

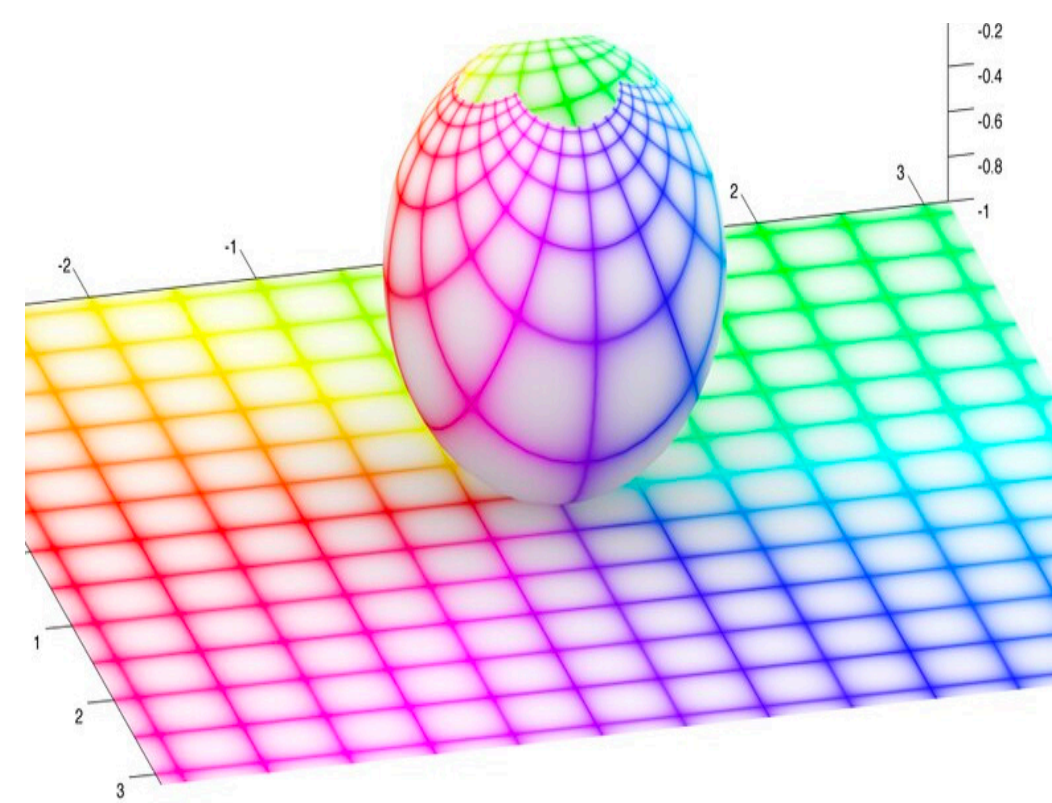
GRAMAR: Graph Machine Regression for assessing the effects of chemical exposures on health outcomes

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★★★★★ 5 ratings | 3 answered questions

