A reproducible comparative study of categorical kernels for Gaussian process regression, with new clustering-based nested kernels

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10/10/2025

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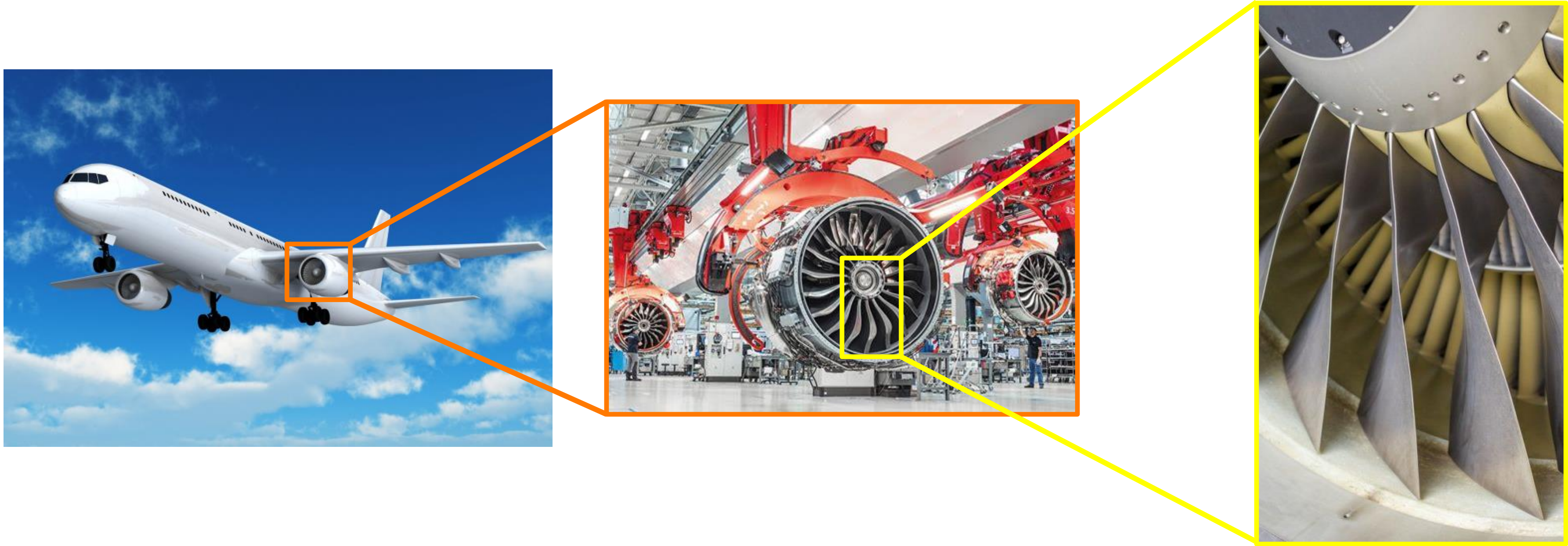
CMAP

Objectives



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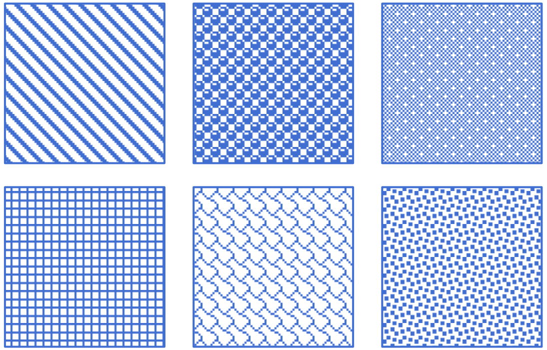
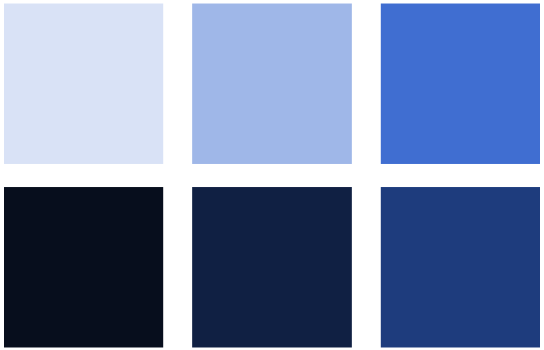


Input 1: weaving



Input 2: type of material

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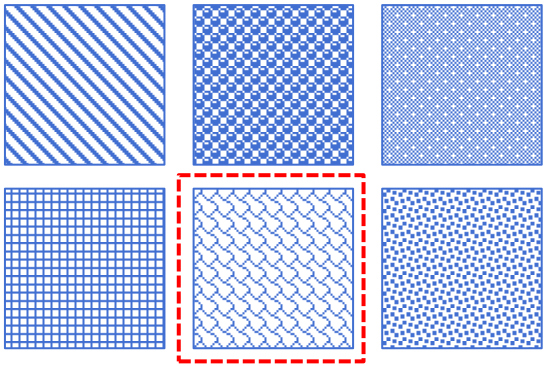
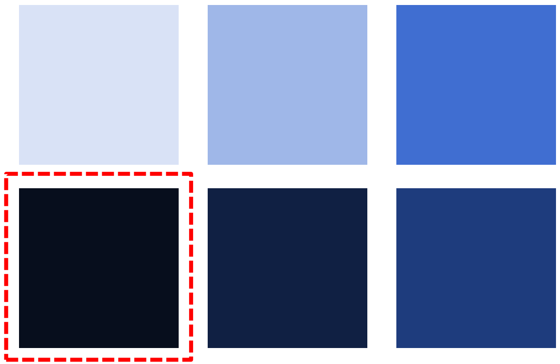


Input 1: weaving



Input 2: type of material

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GP in mixed spaces

$$f : \mathbb{R}^n \times \mathcal{Z} \to \mathbb{R}$$

$\mathbb{R}^n$: Continuous inputs

$\mathcal{Z}$: Categorical inputs

$$\mathcal{Z} = \prod_{i=1}^{m} \mathcal{Z}_i$$

$\mathcal{Z}_i$: Unordered set, finite number of levels

e.g. $\mathcal{Z}_i = \{A, B, \dots, E\}$

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GP in mixed spaces

$$f : \mathbb{R}^n \times \mathcal{Z} \to \mathbb{R}$$

Continuous inputs ($\mathbb{R}^n$) — Categorical inputs ($\mathcal{Z}$)

$$\mathcal{Z} = \prod_{i=1}^{m} \mathcal{Z}_i$$

$\mathcal{Z}_i$ → Unordered set, finite number of levels

e.g. $\mathcal{Z}_i = \{A, B, \dots, E\}$

$$k_{mixed}(\,(x,z),(x',z')\,) = k_{cont}(x,x') \times \prod_{i=1}^{m} k(z_i, z_i') \qquad \text{for } (x,z),(x',z') \in \mathbb{R}^n \times \mathcal{Z}$$

How to choose the categorical kernel k? → In the following, $\mathcal{Z} = \{1, \cdots, C\}$

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1- Review of existing approaches

a) Encoding

b) Covariance matrix parametrization

2- Experiments for datasets with known group structure

3- Automatic selection of groups

4- Experiments for datasets with no known group structure

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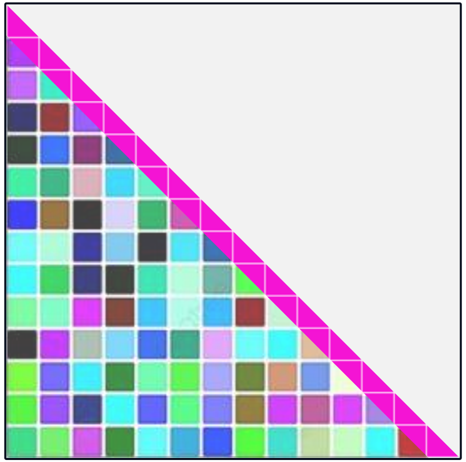
One-hot encoding

Level	Encoding
1	$E(1) = (1, 0, 0 \cdots, 0)$
2	$E(2) = (0, 1, 0 \cdots, 0)$
$\vdots$	
C	$E(C) = (0, 0, 0 \cdots, 1)$

C parameters



$$k(z, z') = \prod_{i=1}^{C} e^{-\frac{\left(E(z)_i - E(z')_i\right)^2}{2\,\theta_i^2}} = \delta_{z,z'} + e^{-\frac{1}{2}\left(\theta_z^{-2} + \theta_{z'}^{-2}\right)}\left(1 - \delta_{z,z'}\right)$$

ARD RBF kernel between encodings

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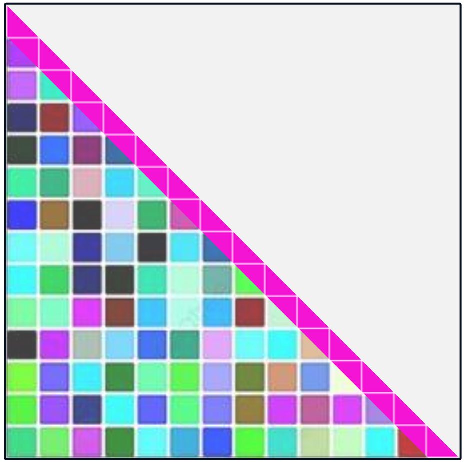
Latent Variables (LVGP)

[Zhang et al., 2020]

$2C - 3$ parameters

$\phi: \{1, \cdots, C\} \rightarrow \mathbb{R}^2$: learned function



$$k(z, z') = e^{-\|\phi(z) - \phi(z')\|_2^2}$$

ARD RBF kernel between learned representations in dimension 2

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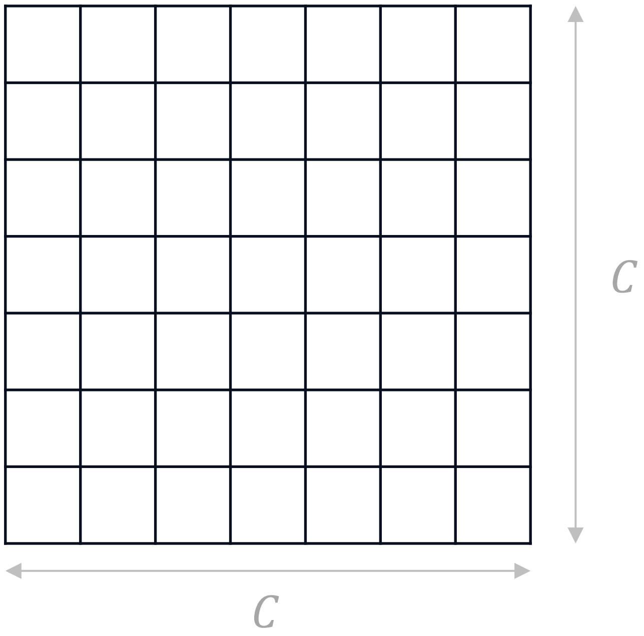
Matrix parametrization

$$k : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$$

$$\sim$$

$T =$



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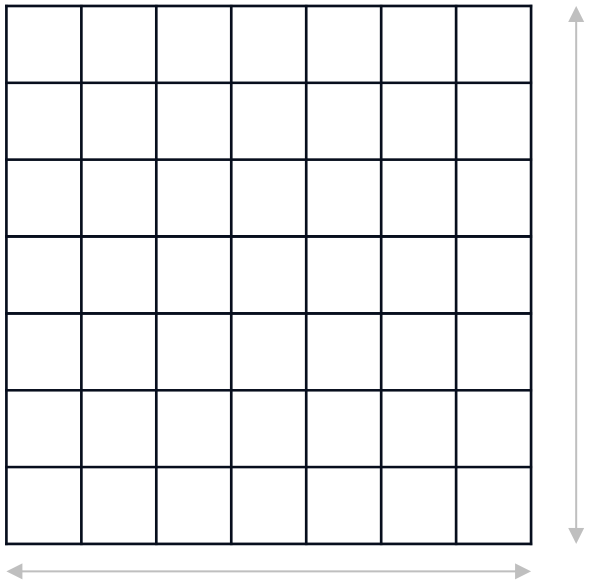

