Enhancing Geometrically Designed Spline (GeDS) Regression through Generalized Additive Models and Functional Gradient Boosting

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1. Motivation

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  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

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- **STAGE A** constructs a least squares linear spline fit to the data.
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- **STAGE B**
  - Builds smoother higher order spline fits using Schoenberg's variation diminishing spline (VDS) approximation, based on the linear fit from Stage A.
  - For each higher spline order (quadratic, cubic...), compute the *averaging knot location* and re-estimate the spline coefficients by LS.

Properties of GeDS estimated knots and regression coefficients:

- *Schoenberg variation diminishing optimality* of the estimated knots (Kaishev et al., 2006b).
- *Asymptotic normality* of estimators in the case of normal noise, which allows for the construction of pointwise asymptotic confidence intervals that effectively converge (Kaishev et al., 2006a).
- Asymptotic conditions on the rate of growth of the knots for *negligible bias/variance ratio* (Kaishev et al., 2006a).

3. Generalized Additive Models with GeDS

The **Generalized Additive Model (GAM)** assumes the response variable, $Y \sim E.F.$, and relates its conditional expectation, $\mu = \mathbb{E}\left[Y|X\right]$, to the predictor variables, $X_1, ..., X_P$, via a link function $g(\cdot)$:

$$g(\mu) = \alpha + \sum_{j=1}^{P} f_j(X_j), \text{ with } \mathbb{E}\left[f_j(X_j)\right] = 0, \quad j = 1, ..., P \tag{1}$$

Hastie and Tibshirani, 1990 — *local-scoring* and *backfitting* algorithms in conjunction with scatterplot smoothers, to fit GAMs.

GAM with GeD Splines: Local-scoring algorithm using GeD splines as the function smoothers, f_j, within the backfitting algorithm.

3.1. Simulated data application

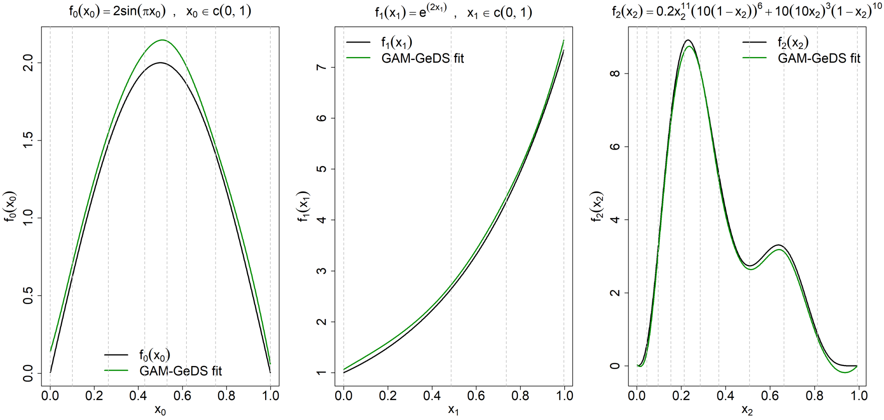
Consider the function (Gu and Wahba, 1991):

$$f(\mathbf{x}) = \underbrace{2 \times \sin(\pi \times x_0)}_{f_0(x_0)} + \underbrace{\exp(2x_1)}_{f_1(x_1)} + \underbrace{0.2x_2^{11}(10(1-x_2))^6 + 10(10x_2)^3(1-x_2)^{10}}_{f_2(x_2)}$$

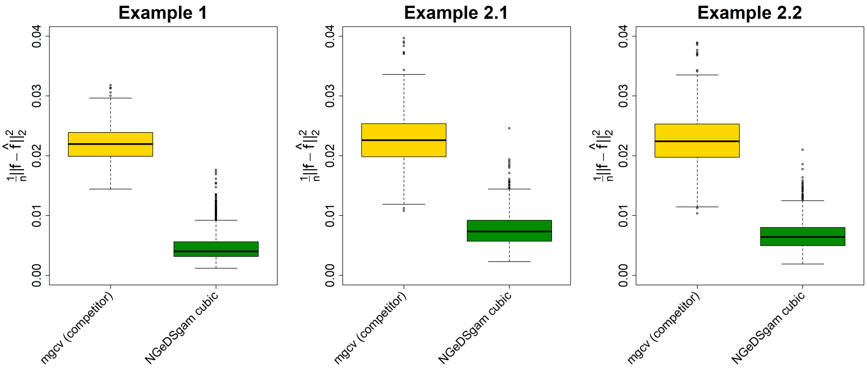
- **Example 1:** Fit $y = f(\mathbf{x}) + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$, and also include a noise predictor x_3.
- **Example 2:** replace $f_0(x_0)$ by a factor variable x_0 with 4 levels.
  - **2.1**: Include the noise predictor x_3.
  - **2.2**: Delete the noise predictor x_3.