About this method

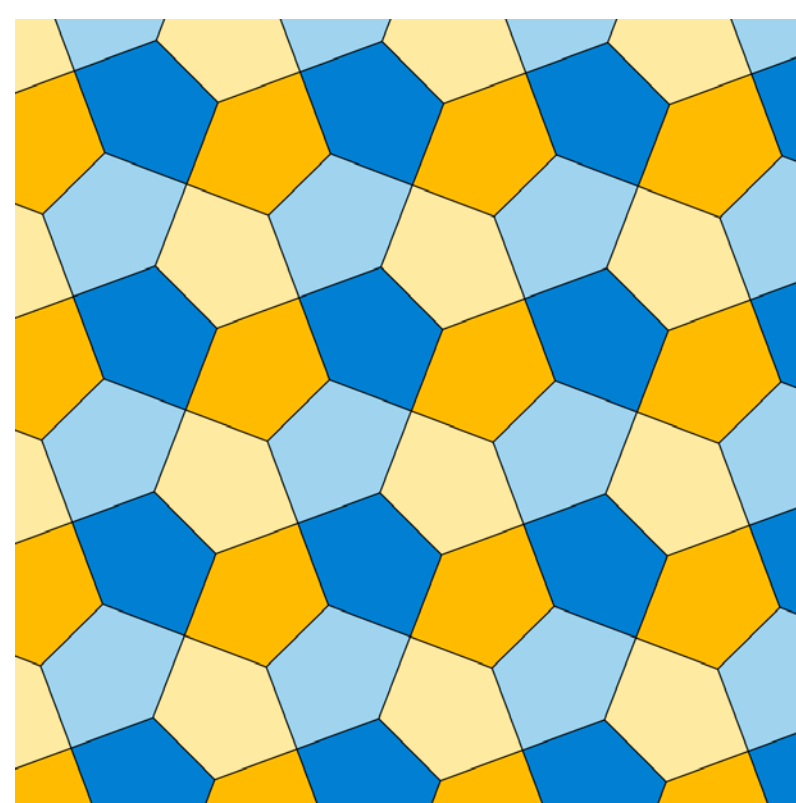
- Flexible regression modeling of large scale data in which several correlated inputs may have nonlinear effects on outputs
- Targets estimation of a smooth response surface, similar to standard GP regression
- Eliminates Gaussian process bottlenecks by inducing conditional independence
- Sparse directed acyclic graph (DAG) outlines conditional independence assumptions
- Based on successful family of methods for geostatistical data
- Based on projecting the input space to lower dimensions
- Open source R packages available for a variety of settings (incl. univariate, multivariate, multi-type, GP factor models)

Steps to reproduce this method



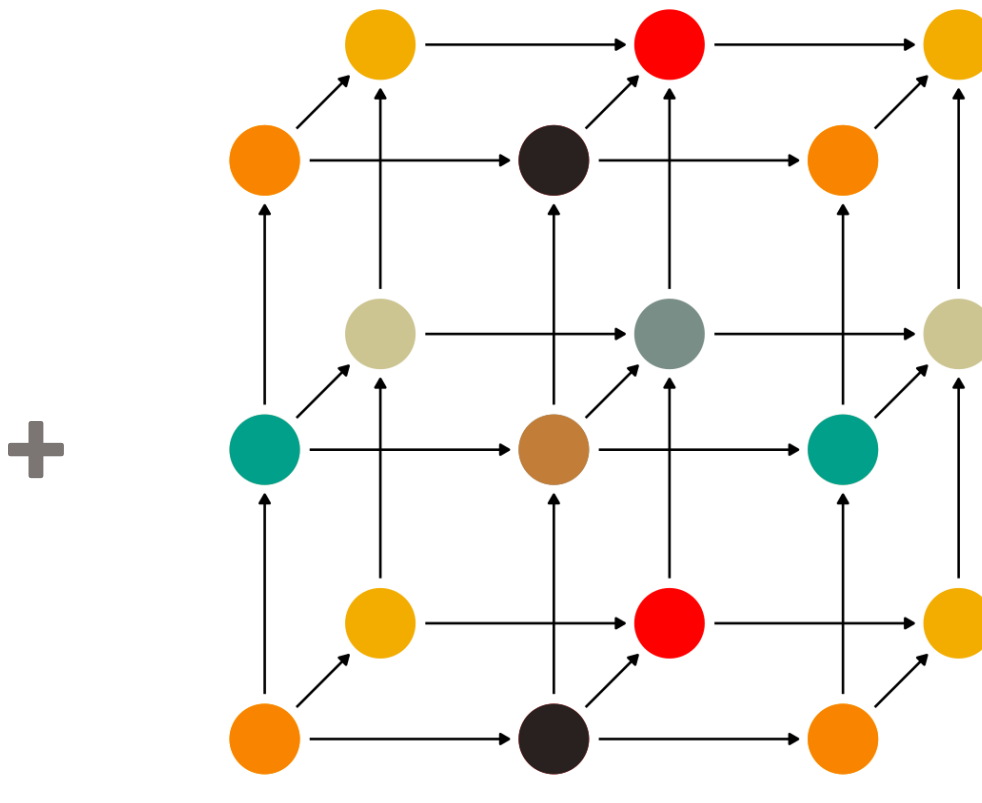
Project input space into a lower dimensional space:

- PCA
- Laplacian Eigenmaps
- other feature-preserving projections



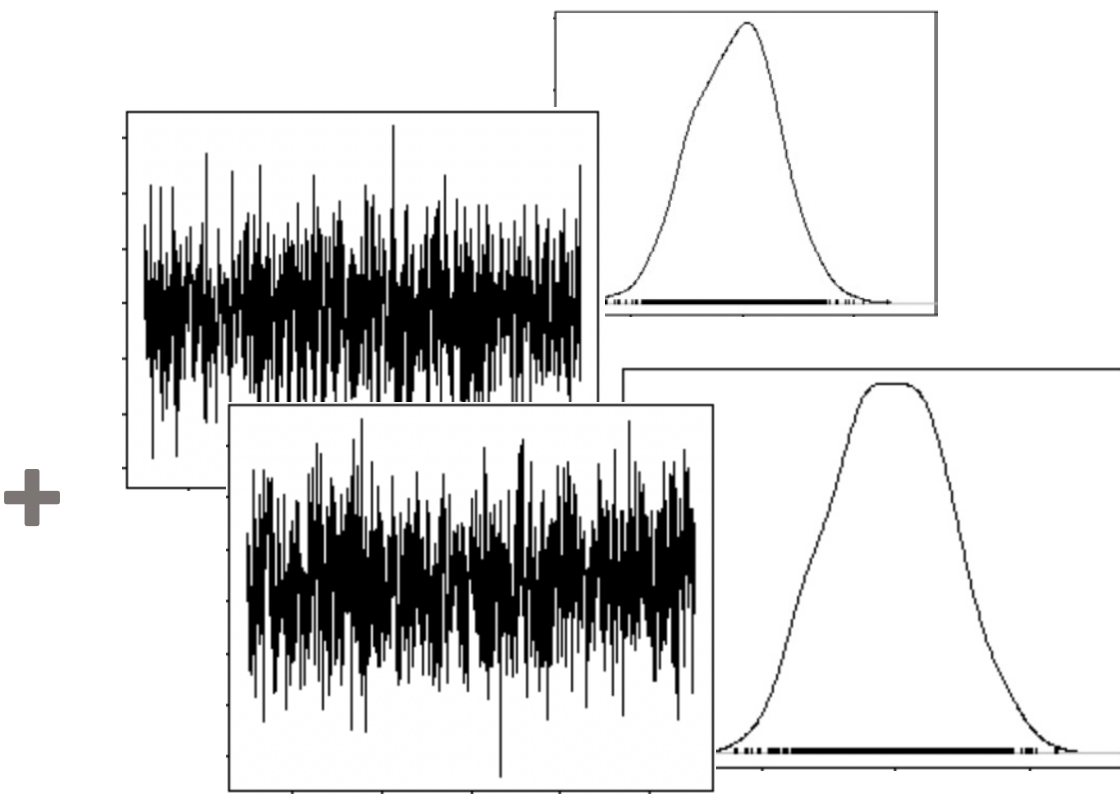
Partition the newly-created input space

- Voronoi tessellation
- axis-parallel
- naive
- others



Link each region to a node in a DAG. Assume DAG is sparse.