C

C

T symmetric positive definite matrix

Cholesky decomposition

$$T = LL^T \qquad L = L(\underline{\theta})$$

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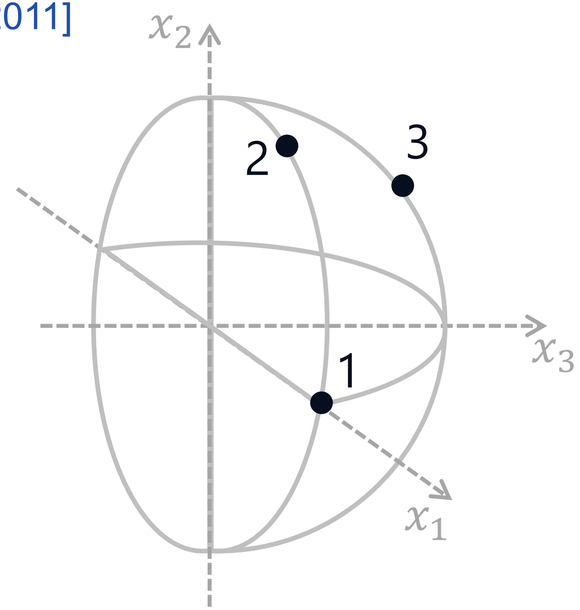
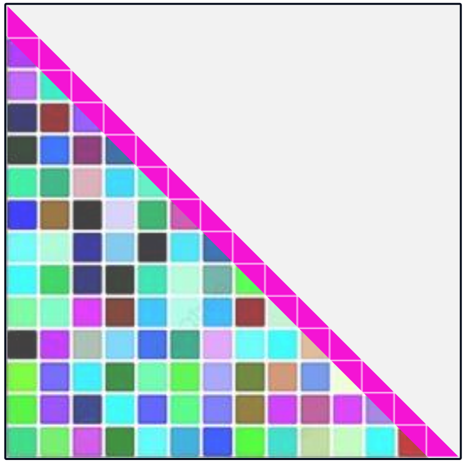
Homoscedastic Hypersphere (Ho)

[Zhou et al., 2011]

$\frac{1}{2}C(C-1)$ parameters





$$L = \begin{bmatrix} 1 & 0 & 0 \\ \cos(\theta_{21}) & \sin(\theta_{21}) & 0 \\ \cos(\theta_{31}) & \sin(\theta_{31})\cos(\theta_{32}) & \sin(\theta_{31})\sin(\theta_{32}) \end{bmatrix}$$

$\theta_{ij} \in \left(0, \frac{\pi}{2}\right) \rightarrow$ Positive correlations

$\theta_{ij} \in (0, \pi) \rightarrow$ Negative correlations

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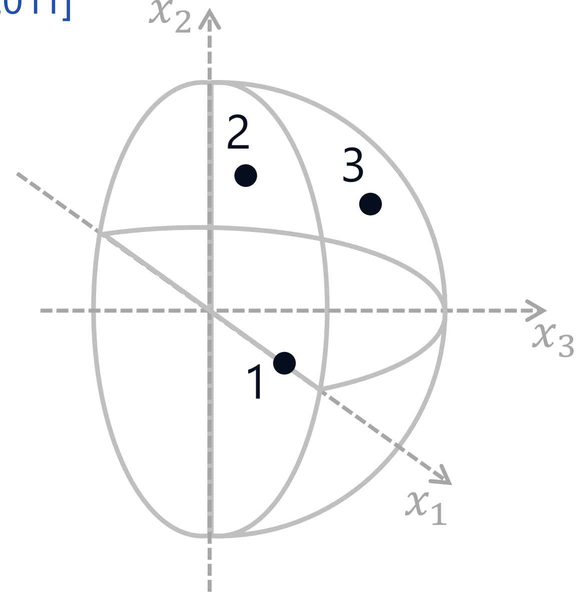
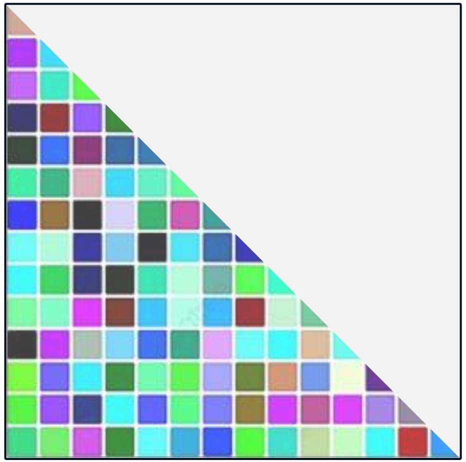
Heterоscedastic Hypersphere (He)

[Zhou et al., 2011]

$\frac{1}{2}C(C+1)$ parameters





$$L = \begin{bmatrix} \theta_{10} & 0 & 0 \\ \theta_{20}\cos(\theta_{21}) & \theta_{20}\sin(\theta_{21}) & 0 \\ \theta_{30}\cos(\theta_{31}) & \theta_{30}\sin(\theta_{31})\cos(\theta_{32}) & \theta_{30}\sin(\theta_{31})\sin(\theta_{32}) \end{bmatrix}$$

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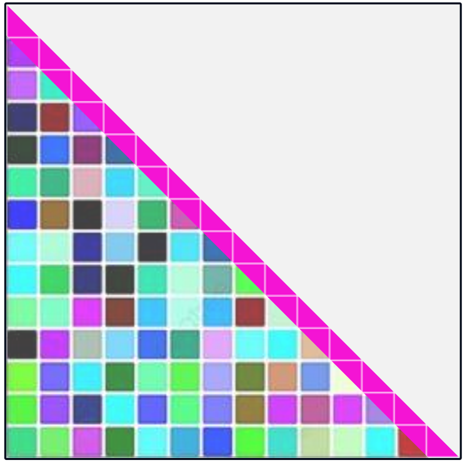
Exp Homoscedastic Hypersphere(EHH)
[Saves et al., 2023]

$\frac{1}{2}C(C+1)$ parameters



L : homoscedastic hypersphere

$$\tau_{z,z'} = \log((LL^T)_{z,z'} - 1)$$

$$k(z,z') = \delta_{z,z'} + e^{-2\tau_{z,z'}}(1-\delta_{z,z'})$$

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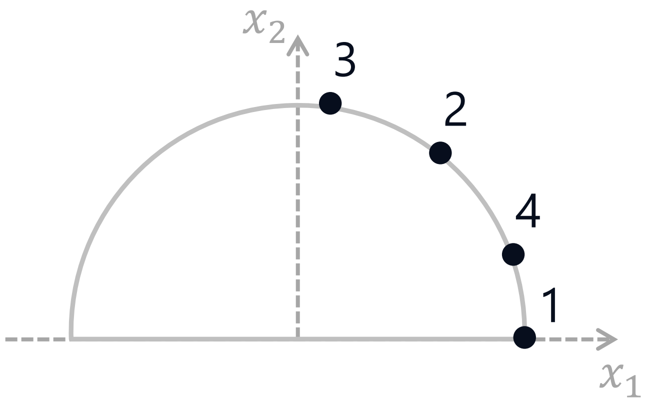
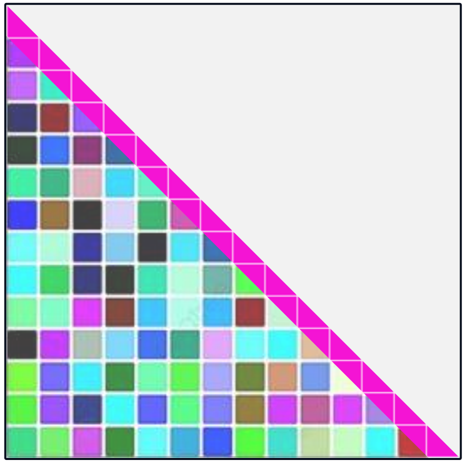
Low rank Hypersphere (Ho_2)

[Kirchhoff et al., 2020]

$C - 1$ parameters





Rank 2

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \sin(\theta_{21}) & \cos(\theta_{21}) & 0 & 0 \\ \sin(\theta_{31}) & \cos(\theta_{31}) & 0 & 0 \\ \sin(\theta_{41}) & \cos(\theta_{41}) & 0 & 0 \end{bmatrix}$$

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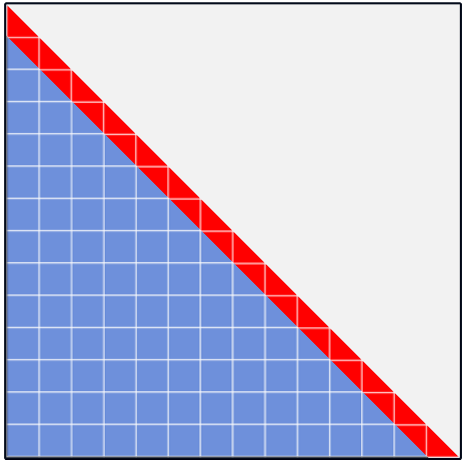
Compound symmetry (CS)

[Katz., 2011]

2 parameters

$$k(z, z') = v\delta_{z,z'} + c(1 - \delta_{z,z'})$$

$$v > 0\ , \quad \frac{c}{v} \in \left(\frac{-1}{C-1}, 1\right)$$



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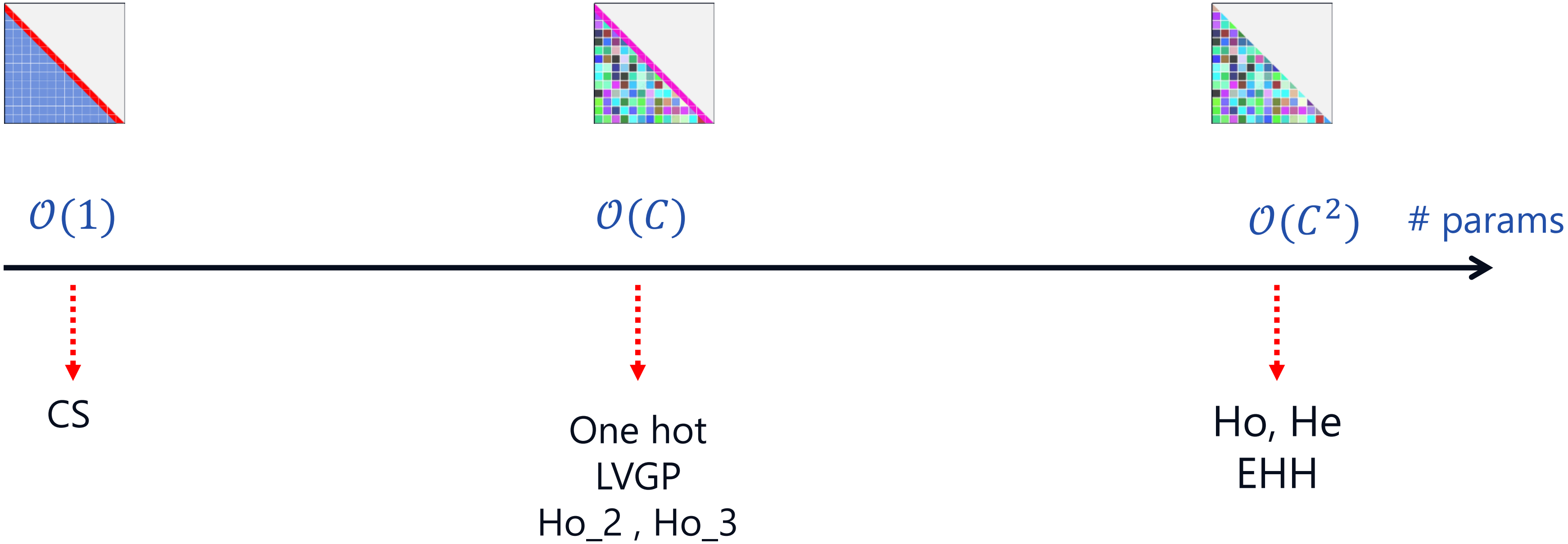
Summary of the methods



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Nested Kernels

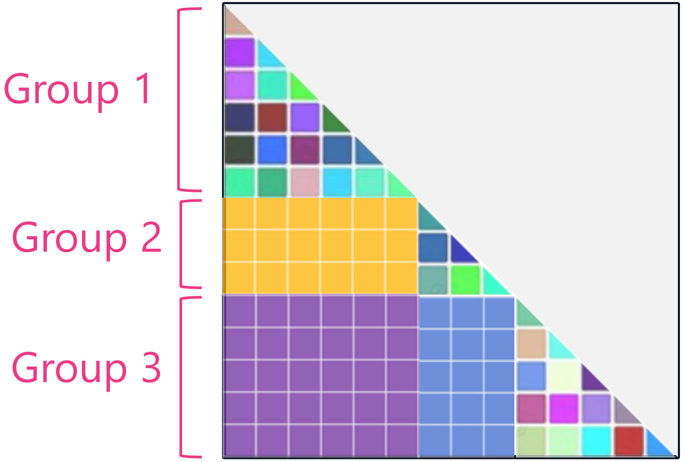
[Roustant et al., 2020]

$$\sum_{l=1}^{\gamma} \frac{n_l(n_l+1)}{2} + \frac{\gamma(\gamma+1)}{2} \quad \text{parameters}$$