➥ Generate $1,000$ random samples, $\{X_i, Y_i\}_{i=1}^N$, with $N = 400$ for example 1 and $N = 200$ for example 2; $x_0, x_1, x_2, x_3 \sim$ Uniform$(0, 1)$.

Example 1: GAM-GeDS (partial) fits



Example 1, 2.1 & 2.2: MSE boxplots



4. Functional Gradient Boosting with GeDS

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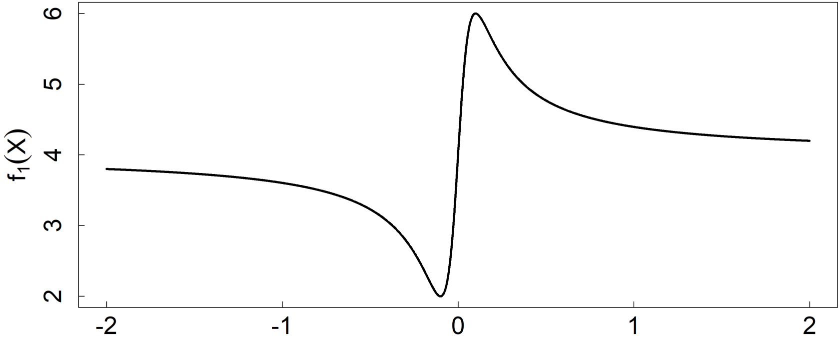
- **"Black-box models"**

➠ Final FGB-GeDS boosted model expressed as a **single spline model**, which simplifies its evaluation and enhances interpretability.

4.1. Simulated data application

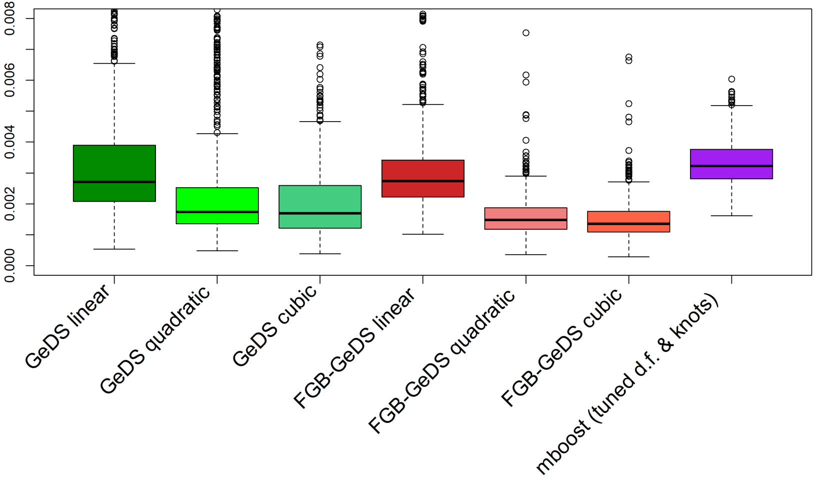
Consider the following function:

$$f_1(x) = 40\frac{x}{1+100x^2} + 4 \quad , \quad x \in c(-2, 2)$$

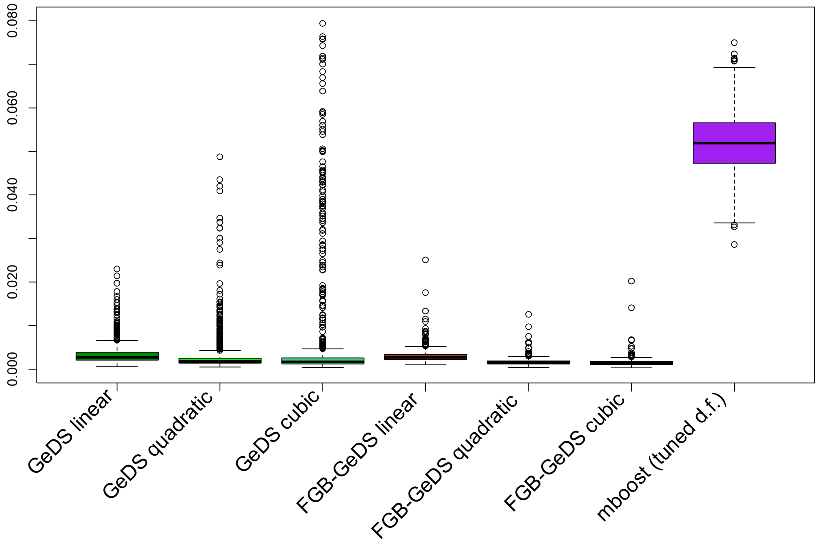


- For each, generate $1,000$ random samples, $\{X_i, Y_i\}_{i=1}^{N}$ with $Y_i \sim \mathcal{N}(\mu_i, \sigma)$, $\sigma = 0.2$, $\mu_i = \eta_i = f_1(X_i)$.

