T \succeq 0 \iff \tilde{T} \succeq 0$$

where $\tilde{T}$ is a $G \times G$ matrix obtained by averaging each block.
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where \( \tilde{T} \) is a \( G \times G \) matrix obtained by averaging each block.

Sketch of proof

\( \implies \) If \( T = \text{Cov}(y) \), then \( \tilde{T} = \text{Cov}(\bar{y}_1, \ldots, \bar{y}_G) \).
Positive definiteness condition - Algebraic point of view

**Theorem 1**

For all GCS block matrices $\mathbf{T}$,

$$
\mathbf{T} \succeq 0 \iff \widetilde{\mathbf{T}} \succeq 0
$$

where $\widetilde{\mathbf{T}}$ is a $G \times G$ matrix obtained by averaging each block.

**Sketch of proof**

$\Rightarrow$ If $\mathbf{T} = \text{Cov}(\mathbf{y})$, then $\widetilde{\mathbf{T}} = \text{Cov}(\overline{y_1}, \ldots, \overline{y_G})$.

$\Leftarrow$

$$
\begin{pmatrix}
W_1 & (c_{g,g'}) \\
& \vdots \\
(c_{g',g}) & W_G
\end{pmatrix}
= \begin{pmatrix}
\overline{W_1} & (c_{g,g'}) \\
& \vdots \\
(c_{g',g}) & \overline{W_G}
\end{pmatrix}
+ \begin{pmatrix}
W_1 - \overline{W_1} & (0) \\
& \vdots \\
(0) & W_G - \overline{W_G}
\end{pmatrix}
$$
Positive definiteness condition - Algebraic point of view

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Positive definiteness condition - Probabilistic point of view

A hierarchical Gaussian model

\[ \eta_{g/\ell} = \mu_g + \lambda_{g/\ell}, \quad g = 1, \ldots, G, \quad \ell \in \mathcal{G}_g \]

with:

1. \( \mu \sim \mathcal{N}(0, \mathbf{B}^*) \) with \( \mathbf{B}^* \) invertible, \( \lambda_{g/\cdot} \sim \mathcal{N}(0, \mathbf{W}_g^*) \), with \( \mathbf{W}_g^* \) invertible.
2. \( \lambda_{1/\cdot}, \ldots, \lambda_{G/\cdot}, \mu \) are independent.

→ response part of a nested two-way ANOVA model, with Gaussian ind. priors.
Positive definiteness condition - Probabilistic point of view

A hierarchical Gaussian model

\[ \eta_{g/\ell} = \mu_g + \lambda_{g/\ell}, \quad g = 1, \ldots, G, \quad \ell \in \mathcal{G}_g \]

with:
- \( \mu \sim \mathcal{N}(0, B^*) \) with \( B^* \) invertible, \( \lambda_{g/\ell} \sim \mathcal{N}(0, W_g^*) \), with \( W_g^* \) invertible.
- \( \lambda_1/., \ldots, \lambda_G/., \mu \) are independent.

→ response part of a nested two-way ANOVA model, with Gaussian ind. priors.

Theorem 2 - Representations of GCS block covariance matrices

\[ T \succeq 0 \iff T = \text{Cov}(\eta|\lambda_1/., = \cdots = \lambda_G/., = 0) \]

with

\[ W_g = B^*_{g,g} J_{n_g} + W_g^* \]
\[ B_{g,g'} = B^*_{g,g'} J_{n_g,n_g'} \]

where \( W_g^* = \text{Cov}(\lambda_{g/.|\lambda_{g/.,} = 0}) \) are centered.
Remarks - CS covariance matrices and negative correlations

- For $G = 1$ this gives a representation of valid CS covariance matrices, including the range of negative correlations.

Ex for $d = 2$, assume $\lambda_1, \lambda_2$ i.i.d $\mathcal{N}(0, \nu_\lambda)$, so that we have two parameters $\nu_\mu, \nu_\lambda$, which is the correct number of parameters for CS cov.mat. Compare with / without condition $\lambda_1 + \lambda_2 = 0$,

$$\eta_1 = \mu + \lambda_1$$
$$\eta_2 = \mu + \lambda_2$$
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- Limitation for groups with strong negative correlation

**Proposition (Exclusion property)**

If $W_g$ is a cov. mat. with minimal negative correlation, i.e. $\overline{W}_g = 0$, then $y_g \perp \! \! \! \perp y_{-g}$. 
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\begin{align*}
\eta_1 &= \mu + \lambda_1 \\
\eta_2 &= \mu + \lambda_2
\end{align*}
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Proposition (Exclusion property)

If $W_g$ is a cov. mat. with minimal negative correlation, i.e. $\overline{W_g} = 0$, then $y_g \perp \! \! \! \perp y_{-g}$.