Requires γ groups of levels:

$$\{1, \cdots, C\} = \bigcup_{1 \le l \le \gamma} G_l \qquad (G_l \text{ of size } n_l)$$

$$T = \begin{bmatrix} W_1 & B_{12} & B_{13} \\ B_{21} & W_2 & B_{23} \\ B_{31} & B_{32} & W_3 \end{bmatrix}$$



Block covariance matrix
- Cov « Within group »
- Cov « Between groups »

Nested_He_He

Between Within

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Nested Kernels

[Roustant et al., 2020]

$$\sum_{l=1}^{\gamma} \frac{n_l(n_l+1)}{2} + 2 \quad \text{parameters}$$

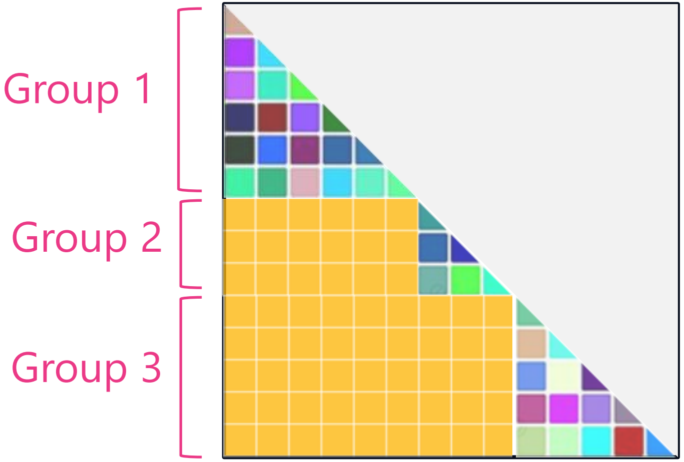
Requires γ groups of levels:

$$\{1, \cdots, C\} = \bigcup_{1 \le l \le \gamma} G_l \qquad (G_l \text{ of size } n_l)$$

$$T = \begin{bmatrix} W_1 & B_{12} & B_{13} \\ B_{21} & W_2 & B_{23} \\ B_{31} & B_{32} & W_3 \end{bmatrix}$$

Block covariance matrix

- Cov « Within group »
- Cov « Between groups »



Nested_CS_He

Between — Within

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Nested Kernels

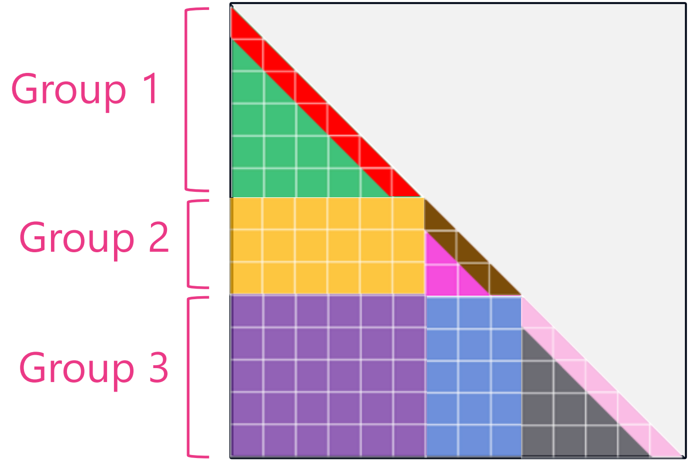
[Roustant et al., 2020]

$$\gamma + \frac{\gamma(\gamma+1)}{2}$$ parameters

Requires γ groups of levels:

$$\{1, \cdots, C\} = \bigcup_{1 \le l \le \gamma} G_l \qquad (G_l \text{ of size } n_l)$$

$$T = \begin{bmatrix} W_1 & B_{12} & B_{13} \\ B_{21} & W_2 & B_{23} \\ B_{31} & B_{32} & W_3 \end{bmatrix}$$



Block covariance matrix

- Cov « Within group »
- Cov « Between groups »

Nested_Ho_CS

Between

Within

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Nested Kernels

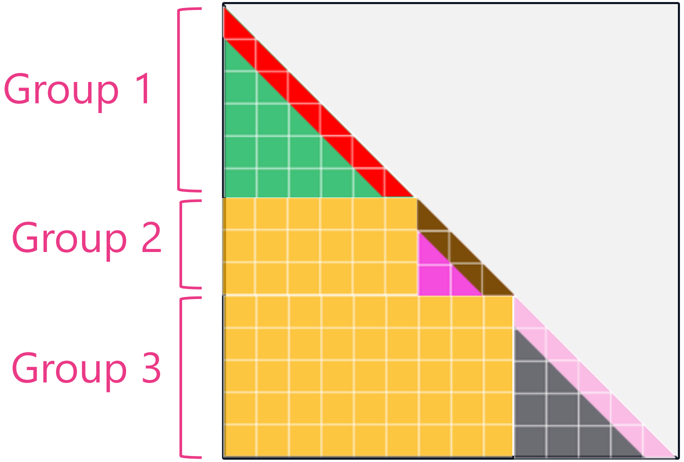
[Roustant et al., 2020]

$\gamma + 2$ parameters

Requires γ groups of levels:

$$\{1, \cdots, C\} = \bigcup_{1 \leq l \leq \gamma} G_l \qquad (G_l \text{ of size } n_l)$$

$$T = \begin{bmatrix} W_1 & B_{12} & B_{13} \\ B_{21} & W_2 & B_{23} \\ B_{31} & B_{32} & W_3 \end{bmatrix}$$



Block covariance matrix
- Cov « Within group »
- Cov « Between groups »

Nested_CS_CS

Between Within

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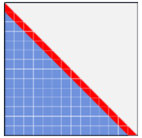
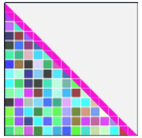
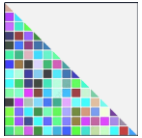
Summary of the methods







$\mathcal{O}(1)$ $\mathcal{O}(C)$ $\mathcal{O}(C^2)$ # params

CS

One hot
LVGP
Ho_2 , Ho_3

Ho, He
EHH

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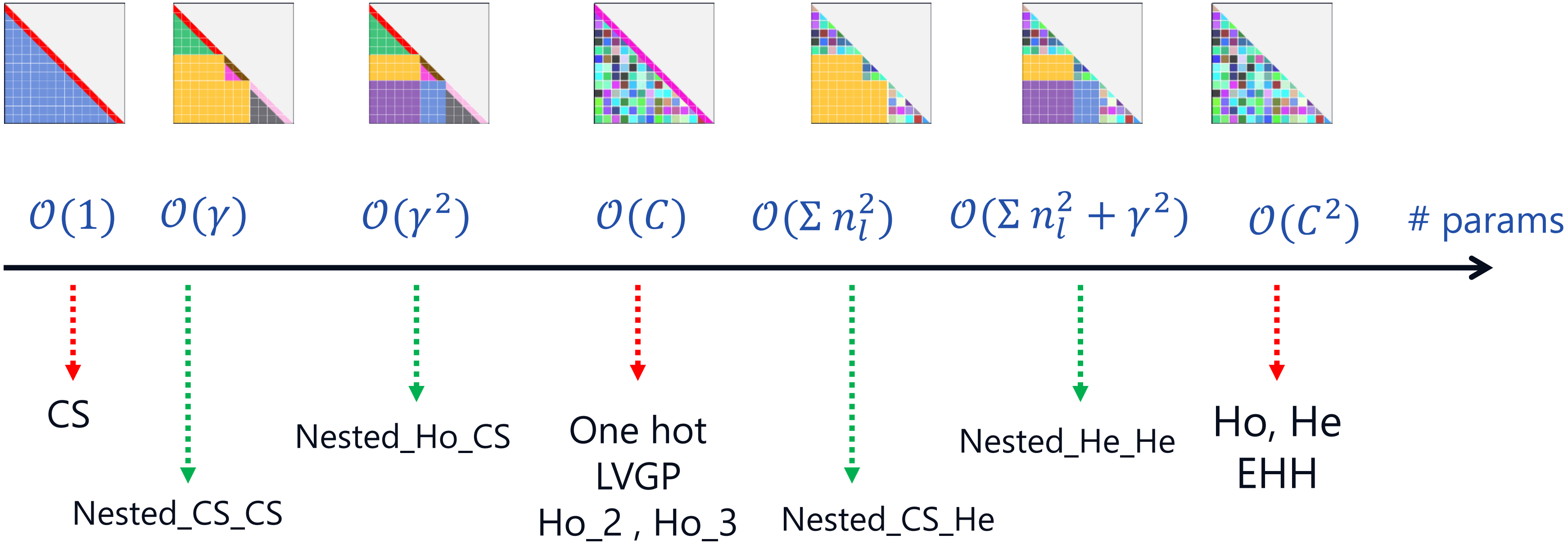

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a) Encoding

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c) Kernels from the BO litterature

2- Experiments for datasets with known group structure

3- Automatic selection of groups

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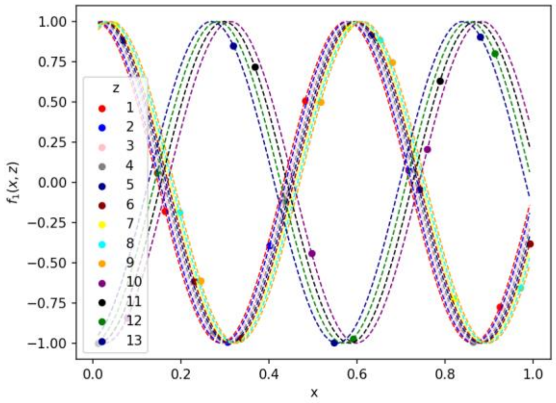
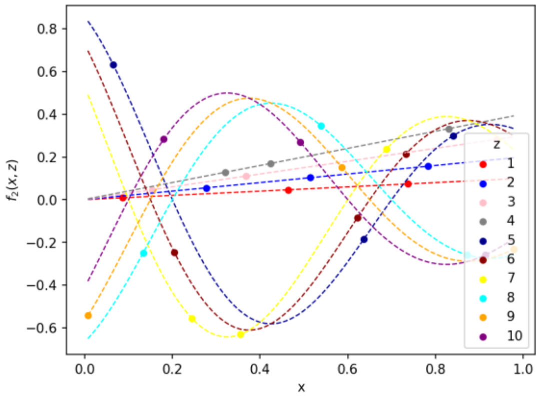
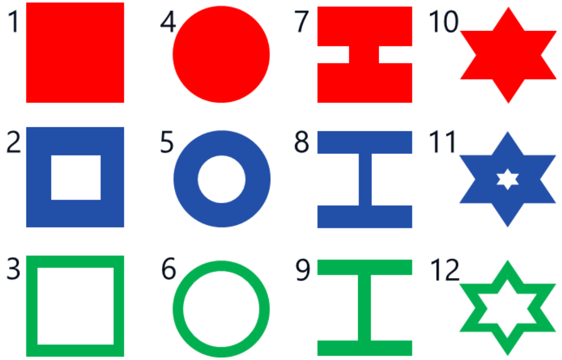
Datasets with known group structure







Name	Cont	Cat	Train	Test	Groups	Source
f_1	1	1 (13)	39/78/117/156/195	1001	True	Roustant et al. (2020)
f_2	1	1 (10)	30/60/90/120/150	1000	True	Roustant et al. (2020)
Beam bending	2	1 (12)	36/72/108/144/180	1000	True	Roustant et al. (2020)

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Presentation of the methods/kernels

Category	Name	Description
Hypersphere	Ho	Homoscedastic, only positive correlations
	Ho_NC	Homoscedastic, allowing negative correlations
	He	Heteroscedastic, only positive correlations
	He_NC	Heteroscedastic, allowing negative correlations
	Ho_2	Homoscedastic, only positive correlations (rank 2)
	Ho_3	Homoscedastic, only positive correlations (rank 3)
	EHH	Exponential Homoscedastic Hypersphere
LVGP	LVGP	Latent dimension 2
CS	CS	Compound symmetry
One-hot	One_hot	One hot encoding
No cat	No cat	Only continuous variables