- Fast density evaluation in original input space
- Graph coloring



Posterior sampling via MCMC:

- collapsed: sparse Cholesky
- non-collapsed: parallel Gibbs/Langevin/HMC

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Technical specifications

Input space dimension	Suppose $z_i \in \mathbb{R}^d$ is a vector of inputs for subject i . We store all subjects' inputs in matrix \mathbf{Z} .
Target model	$y_i = \mathbf{x}_i^\top \boldsymbol{\beta} + f(z_i) + \varepsilon_i$, $\varepsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$, assume $f(\cdot) \sim \Pi_\theta$. At \mathbf{Z} , in vector form $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{f}_\mathbf{Z} + \boldsymbol{\varepsilon}$.
Projection step	Project \mathbf{Z} to \mathbf{Z}^* so that $z_i^* \in \mathbb{R}^2$. On the new space, we can build a sparse DAG process (MGP, NNGP, MRA, SpamTrees, Vecchia-like).
Sparse GP choice	If MGP, then \mathbf{Z}^* is partitioned into m blocks. If NNGP, then for every z_i^* we have a list of neighbors.
DAG factorization	Partition & sparse DAG factorization: $\pi_\theta(\mathbf{f}_\mathbf{Z}) = N(\mathbf{f}_1; \mathbf{0}, \mathbf{C}_1)N(\mathbf{f}_2; \mathbf{H}_2 \mathbf{f}_{\text{Pa}(2)}, \mathbf{R}_2) \cdots N(\mathbf{f}_m; \mathbf{H}_m \mathbf{f}_{\text{Pa}(m)}, \mathbf{R}_m)$. Note that \mathbf{Z} (and thus, $\mathbf{f}_\mathbf{Z}$) is also partitioned into m blocks $\{z_1, \dots, z_m\}$, each of which is 1:1 with the partition in \mathbf{Z}^* space.
Notation for conditional Gaussians	Product of conditional Gaussians: $\mathbf{H}_i = \mathbf{C}_{i, \text{Pa}(i)} \mathbf{C}_{\text{Pa}(i)}^{-1}$, $\mathbf{R}_i = \mathbf{C}_i - \mathbf{H}_i \mathbf{C}_{\text{Pa}(i), i}$ using a pre-specified kernel operating on \mathbf{Z} (thus, unrelated to the specific chosen projection)
MCMC computations	Graph coloring leads to parallel Gibbs. Sparse DAG leads to sparse precision matrix and fast collapsed samplers.

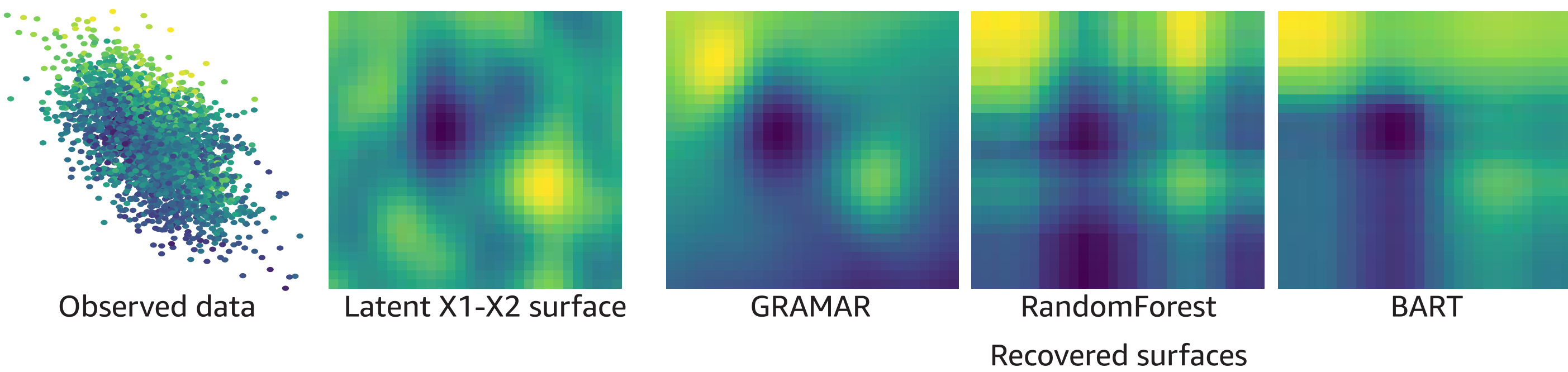
User reviews

Yurin Competent

★★★★★ Almost gave up on GPs, until I found GRAMAR!

