

Augmented Spline Regression for Advanced Data Analysis: Generalized Additive Models & Functional Gradient Boosting with Geometrically Designed (GeD) Splines

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Geometrically Designed Splines (GeDS)

Free-knot spline regression technique based on a ***residual-driven (locally-adaptive) knot insertion scheme*** that produces a piecewise linear spline fit, over which ***smoother higher order spline fits*** are subsequently built (Kaishev et al., 2016, Dimitrova et al., 2023).

* GeD spline methodology is extended further by:

1. **GAM-GeDS**: encompassing **Generalized Additive Models (GAM)**, thereby making GeDS highly multivariate.
2. **FGB-GeDS**: incorporating **Functional Gradient Boosting (FGB)**, improving the construction of the underlying spline regression model.

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- Applications in highly multivariate contexts: AI (e.g., image recognition/processing); robotics (e.g. motion planning for humanoid robots).
 - Implemented in the R package **GeDS**, available from CRAN:
<https://cran.r-project.org/package=GeDS>

4. Functional Gradient Boosting with GeDS (FGB-GeDS)

- Functional Gradient Boosting (Friedman, 2001).

* FGB-GeDS deals with major limitations of mainstream boosting algorithms:

- "Prone to overfitting"
 - ➡ Optimal number of boosting iterations determined by a **stopping rule** based on a ratio of consecutive deviances.
- "Large number of parameters and unstable performance"
 - ➡ Strength of the base learners is **automatically regulated by the GeDS** technique itself, and flexibly controlled through the GeDS parameters.
- "Black-box models"
 - ➡ Final FGB-GeDS boosted model expressed as a **single spline model**, which simplifies its evaluation and enhances interpretability.

Task: Fourier Transform Computation of Materials Science Data

Given a sample, $\mathcal{L} = \{F(Q_i), Q_i\}_{i=1}^N$, $0 < Q_1 < \dots < Q_N < \tilde{Q}_{\max}$, we are interested in estimating the **Fourier transform** (imaginary part):

$$G(r) = \frac{2}{\pi} \int_0^{Q_{\max}} F(Q) \sin(Qr) dQ.$$

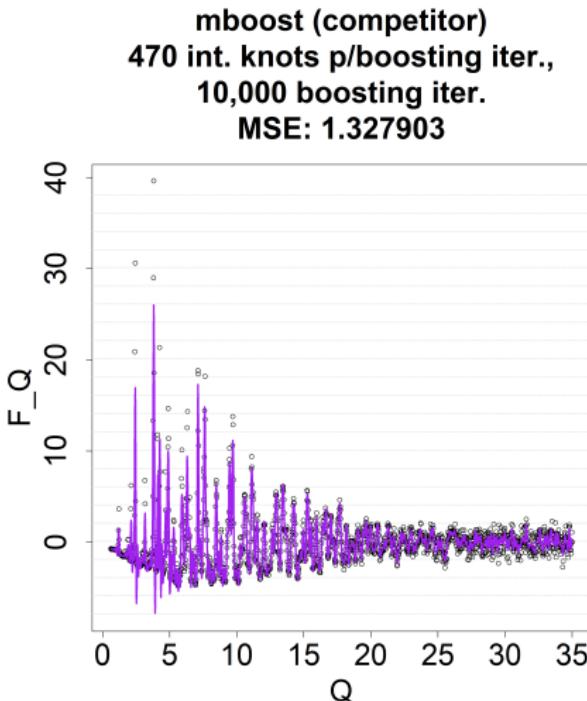
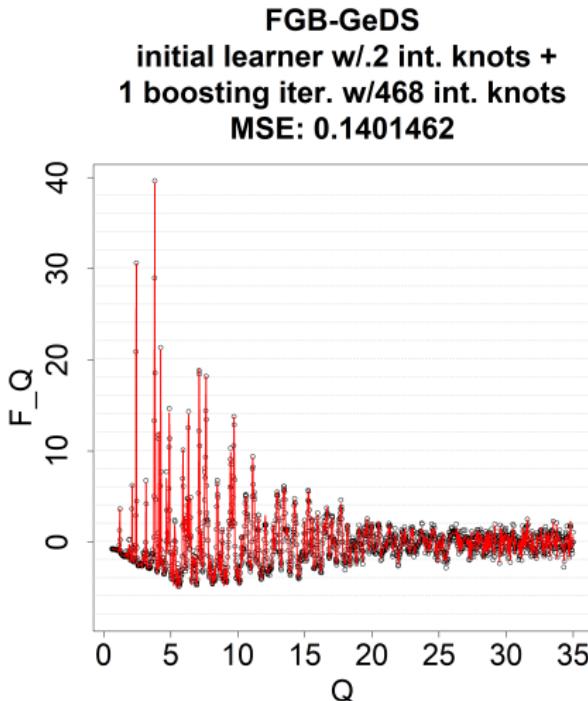
Assuming Q_{\max} is known, this involves two steps:

- Step 1.** Estimate $F(Q)$ through a GeDS fit $\equiv S(Q)$ to the sample \mathcal{L} .
- Step 2.** Compute $G(r)$ using the fitted GeDS model, $S(Q)$.

For the time being, let us assume $Q_{\max} \equiv \tilde{Q}_{\max}$, though in general $Q_{\max} < \tilde{Q}_{\max}$:

- ➡ Signal in the data prevails up to a certain point; beyond this, only noise remains.
- ➡ Sequential (and costly) data collection: cut off at the appropriate Q_{\max} for an optimal experimental design.

Step 1. Fit $F(Q)$, e.g., with an FGB-GeDS model



Step 2. Compute the Fourier transform of gold

Proposition

For the $\sin()$ transform,

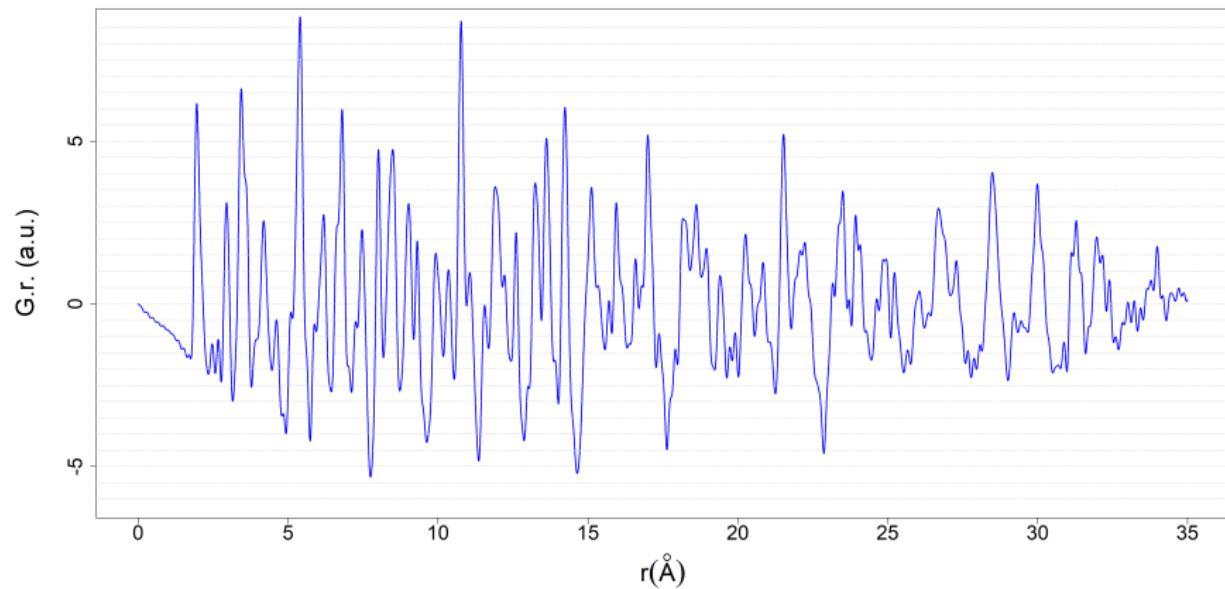
$$G(r) = \frac{2}{\pi} \int_0^{Q_{\max}} F(Q) \sin(Qr) dQ$$

of the function $F(Q)$, approximated by $S(Q)$ of order $n = 2s$, $s = 1, 2, 3, \dots$ we have

$$G(r) \approx \frac{(-1)^s 2(n-1)!}{\pi r^n} \sum_{i=1}^p \hat{\theta}_i (t_{i+n} - t_i) \sum_{j=i}^{i+n} \frac{\sin(t_j r)}{\prod_{\substack{l=i \\ l \neq j}}^{i+n} (t_j - t_l)},$$

where $r \in \mathbb{R}^+$, $p = k + n$; $\hat{\theta}_i$, $i = 1, \dots, p$ are the GeDS regression coefficients.

Step size of r is 0.01



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