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Presentation of the methods/kernels

Category	Name	Description
Nested	Nested_CS_He	Between = CS, Within = He
	Nested_He_He	Between = He, Within = He
	Nested_Ho_CS	Between = Ho, Within = CS
	Nested_CS_CS	Between = CS, Within = CS

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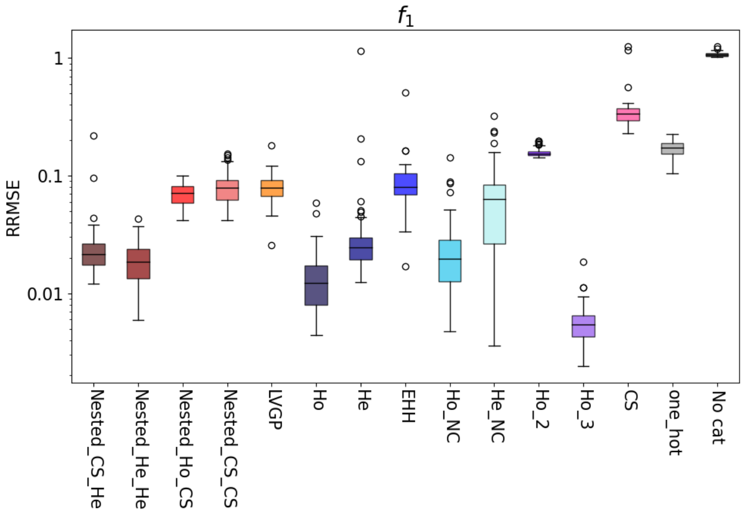
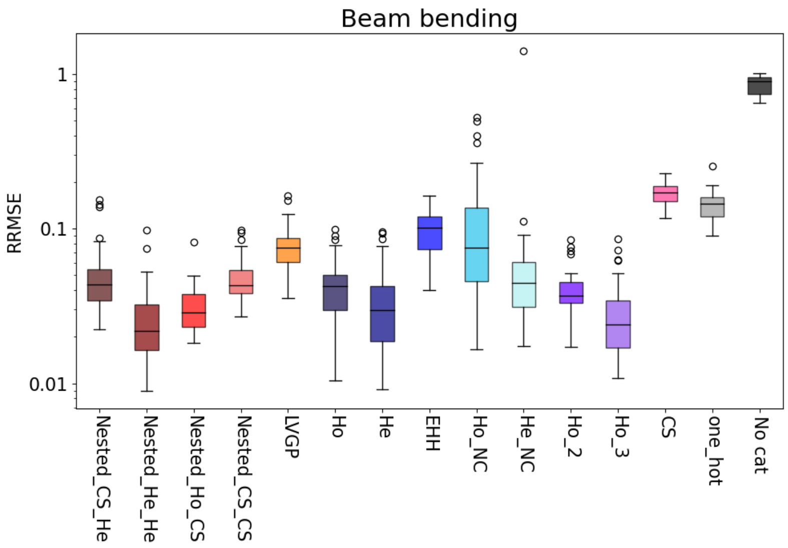
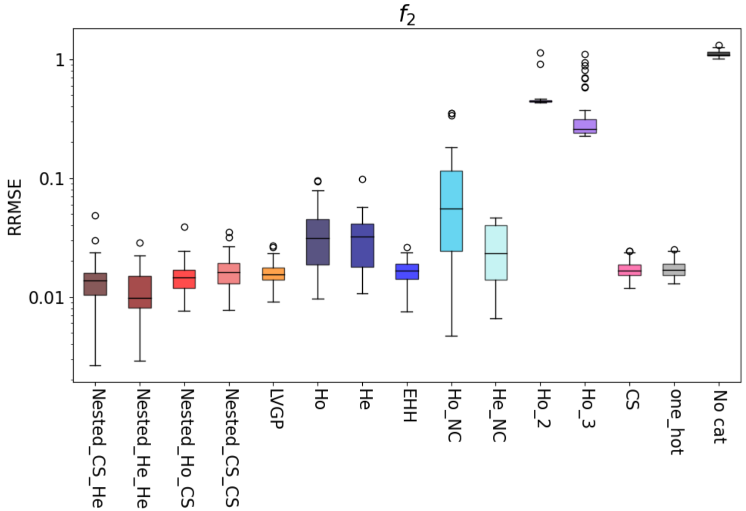
Individual results







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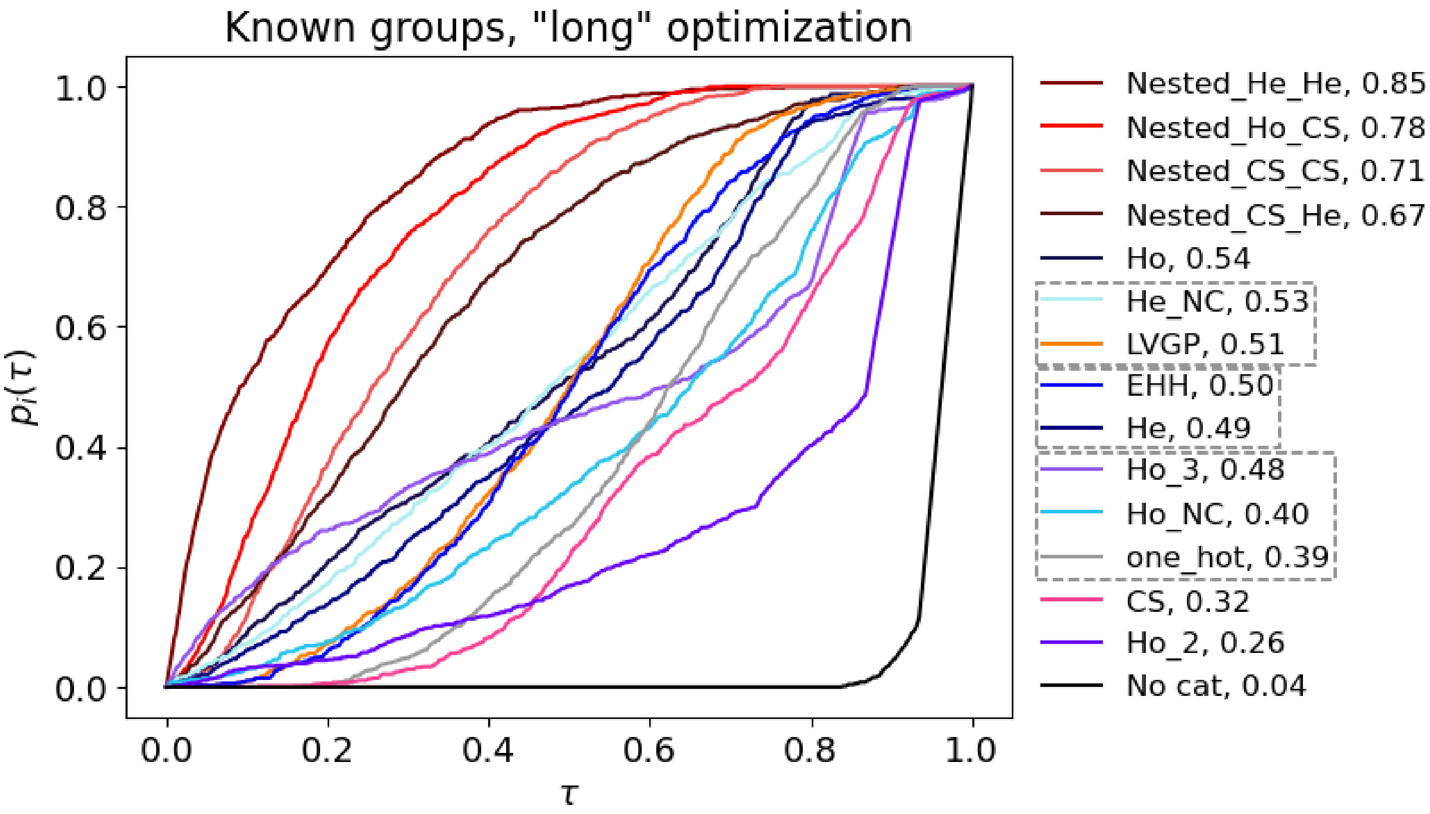
Performance profiles (known groups)



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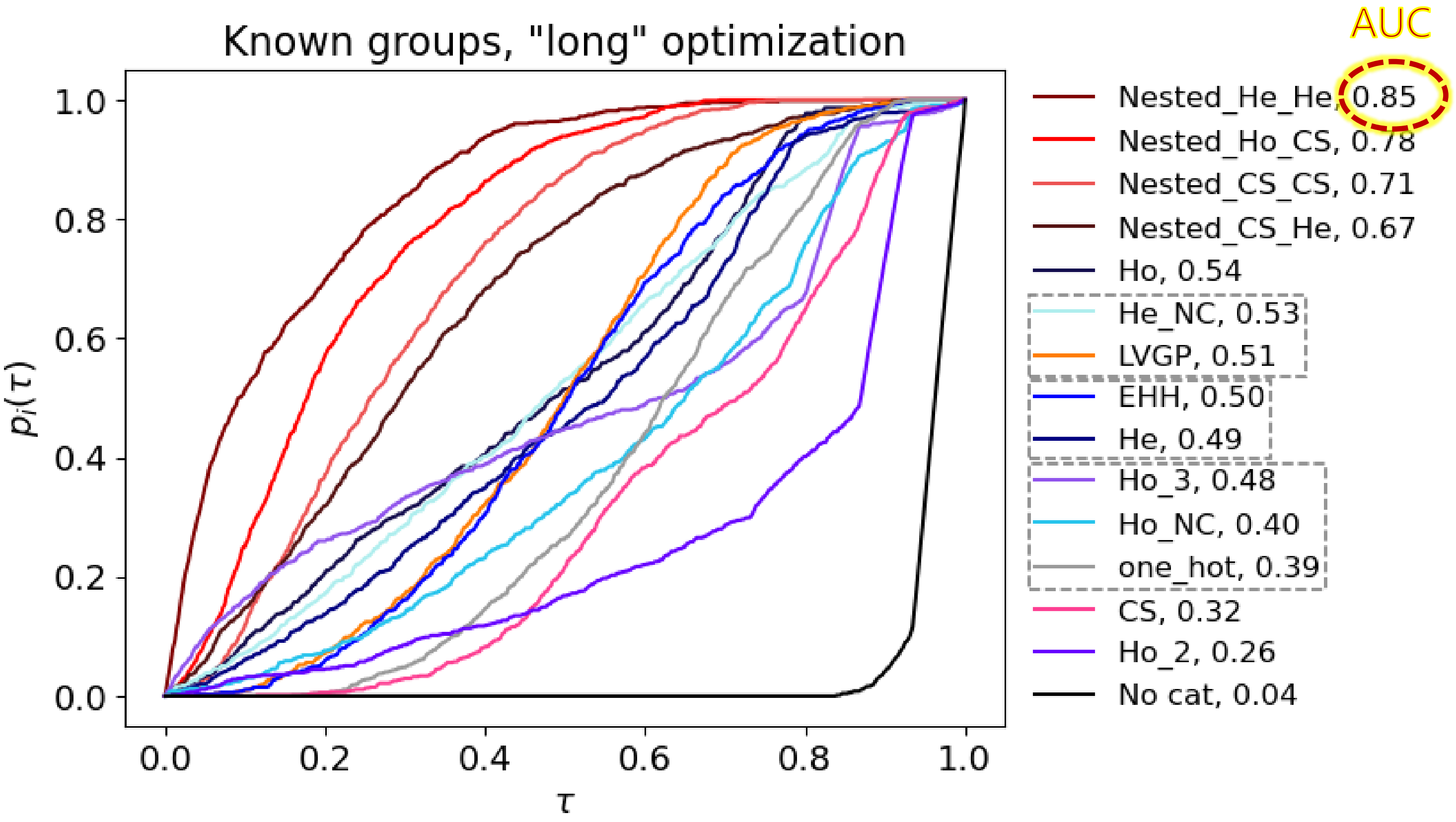
Performance profiles (known groups)