GeDS	10 int. knots
FGB-GeDS	Init. learner with 2 int. knots + 1 boosting iter. with 8 int. knots
mboost (competitor)	10,000 boosting iter. with 36 int. knots per iter.



➠ And setting **mboost** to have 10 int. knots p/boosting iter. (i.e., $\simeq$ **FGB-GeDS**):



4.2 Task: Fourier Transform Computation of Materials Science Data

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

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

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, $S(Q)$.

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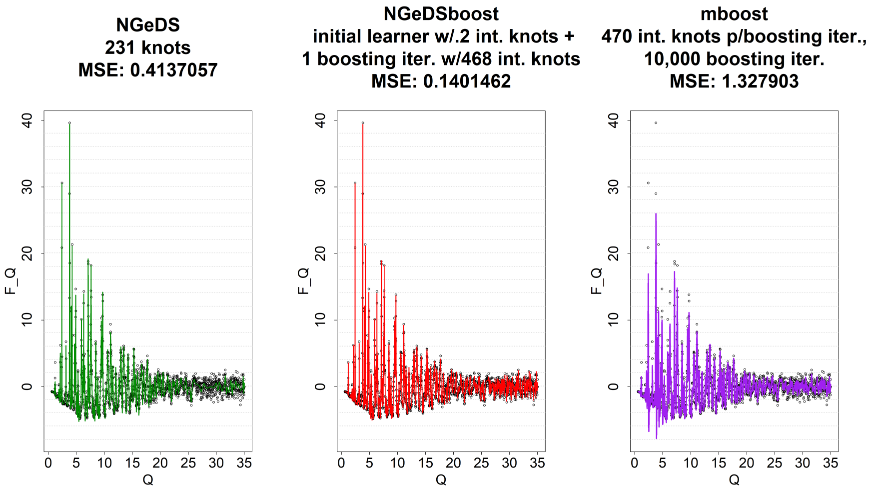
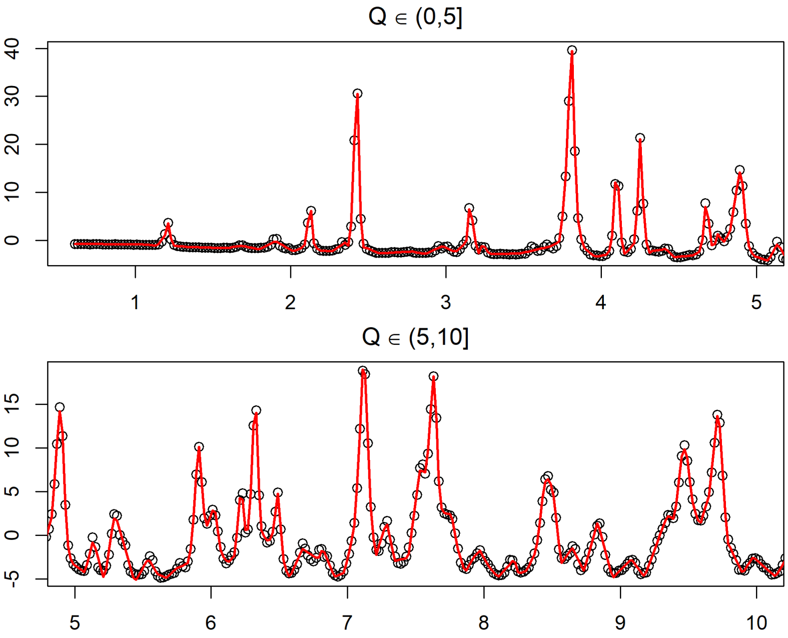
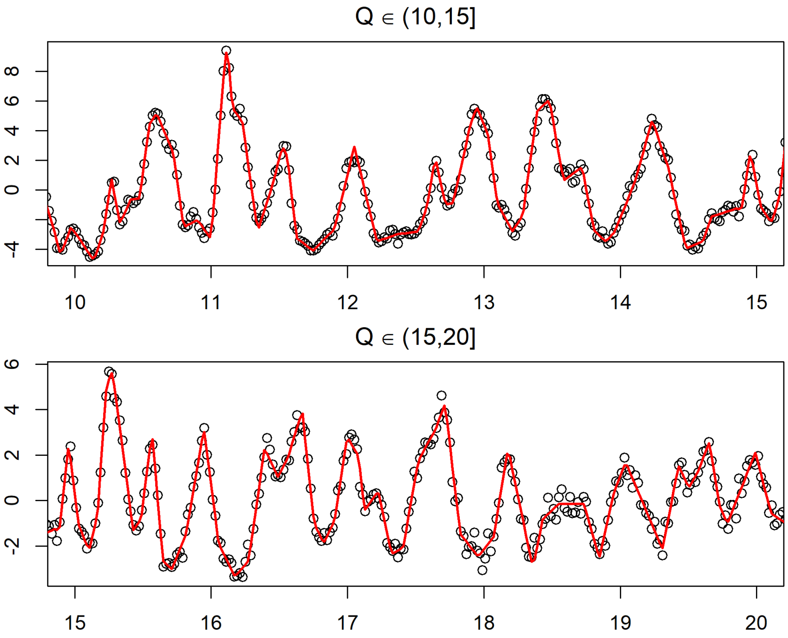
For the time being, let us assume $Q_{\text{max}} \equiv \widetilde{Q}_{\text{max}}$, though in general $Q_{\text{max}} < \widetilde{Q}_{\text{max}}$:

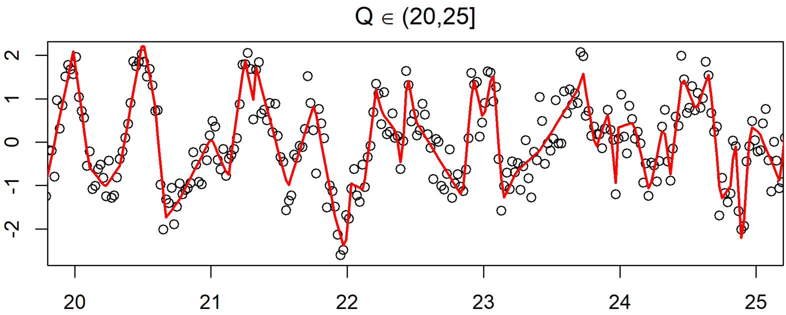
- Signal in the data prevails up to a certain point; beyond this, only noise remains.
- Sequential (and costly) data collection: cut off at the appropriate Q_{max} for an optimal experimental design.

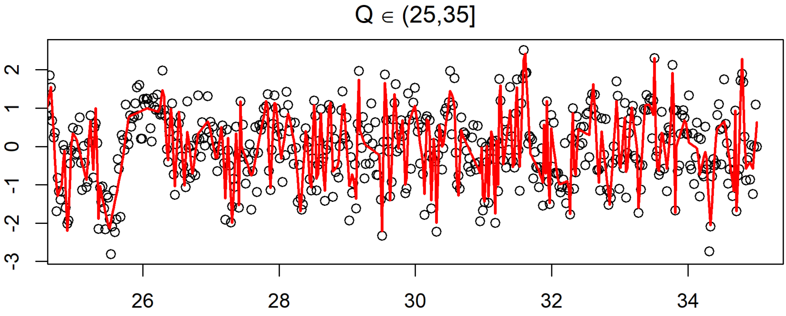
Step 1. Fit $F(Q)$, e.g, with a GeDS model