Sketch of proof

If $\overline{W_g} = 0$, then $\overline{T_{g,g}} = 0$.

Since $\overline{T}$ is p.s.d., we must have $0 = \overline{T_{g,g'}} = c_{g,g'}$ for all $g' \neq g$. 
Remarks - Centered covariance matrices

Centered matrices $W^*_g$ can be parameterized.

Let $A$ be a $L \times (L - 1)$ matrix whose columns form an orthonormal basis of $\mathbf{1}_L^\perp$. A centered matrix $W^*$ is written in an unique way

$$W^* = AMA^\top$$

where $M$ is a covariance matrix of size $L - 1$.

As an example, $A$ can be obtained by normalizing the columns of a Helmert contrast matrix (Venables and Ripley (2002), §6.2.):

$$
\begin{bmatrix}
-1 & -1 & -1 & \cdots & -1 \\
1 & -1 & -1 & \cdots & -1 \\
0 & 2 & -1 & \cdots & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & 3 & \cdots & -1 \\
0 & \cdots & \cdots & \cdots & L - 1
\end{bmatrix}
$$
**Parameterization of block covariance matrices**

<table>
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<tr>
<th>Form of $T$</th>
<th>Parametric setting</th>
<th>Number of parameters</th>
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<tr>
<td>$W_g$</td>
<td>$B_{g,g'}$</td>
<td></td>
</tr>
<tr>
<td>CS</td>
<td>$c_{g,g'} \equiv c$</td>
<td>$\propto I_{n_g-1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\propto I_{n_g-1}$</td>
</tr>
<tr>
<td>General</td>
<td>$c_{g,g'} \equiv c$</td>
<td>General</td>
</tr>
<tr>
<td>General</td>
<td>$c_{g,g'}$</td>
<td>General</td>
</tr>
</tbody>
</table>

Reminder:

$$W_g = B_{g,g}'^* J_{n_g} + A_g M_g A_g^T$$

$$B_{g,g'} = B_{g,g'}^* J_{n_g,n_g'}$$
Group selection for group kernels

- Form considered:

\[ T = \begin{pmatrix}
W_1 & (c_{1,2}) & \cdots & (c_{1,G}) \\
(c_{1,2}) & W_2 & \ddots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
(c_{1,G}) & \cdots & (c_{G-1,G}) & W_G
\end{pmatrix} \]

- Constant between-group covariances
- Within-group covariances, s.t. \( W_g - W_g J_{n_g, n_g} \succeq 0 \)

- Particular case: \( W_g \) is exchangeable, i.e. \( W_g = \begin{pmatrix}
v_g & c_g & \cdots & c_g \\
c_g & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & c_g \\
c_g & \cdots & c_g & v_g
\end{pmatrix} \)
Group selection for group kernels

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- Constant between-group covariances
- Within-group covariances, s.t. \( W_g - \overline{W_g} J_{n_g,n_g} \succeq 0 \)

- Particular case: \( W_g \) is exchangeable, i.e.

\[
W_g = \begin{pmatrix}
v_g & c_g & \cdots & c_g \\
c_g & \ddots & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
c_g & \cdots & c_g & v_g
\end{pmatrix}
\]

→ If groups are perfectly homogeneous (\( c_g = v_g \)), then \( T \) has rank \( \leq G \)
A first algorithm for group selection

A model-based algorithm

1. Estimate a first GP model for \((x, u)\) by replacing \(T\) by a proxy kernel \(T_{\text{prox}}\).
2. Apply a clustering algorithm on levels, using the \(L^2\) distance given by \(T_{\text{prox}}\):

\[
d(\ell, \ell')^2 = E([Z_u - Z_{u'}]^2) = T_{\text{prox}}(\ell, \ell) + T_{\text{prox}}(\ell', \ell') - 2 T_{\text{prox}}(\ell, \ell')
\]
**A first algorithm for group selection**