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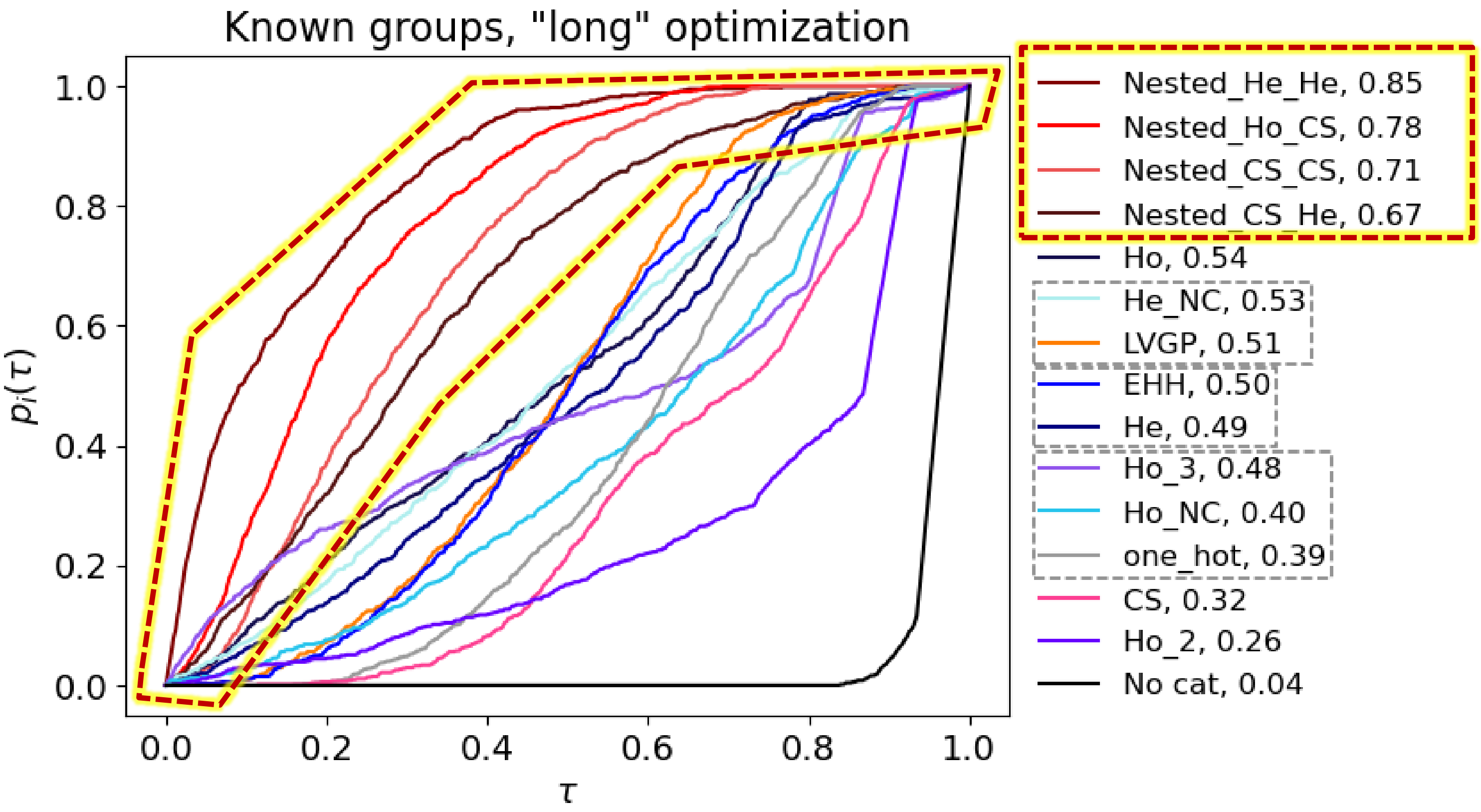

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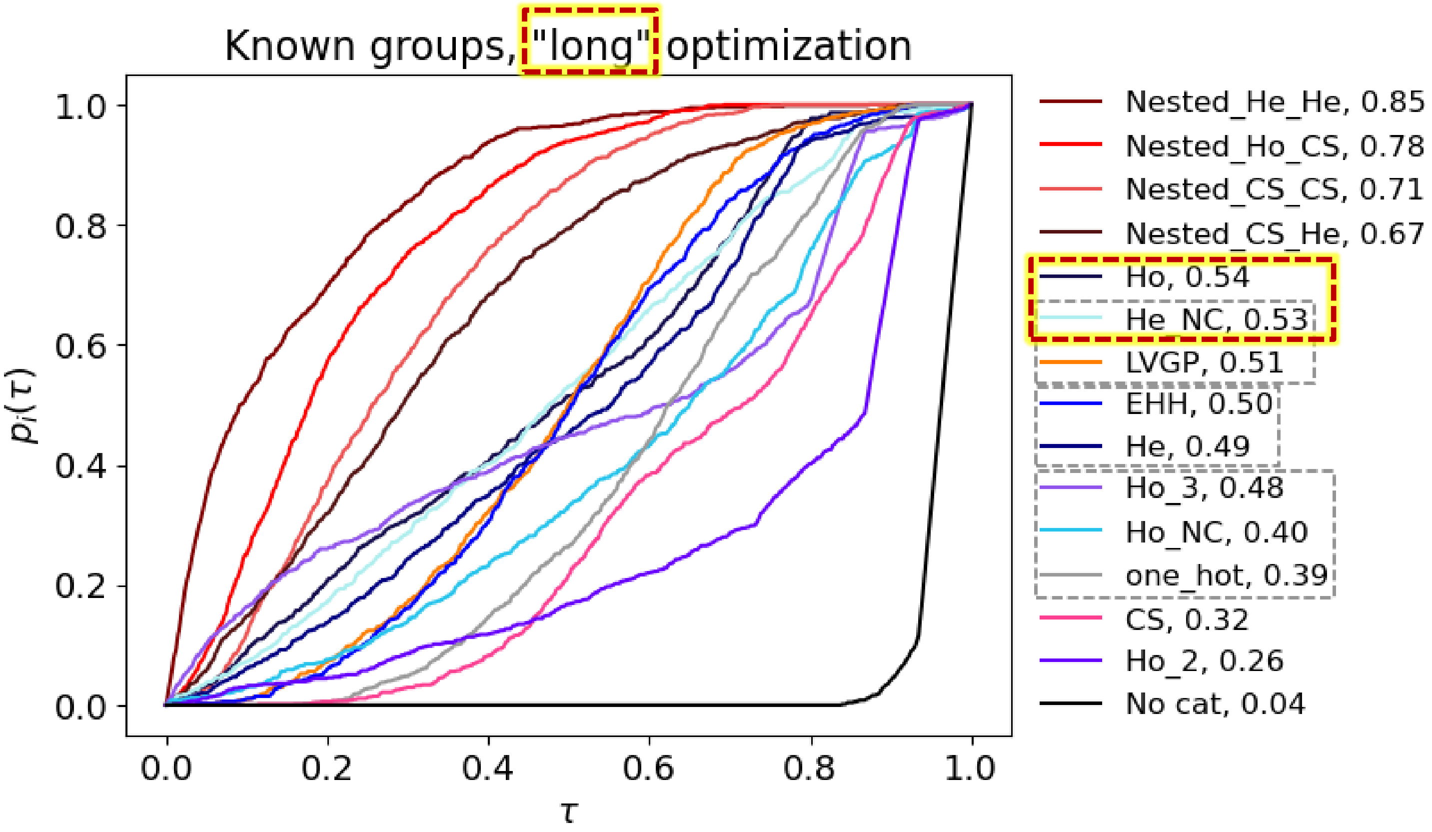
Performance profiles (known groups)



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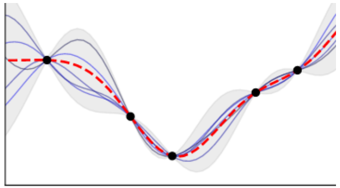
Selection of groups when they are not known

<u>Objective:</u> Use Nested kernels. <u>Issue:</u> no known groups [Roustant et al., 2020]

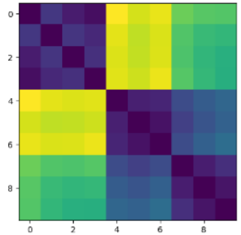
1- Train a GP#1

Kernel = LVGP



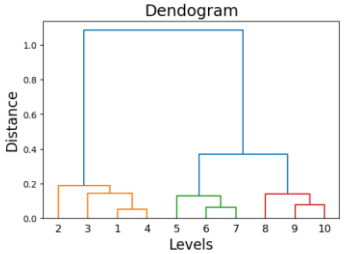
2- Get T^{prox} from GP#1

$$d(z,z') = \left(T^{prox}_{z,z} + T^{prox}_{z',z'} - 2T^{prox}_{z,z'}\right)^{1/2}$$



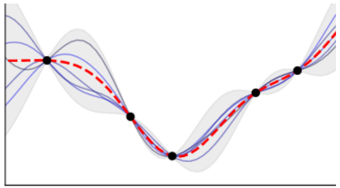
3- Clustering

Hierarchical, from d



4- Train a GP#2

Kernel = Nested



✘ Requires to train another GP model before to get the groups

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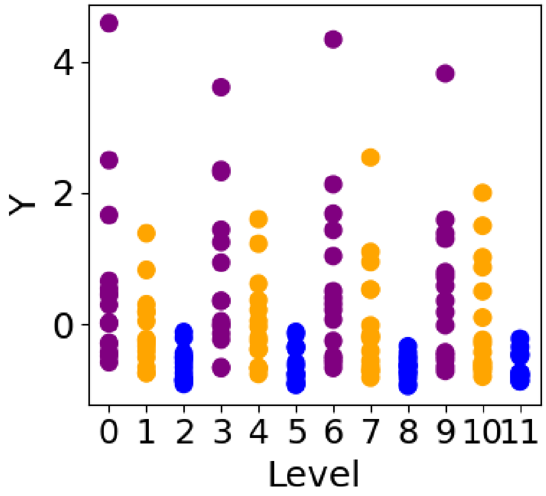
Target encodings



Train inputs $(x^{(i)}, z^{(i)})$ and outputs $y^{(i)}$

$$\nu_c = \frac{1}{|i: z^{(i)} = c|} \sum_{i: z^{(i)} = c} \delta_{y^{(i)}}$$

Target encoding of the level c

Choose $d(z, z') = \mathcal{D}(\nu_z, \nu_{z'})$

Divergence between empirical measures

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Target encodings

In practice, since ν_c is of small size (<10), we can use:

μ_c mean and σ_c SD of ν_c

$$\mathcal{D}(z,z') = \|(\mu_z,\sigma_z) - (\mu_{z'},\sigma_{z'})\|_2$$

Train inputs $(x^{(i)}, z^{(i)})$ and outputs $y^{(i)}$

$$\nu_c = \frac{1}{|i: z^{(i)} = c|} \sum_{i:z^{(i)}=c} \delta_{y^{(i)}}$$

Target encoding of the level c

Choose $d(z,z') = \mathcal{D}(\nu_z, \nu_{z'})$

Divergence between empirical measures

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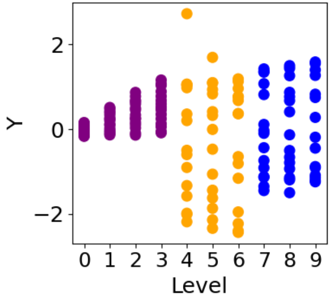
New selection of groups when they are not known

<u>Objective:</u> Use Nested kernels.