Size: n=3000, d=15 | Verified analysis

I tried this on some simulated data with 15 correlated inputs. Lo and behold this thing crunches numbers F A S T, 50x faster than BKMR!

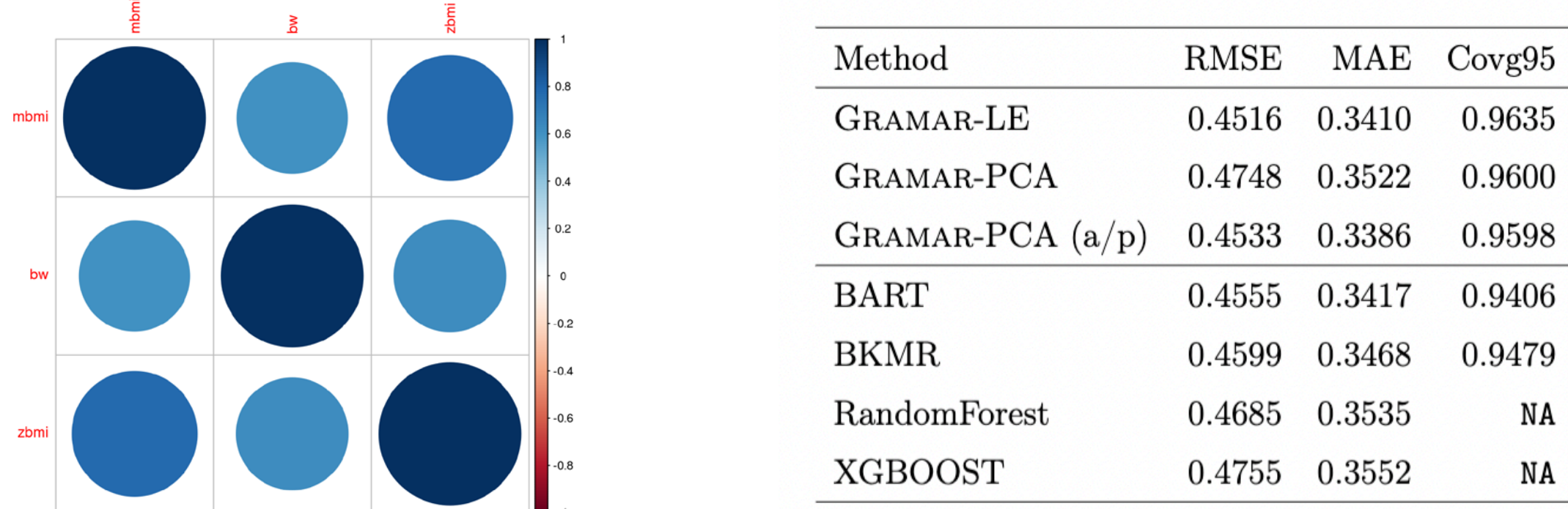


Imma Jenyius

★★★★★ Works well on HELIX exposure data

Size: n=1096, d=51 | Verified analysis

I used GRAMAR on a multivariate outcome to estimate latent correlations. Fantastic! It only took 33 seconds when BKMR doesn't even work on multivariate outcomes and takes minutes for univariate data!



Get to Know Us

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Analyze Data with Us

The **grammar** R package
github.com/mkln/grammar
The **meshed** R package
CRAN.R-project.org/package=meshed

Let Us Help You

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