Q ∈ (0,5]
40
30
20
10
0
1
2
3
4
5
Q ∈ (5,10]
15
10
5
0
-5
5
6
7
8
9
10


Q ∈ (10,15]
8
6
4
2
0
-4
10
11
12
13
14
15
Q ∈ (15,20]
6
4
2
0
-2
15
16
17
18
19
20


Q ∈ (20,25]
2
1
0
-1
-2
20
21
22
23
24
25


Q ∈ (25,35]
2
1
0
-1
-2
-3
26
28
30
32
34

Step 2. Compute the Fourier transform

Proposition

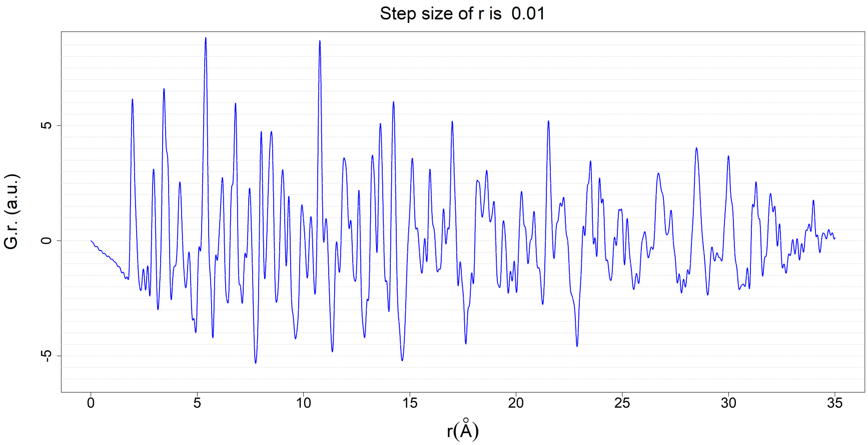
For the $\sin()$ transform,

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

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

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

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


Step size of r is 0.01
G.r. (a.u.)
r(Å)
-5
0
5
0
5
10
15
20
25
30
35

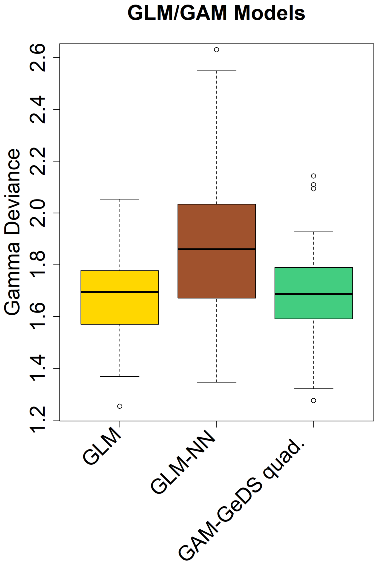
5. Insurance data application

$\underbrace{\text{Motorcycle insurance data swmotorcycle available through the R package CASdatasets (Dutang and Charpentier, 2020).}}$

$\longrightarrow$ We follow Delong et al., 2021 and model **gamma claim sizes**:

1. Gamma GLM regression + Gamma Neural Network regression.
2. `mboost`: FGB with P-splines.
3. GAM-GeDS.
4. FGB-GeDS.

- *Response*: `ClaimAmount/ClaimNb`, i.e., the average claim size.
- *Covariates*: `OwnerAge`; `Gender`; `Area`, `RiskClass`; `VehAge`.
- *Train/Test split*: **80%/20%**.
  - Simulate $\underline{100}$ different splits of data.


GLM/GAM Models
Gamma Deviance
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
GLM
GLM-NN
GAM-GeDS quad.

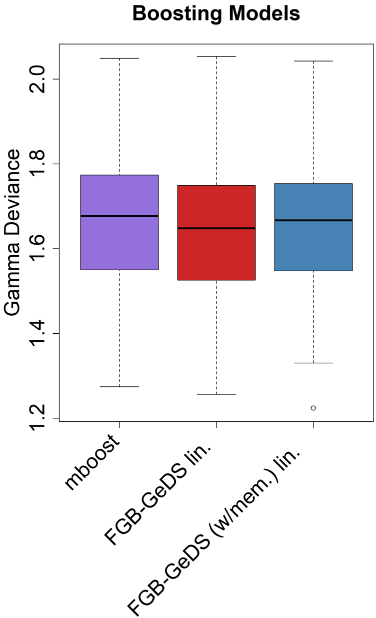

Boosting Models
Gamma Deviance
1.2
1.4
1.6
1.8
2.0
mboost
FGB-GeDS lin.
FGB-GeDS (w/mem.) lin.

Table 1: GLM/GAM Models

	Gamma Deviance			Internal knots
	Train Data	Test Data	Time (sec.)	(OwnerAge+VehAge)
GLM	1.585727	1.694797	0.008708	-
GLM NN	1.719903	**1.859394**	167.224576	-
GAM-GeDS quadratic	1.557612	**1.686492**	0.671260	5

Table 2: Boosting Models

	Gamma Deviance			Internal knots	Boosting
	Train Data	Test Data	Time (sec.)	p/boosting iter. (OwnerAge+VehAge)	iterations
mboost	1.610290	**1.676810**	0.156095	4	100
FGB-GeDS linear (2 starting knots)	1.575972	**1.648345**	0.130963	2	1
FGB-GeDS w/mem. linear (1 starting knot)	1.575536	1.667158	0.129040	1	3

Concluding remarks

- GeDS is able to perform well both with more intricate, wiggly data, as well as with more disperse data.
- Broad scope of applications (insurance data, materials science data

Further extensions:

- Quantile regression (Hendricks and Koenker, 1992).
- Varying coefficients regression (Hastie and Tibshirani, 1993).
- Density estimation.

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