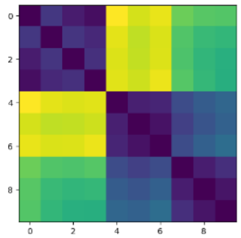
<u>Issue:</u> no known groups

1- Target encodings



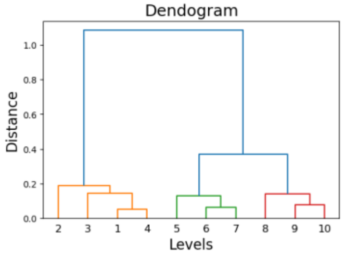
2- MSD distance matrix

$$d(z,z') = \mathcal{D}(\nu_z, \nu_{z'})$$



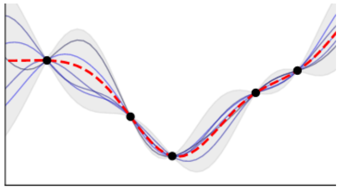
3- Clustering

Hierarchical, from d



4- Train a GP

Kernel = Nested



✓ Only one GP training is required

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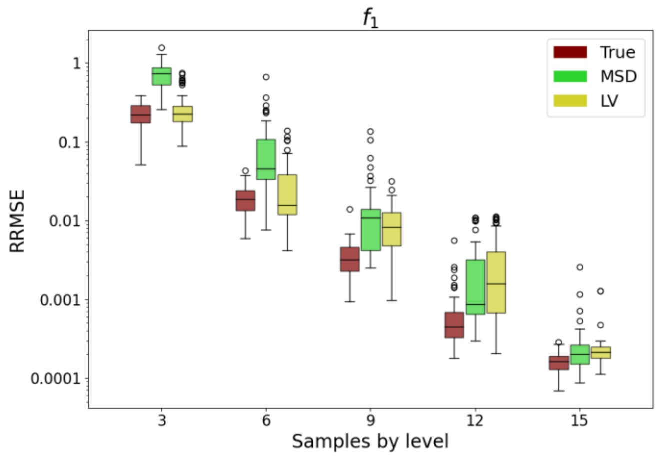
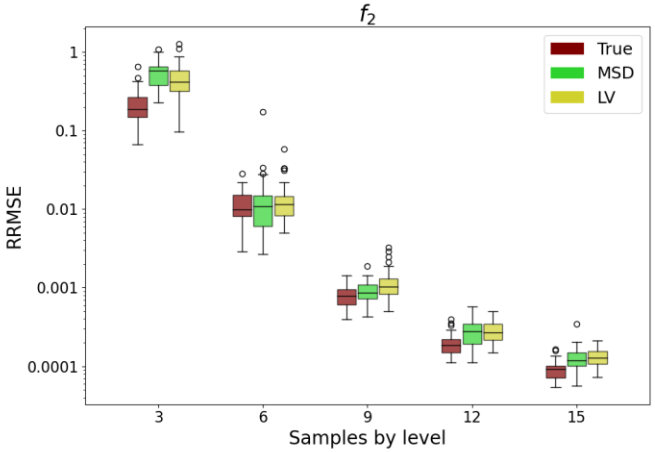
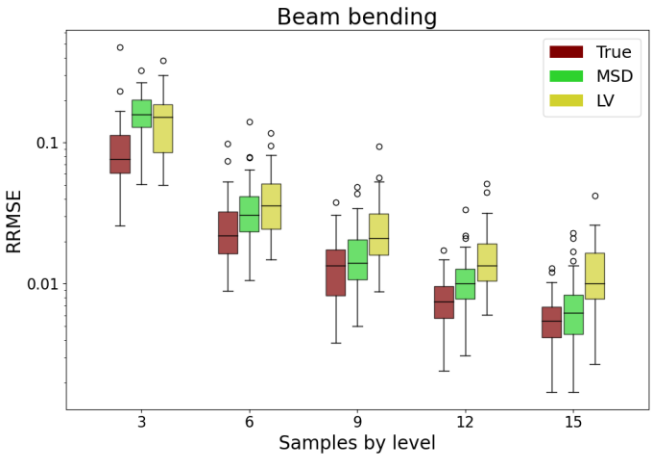
Impact of the group selection strategy: scores







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1- Review of existing approaches

a) Encoding

b) Covariance matrix parametrization

c) Kernels from the BO litterature

2- Experiments for datasets with known group structure

3- Automatic selection of groups

4- Experiments for datasets with no known group structure

Datasets with no known group structure

Name	Cont	Cat	Train	Test	Groups	Source
Borehole	6	2 (3-4)	36/72/108/144/180	1008	False	Zhang et al. (2020)
Borehole2	6	1 (12)	36/72/108/144/180	1008	False	Zhang et al. (2020)
OTL	4	2 (4-6)	72/144/216	1008	False	Zhang et al. (2020)
OTL2	4	1 (24)	72/144/216	1008	False	Zhang et al. (2020)
Piston	5	2 (5-3)	45/90/135	1005	False	Zhang et al. (2020)
Piston2	5	1 (15)	45/90/135	1005	False	Zhang et al. (2020)
Goldstein	2	1 (9)	27/54/81/108/135	999	False	Pelamatti et al. (2021)

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Presentation of the methods/kernels

Category	Name	Description
Hypersphere	Ho	Homoscedastic, only positive correlations
	Ho_NC	Homoscedastic, allowing negative correlations
	He	Heteroscedastic, only positive correlations
	He_NC	Heteroscedastic, allowing negative correlations
	Ho_2	Homoscedastic, only positive correlations (rank 2)
	Ho_3	Homoscedastic, only positive correlations (rank 3)
	EHH	Exponential Homoscedastic Hypersphere
LVGP	LVGP	Latent dimension 2
CS	CS	Compound symmetry
One-hot	One_hot	One hot encoding
No cat	No cat	Only continuous variables

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Presentation of the methods/kernels

Category	Name	Description
Nested (auto LV)	Nested_CS_He_LV	Between = CS, Within = He
	Nested_He_He_LV	Between = He, Within = He
	Nested_Ho_CS_LV	Between = Ho, Within = CS
	Nested_CS_CS_LV	Between = CS, Within = CS
Nested (auto MSD)	Nested_CS_He_MSD	Between = CS, Within = He
	Nested_He_He_MSD	Between = He, Within = He
	Nested_Ho_CS_MSD	Between = Ho, Within = CS
	Nested_CS_CS_MSD	Between = CS, Within = CS

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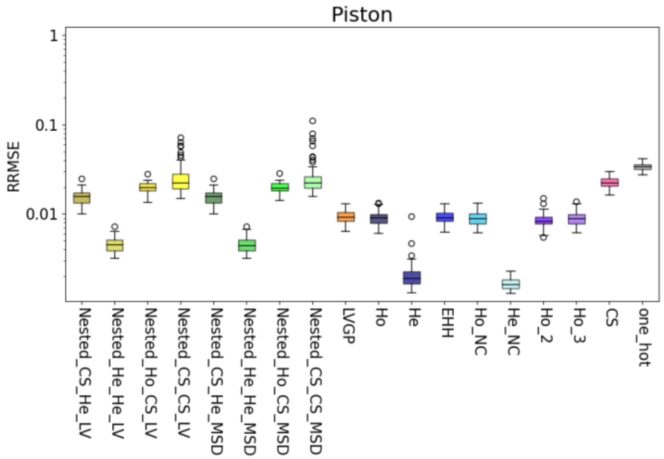
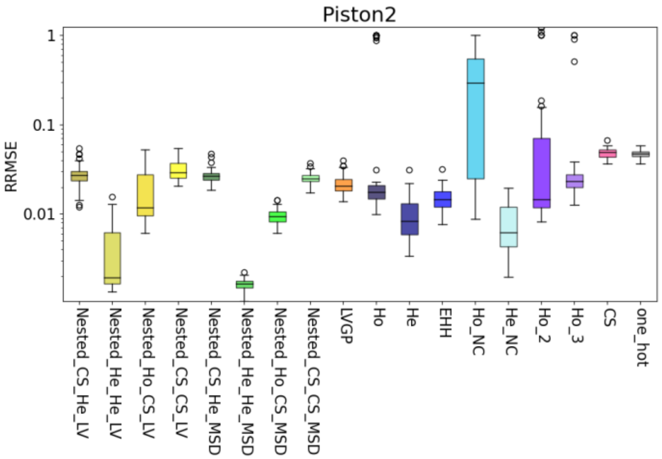
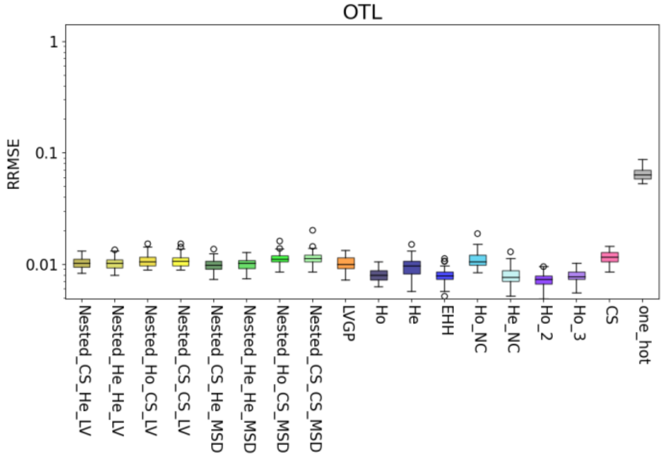
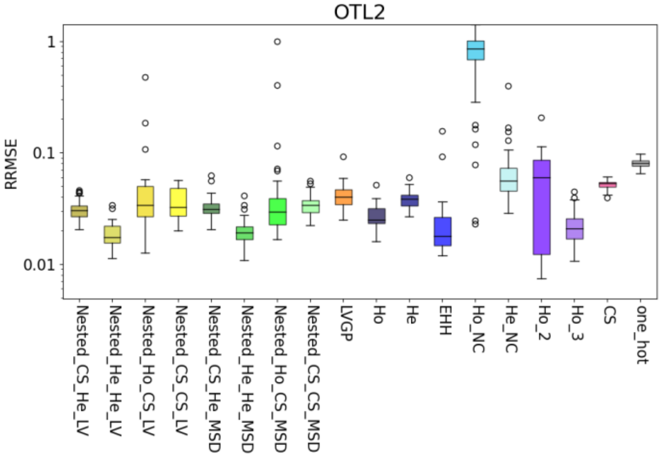
Individual results









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Performance profiles (no known groups)

« long »

Max iter	3000
Max func. evaluations	3000 × (#params + cst)
Tolerance	10^{-10}

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Performance profiles (no known groups)

« long »

Max iter	3000
Max func. evaluations	3000 × (#params + cst)
Tolerance	10^{-10}

« short »

Default in scipy

Max iter	Ø
Max func. evaluations	15000
Tolerance	10^{-9}

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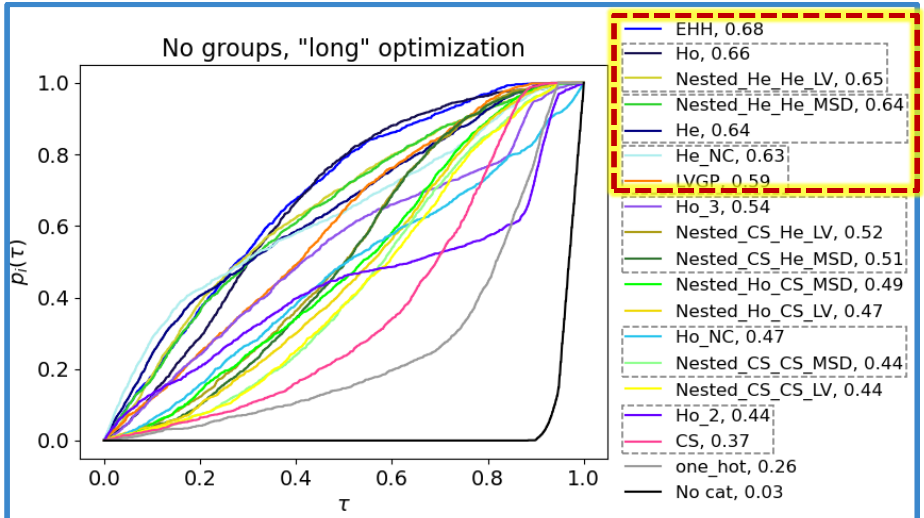
Performance profiles (no known groups)