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\[
 d(\ell, \ell')^2 = E([Z_u - Z_{u'}]^2) \\
 = T_{\text{prox}}(\ell, \ell) + T_{\text{prox}}(\ell', \ell') - 2 T_{\text{prox}}(\ell, \ell')
\]

**Choice of \(T_{\text{prox}}\) and scope of applicability**

- *If there are few homogeneous groups*, a group kernel should be well approximated by a low rank kernel
  - Choose \(T_{\text{prox}}\) as a low-rank kernel (of rank \(\geq G\))
A first algorithm for group selection

A model-based algorithm

1. Estimate a first GP model for \((x, u)\) by replacing \(T\) by a proxy kernel \(T_{\text{prox}}\)
2. Apply a clustering algorithm on levels, using the \(L^2\) distance given by \(T_{\text{prox}}\)

\[
d(\ell, \ell')^2 = \mathbb{E}([Z_u - Z_{u'}]^2) = T_{\text{prox}}(\ell, \ell) + T_{\text{prox}}(\ell', \ell') - 2 T_{\text{prox}}(\ell, \ell')
\]

Choice of \(T_{\text{prox}}\) and scope of applicability

- If there are few homogeneous groups, a group kernel should be well approx. by a low rank kernel
  → Choose \(T_{\text{prox}}\) as a low-rank kernel (of rank \(\geq G\))

- If groups are homogeneous and levels are ordered, they should be visible as jumps in the warping function
  → Choose \(T_{\text{prox}}\) as a warped kernel (with degrees of freedom \(\geq G\))
Performance assessment of the group selection algorithm

Figure – Four simulations of a GP model $Z$ with tensor-product kernel $k(\mathbf{w}, \mathbf{w'}) = k_{\text{cont}}(x, x')k_{\text{cat}}(u, u')$. $k_{\text{cont}}$: Matérn kernel with lengthscale $\theta = 0.4$. $k_{\text{cat}}$: GCS group kernel (10 levels, 2 groups of same size). Within-group correlation : 0.8. Between-group correlation : $-0.5$. 

(a) Simulation 1
(b) Simulation 2
(c) Simulation 3
(d) Simulation 4
Performance assessment of the group selection algorithm

<table>
<thead>
<tr>
<th>$\rho_{\text{bet}}$</th>
<th>$-0.5$</th>
<th>$0$</th>
<th>$0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Misclassif. rate (95% conf. int)</td>
<td>[12%, 18%]</td>
<td>[18%, 25%]</td>
<td>[26%, 32%]</td>
</tr>
</tbody>
</table>

- For the example of previous slide ($\rho_{\text{bet}} = -0.5$), the misclassif. rate is $\approx 15\%$.
  \[\rightarrow\] All the 10 levels but 1 (or 2) are correctly classified
- Misclassification decreases when groups are less separated ($\rho_{\text{bet}} \uparrow$)
Outline

1. Context and motivation
2. Background on GPs with categorical inputs
3. Group covariance functions
4. Examples and application
5. Conclusion and perspectives
Examples and application

Results on a simple toy example

(a) The example (3 design points per level)

(b) $\hat{T}$ (median $Q^2$)

(c) $Q^2$. Nb. param.: groups = (4, 2, 4, 3, 12), ordinal = (4, 13, 4, 13), other = (26, 24)
A toy example

(d) 1 group
(e) 2 groups
(f) 5 groups (common between-group corr.)

(g) 5 groups (general)
(h) 13 groups
(i) Ordinal

Figure – Estimated correlation kernel $k_{\text{cat}}$, for a design with median $Q^2$. 
A second toy example, with negative within-group correlations

(a) 2 groups

(b) 3 groups
A guiding case-study in nuclear engineering

A particle transport simulator MCNP (Clément, 2016)

1. Computation using Monte Carlo
2. 4 continuous inputs: $L$, density, mean width, lateral surface
3. 3 categorical inputs: energy, form, chemical element.