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Max iter	3000
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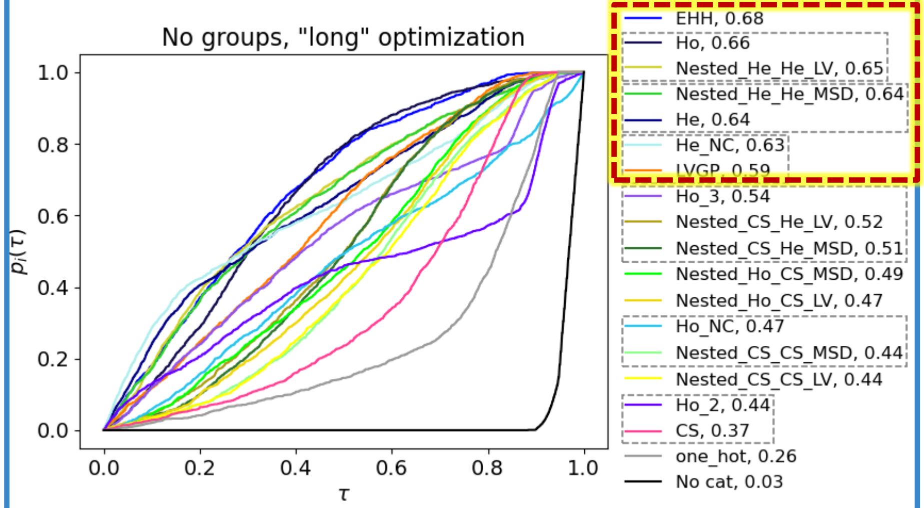
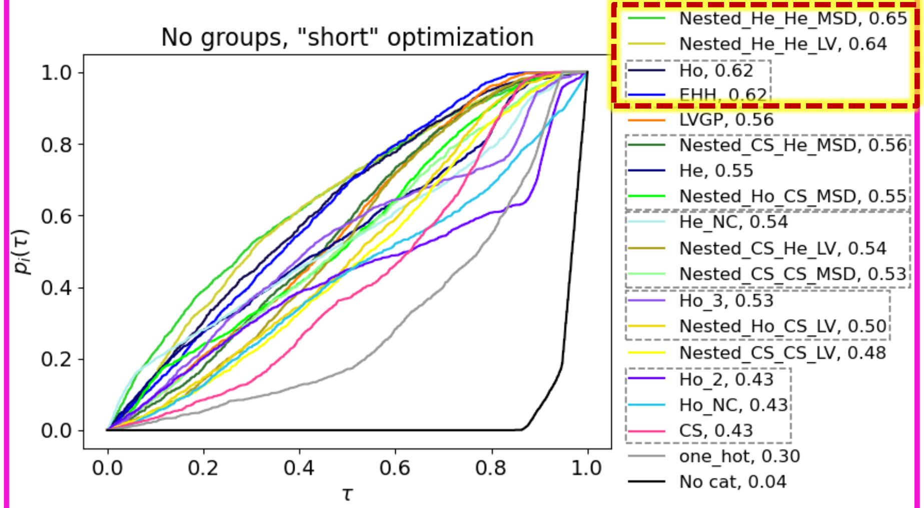
Performance profiles (no known groups)



« long »

Max iter	3000
Max func. evaluations	3000 × (#params + cst)
Tolerance	10^{-10}



« short »

Default in scipy

Max iter	Ø
Max func. evaluations	15000
Tolerance	10^{-9}

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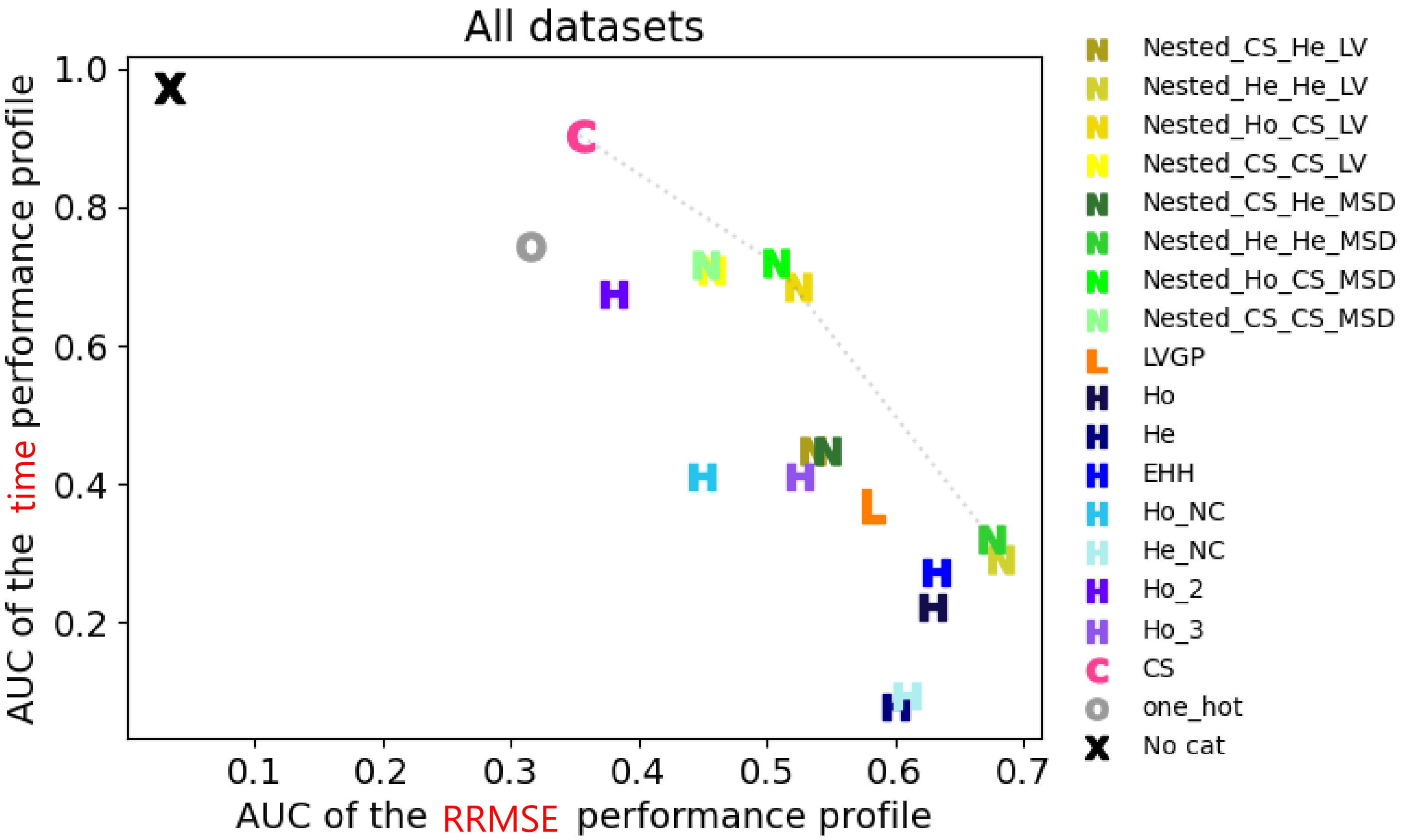
AUCS of perf. profiles: time vs RRMSE (all datasets)



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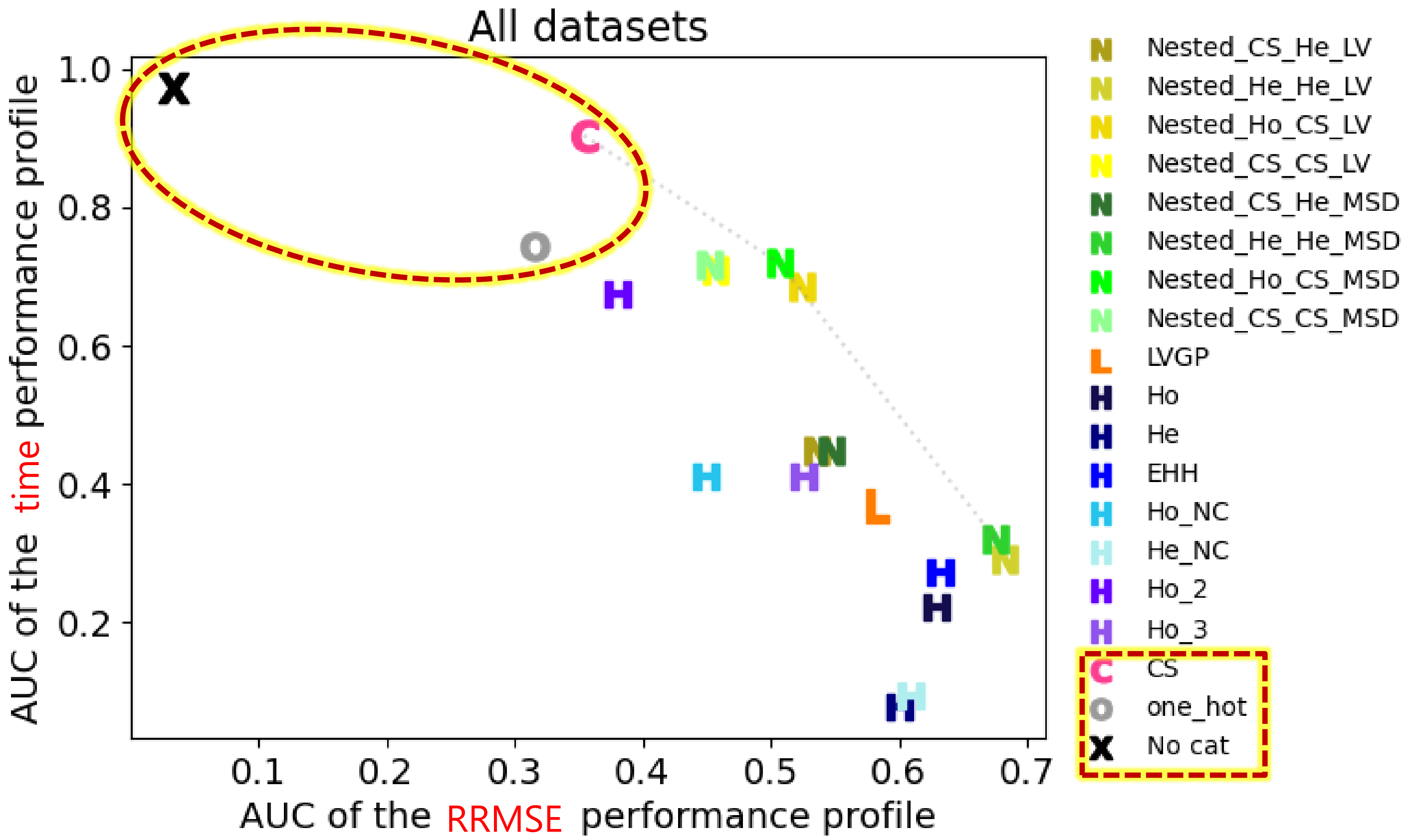

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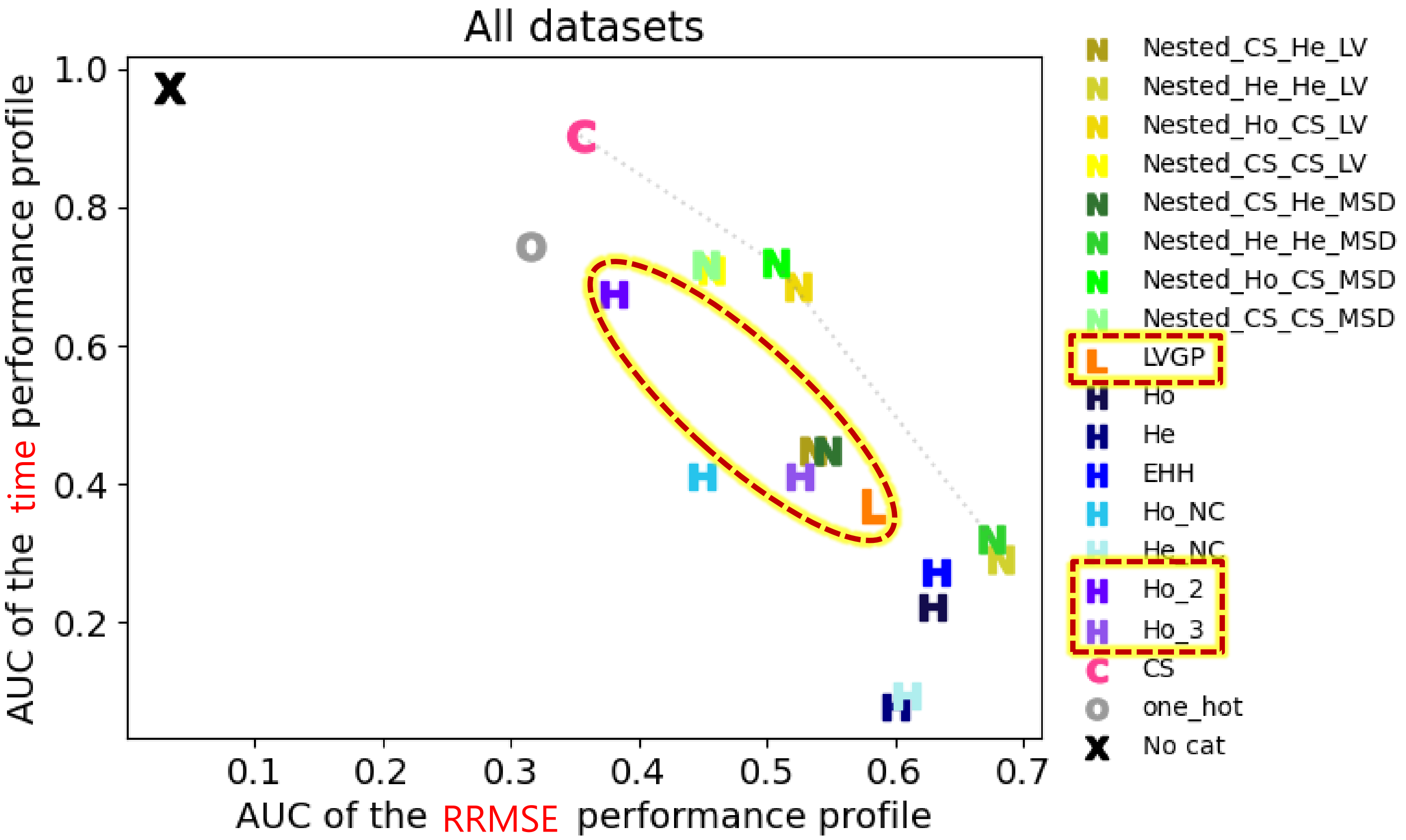

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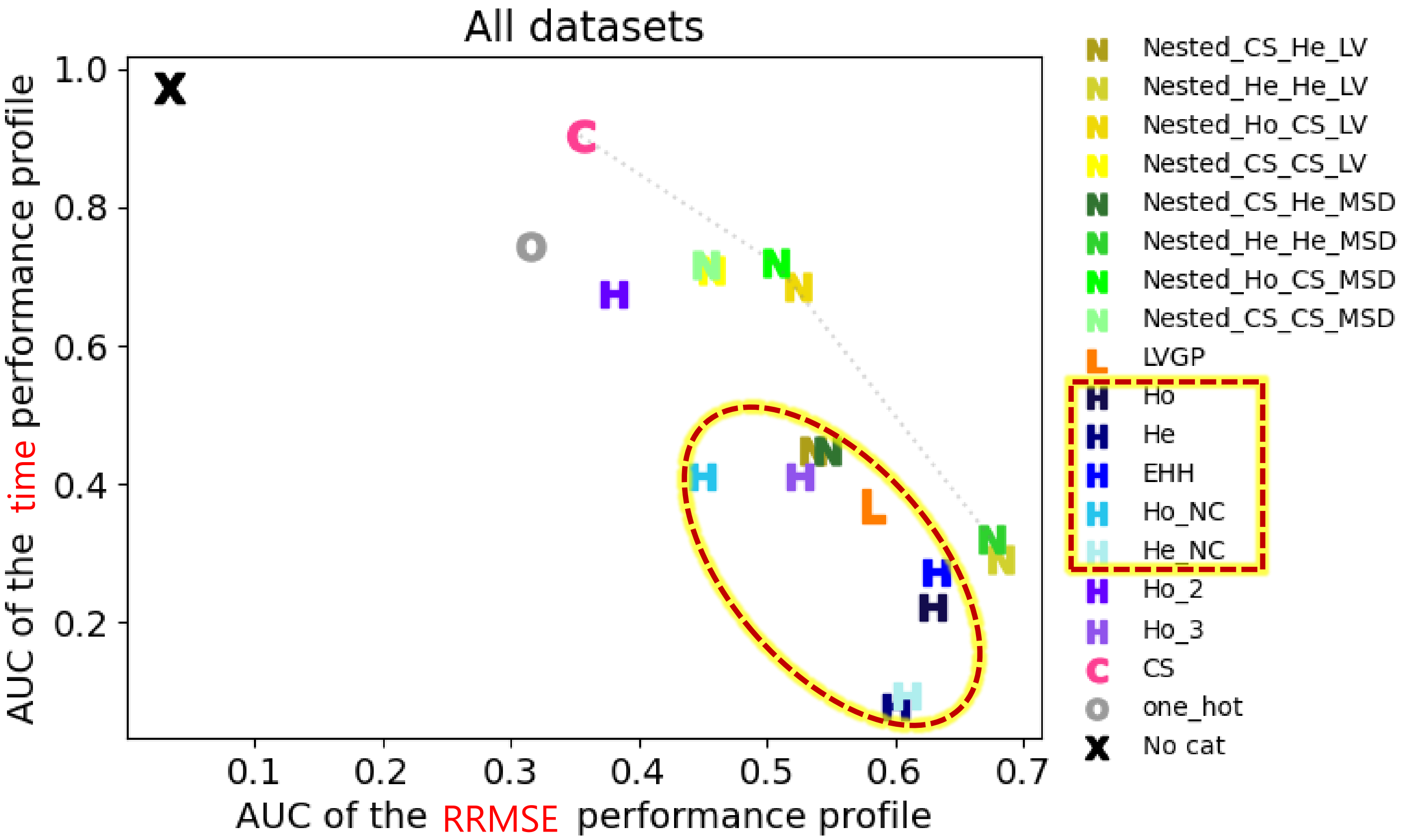

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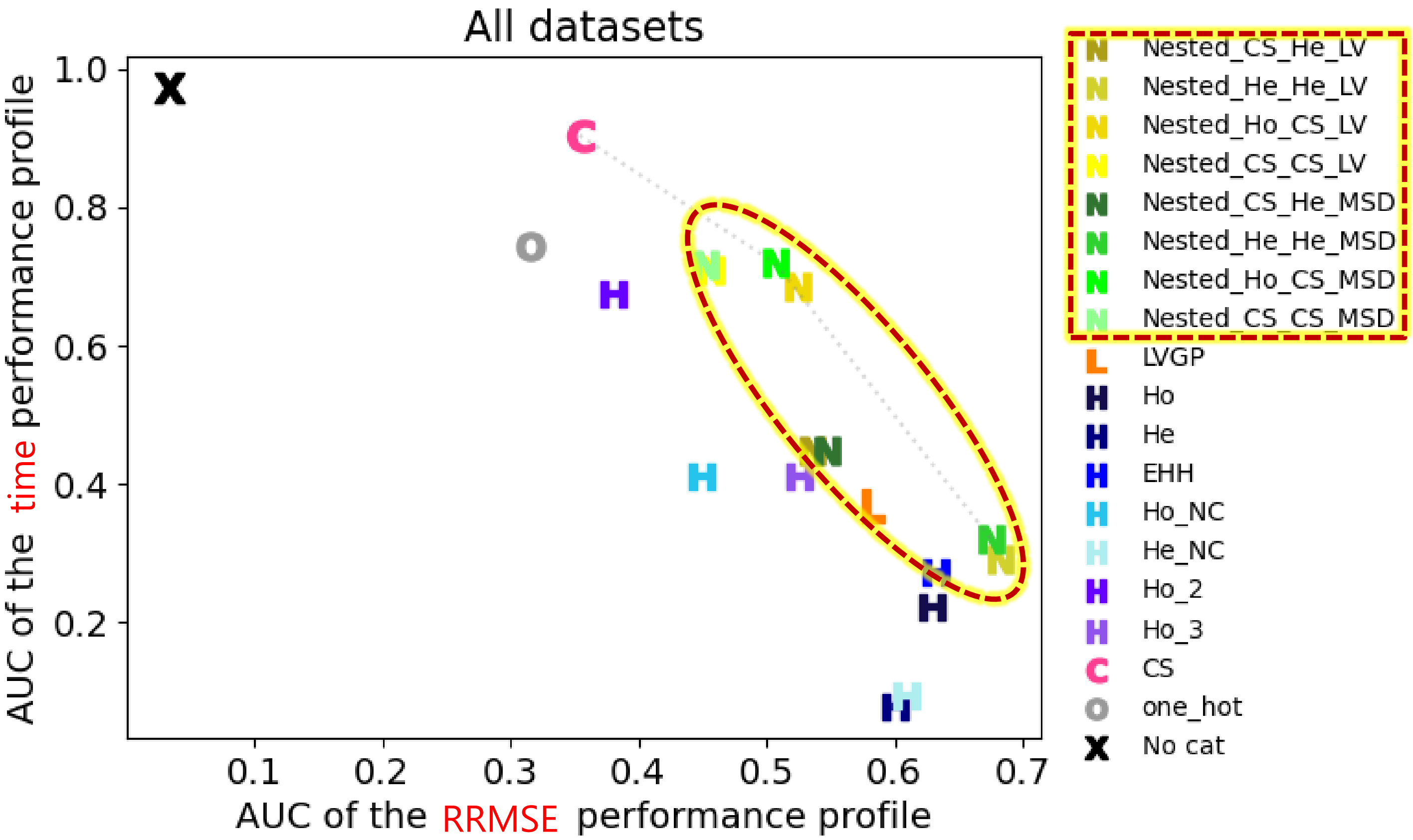

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Conclusion

Contributions

- Reproducible comparative study available at : https://gitlab.com/drti/cat_gp/
  - 23 kernels including: Hypersphere, Nested, LVGP, CS models
  - 42 datasets with varying sizes, continuous and categorical variables with different numbers of levels
  - Datasets with/without known groups
- New global evaluation metrics: **performance profiles**
- New **clustering-based nested kernels** using target encodings

Take home messages

- **Optimization** has an important impact, especially on **hypersphere** models
- **Nested kernels** outperform other kernels when groups are known
- Even when groups are unknown, they are among the best methods with the **automatic group selection** strategies

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Acknowledgments

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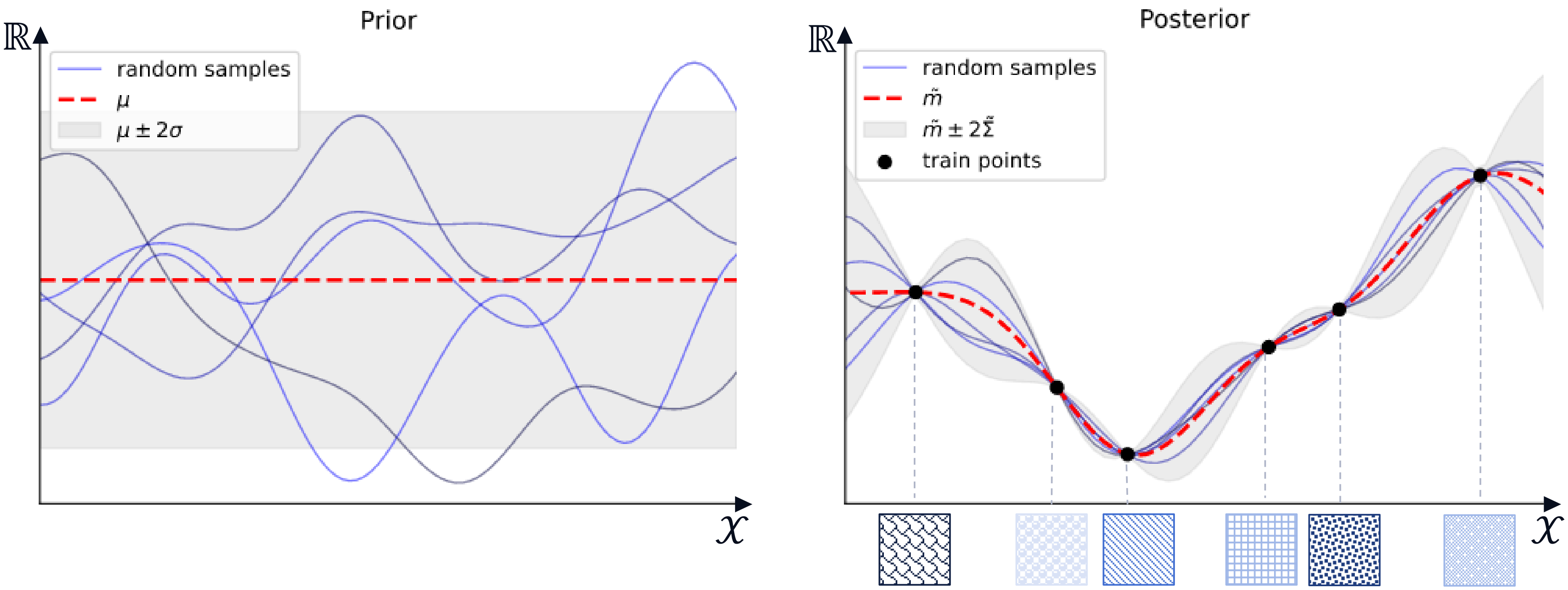
Gaussian process regression



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