Specific problem: a categorical input with a large number of levels

(c) Form (3 levels)  (d) Atomic number: 94 levels!  (e) Energy (6 levels)
## Settings

### Full dataset \((N = 5076)\)
- Simulator runs from a stratified sampling w.r.t. categorical inputs  
  \[\Rightarrow 3 \text{ points for each of the } 6 \times 3 \times 94 = 1692 \text{ combinations of levels}\]
- Latin hypercube of size \(N\) for the continuous inputs

### Design of experiments \((n = 282)\)
Obtained from the full dataset by stratified sampling w.r.t. 'chemical element'  
\[\Rightarrow 3 \text{ points for each of the 94 levels}\]

### Test set \((N - n)\)
Remaining data set
Exploratory analysis - Variables 'Energy' & 'Geometry shape'

Modelling choices:
- 'Energy': ordinal variable
- 'Geometry shape': levels seem approx. exchangeable → CS cov. matrix
Exploratory analysis – Variable 'Chemical Element' (94 levels)

Modelling choice:
- Make the variance depend on the group number
Examples and application

Exploratory analysis – Continuous variables

- Sphere
- Cylinder
- Parallelepiped

Group 1
Group 2
Group 3
Group 4
Group 5

O. Roustant et al. (EMSE) Group kernels for GP models with categorical inputs October 2018 37 / 49
## Prediction accuracy

<table>
<thead>
<tr>
<th></th>
<th>CS</th>
<th>Groups (a)</th>
<th>Groups (b)</th>
<th>Ordinal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q^2</td>
<td>1.00-</td>
<td>0.95-</td>
<td>0.90-</td>
<td>0.85-</td>
</tr>
<tr>
<td></td>
<td>0.95-</td>
<td>0.90-</td>
<td>0.85-</td>
<td>0.80-</td>
</tr>
<tr>
<td></td>
<td>0.90-</td>
<td>0.85-</td>
<td>0.80-</td>
<td>0.75-</td>
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<tr>
<td></td>
<td>0.85-</td>
<td>0.80-</td>
<td>0.75-</td>
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<td></td>
<td>0.80-</td>
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<tr>
<td></td>
<td>0.75-</td>
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**Figure** – Q2 of several GP models (in %), based on 60 random designs \((n = 282)\).

Operation used: **sum**, **product**, **ANOVA**

Nb of param: ‘prod’ = \((12, 21, 30, 14)\), ‘add’ = ‘prod’ + 6, ‘anova’ = ‘prod’ + 7

The nominal approach with groups confirms the atomic order as a right order.
Robustness to group / order misspecification

Remarks
- Choosing groups at random is here equivalent to considering 1 group
- Choosing ordering at random can be more detrimental!
- Low-rank approaches are intractable (with the general param. of $F$)
Some results – Estimated correlations between levels of categorical variables

(a) Chemical element  

(b) Geometric shape
Some results – Estimated correlations between levels of categorical variables

Figure – Estimated kernel for the energy: warping (left) and correlation structure (right).
Towards trees
More on hierarchical GPs

- Wavelet kernels (Amato et al., 2006)
- Treed Gaussian processes (Gramacy, 2007)
- Lattice Kriging (Nychka et al., 2015)
- Multiresolution GPs (Fox and Dunson, 2012)
- Hierarchical GPs (Park and Choi, 2010)
- ...

**Remark:** In these models, the children ("details in subareas") are independent conditionally on the mother ("trend").

This was not the case before since children sum to 0 (cond. on the mother).

Source: Fox and Dunson (2012), Figure 2.
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- A kernel on a discrete space is a positive semidefinite matrix
- Build kernels from old: product, sum, ANOVA, warping, ...
- Heteroscedasticity / level can be handled directly
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1. Prop 1 (Algebra): Checking PSD only involves the number of groups
   → Check if the block average matrix is PSD
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   → The whole range of negative correlations for CS is recovered
   → Children are not independent conditionally on father ≠ tree GPs
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Software implementation

R packages kergp (Deville et al., 2020) (available on CRAN)
and mixgp (Padonou, 2016) (internal).
Open questions and perspectives

Modelling

- How to include trend in models?
- Nominal inputs: How to group levels?
- Ordinal inputs: How to order levels?
Open questions and perspectives

**Modelling**
- How to include trend in models?
- Nominal inputs: How to group levels?
- Ordinal inputs: How to order levels?

**Operational goals**
- How to design optimizers that deal with discrete & continuous inputs?
Références I


