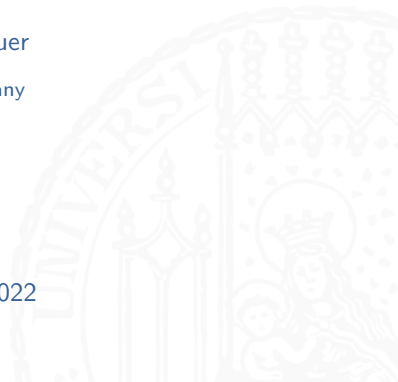


Registration for Incomplete Non-Gaussian Functional Data

Dr. Alexander Bauer

LMU Munich, Germany

JSM | August 9, 2022



LMU Munich



Fabian Scheipl



Helmut Küchenhoff



Alice-Agnes Gabriel

University of Colorado

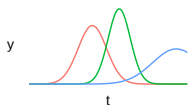


Julia Wrobel

Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



registr 2.0

Wrobel & Bauer (2021)

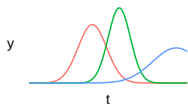


1. Conceptual Basics
2. Novel Approach
 - 2.1. Incomplete Curve Registration
 - 2.2. Incomplete Curve GFPCA
 - 2.3. Joint Approach
3. Simulation Study
4. Implementation in registr package

Incomplete Curve Registration

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Wrobel & Bauer (2021)



1. Conceptual Basics

2. Novel Approach

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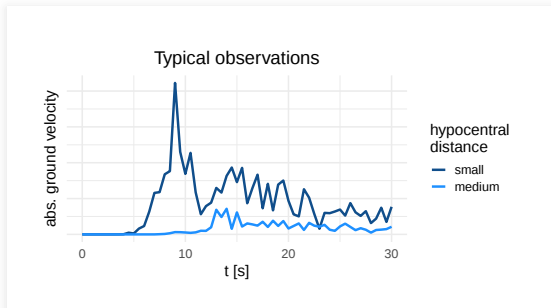
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Application with data on **seismic ground motion propagation**



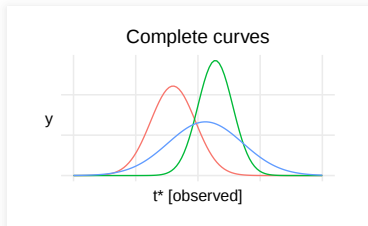
Research Question

Given the occurrence of a seismic event,
what are the driving forces for its strength?

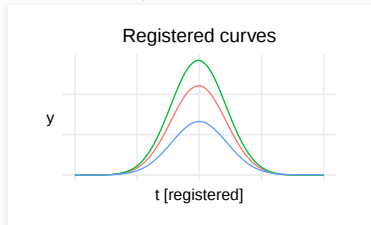
Data

135 simulations of the 1994 Northridge (US) quake,
30s recordings of ground motion at ~ 6000 seismometers

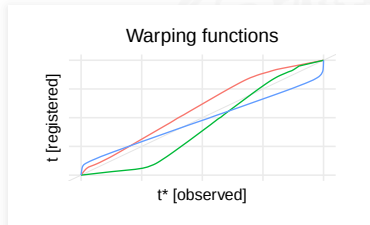
Separating amplitude and phase



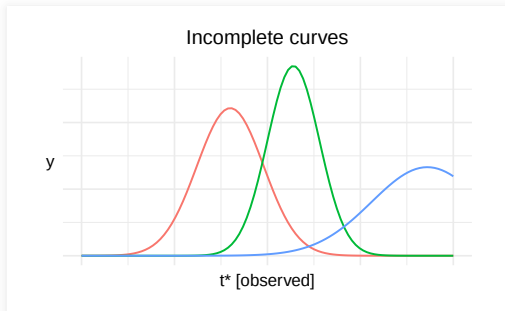
Amplitude variation



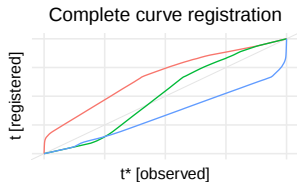
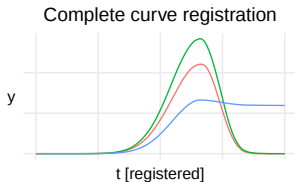
Phase variation



Challenge incomplete curves



Challenge incomplete curves



Common assumption: Processes are observed until their very end

We want a method that ...

- is able to handle incomplete curves
- is able to handle non-Gaussian data
- includes a lower-dimensional representation of the registered curves

Challenge 1

Lack of registration methods for incomplete curves

Challenge 2

Registration methods often only applicable to specific data situations

Complete, Gaussian, densely observed curves on a regular grid

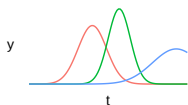
Challenge 3

Lack of good software packages for incomplete curve registration.

Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



registr 2.0

Wrobel & Bauer (2021)



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Notation

$Y_i(t_i^*)$	curve of subject $i = 1, \dots, N$, observed over <i>chronological time domain</i> $T_i^* = [t_{\min,i}^*, t_{\max,i}^*]$
$T = [0, 1]$	<i>internal time domain</i> , with $T_i^* \subseteq T \forall i$
$h_i^{-1} : T_i^* \mapsto T$	inverse warping functions
$Y_i(t) = Y_i(h_i^{-1}(t_i^*))$	aligned curve of subject i

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$h_i^{-1} : T_i^* \mapsto T$	inverse warping functions
$Y_i(t) = Y_i(h_i^{-1}(t_i^*))$	aligned curve of subject i
n_i	number of measurements for curve i
$T_i^* = [t_{\min,i}^*, 1]$	leading incompleteness
$T_i^* = [0, t_{\max,i}^*]$	trailing incompleteness
$T_i^* = [t_{\min,i}^*, t_{\max,i}^*]$	full incompleteness

Only few approaches exist for **registering incomplete curves**

- **Dynamic Time Warping** methods developed for matching time series
 - ⚡ Computationally quite expensive & mostly very heuristic algorithms
- **Bayesian approach** for *fragmented functional data* Matuk et al. (2019)
 - ⚡ Computationally quite expensive
- **SRVF-based approach** for *elastic partial matching* Bryner & Srivastava (2021) based on the **S**quare-**R**oot **V**elocity **F**unction framework
 - Joint estimation scheme for complete curve SRVF and linear domain scaling
 - ⚡ Limited to continuous data & based on derivatives

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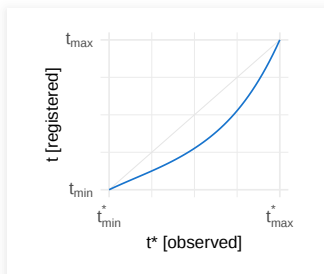
Extend the complete curve **likelihood-based framework** of Wrobel et al. (2019)

- ✓ Applicable for exponential family distributions
- ✓ Joint estimation scheme with Gaussian or Binomial FPCA

Aim: Map the chronological domains T_i^* onto the registered domain T

⇒ **Inverse warping functions** h_i^{-1} map curve $Y_i(t_i^*)$ onto a template $\mu_i(t)$:

$$E[Y_i(h_i^{-1}(t_i^*)) | h_i^{-1}] = \mu_i(t).$$



⇒ Warping functions have to be **monotone and domain-preserving**

Low-dimensional **B-spline representation** of inverse warping functions:

$$h_i^{-1}(t_i^*) = \Theta_h(t_i^*)\beta_i$$

Notation	
Θ_h	design matrix of K_h basis functions, $\in \mathbb{R}_{n_i \times K_h}$
β_i	coefficient vector, $\in \mathbb{R}_{K_h \times 1}$

Low-dimensional **B-spline representation** of inverse warping functions:

$$h_i^{-1}(t_i^*) = \Theta_h(t_i^*)\beta_i$$

Optimization of the **exponential family log-likelihood** for curve i :

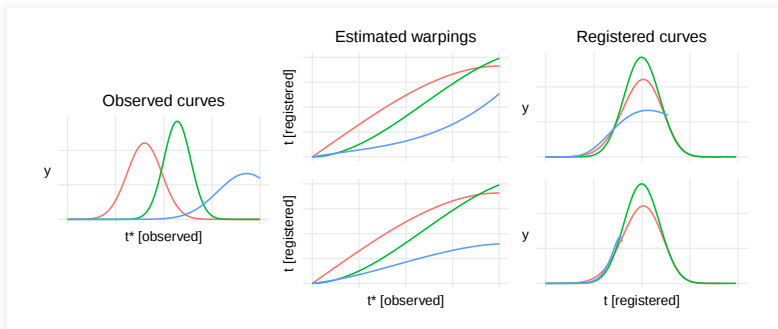
$$\ell(h_i^{-1}|y_i, \mu_i) = \log \left(\prod_{j=1}^{n_i} f_{i,j} [y_i(t_{i,j}^*)] \right),$$

with $f_{i,j}(\cdot)$ the corresponding density with expected value $\mu_i(h_i^{-1}(t_{i,j}^*))$,
and conditional independence

- across functions $[Y_i \perp Y_{i'}] | \mu_i, \mu_{i'}$,
- within functions $[Y_i(t_{ij}) \perp Y_i(t_{ik})] | \mu_i$.

Ensure reasonable warping functions $h_i^{-1}(t_i^*)$

- A constrained optimizer ensures **monotony and domain-preservation** ✓
- Further, they should produce **scientifically reasonable distortions**



Circumventing fixed time intervals

- Allow warping functions to start and / or end anywhere in the overall domain
- Penalize how much the duration of the (observed) time domain is warped

Penalized log-likelihood for full incompleteness

$$\ell_{\text{pen}}(h_i^{-1}|y_i, \mu_i) = \ell(h_i^{-1}|y_i, \mu_i) - \lambda \cdot n_i \cdot \text{pen}(h_i^{-1}),$$

with
$$\text{pen}(h_i^{-1}) = ([h_i^{-1}(t_{\max,i}^*) - h_i^{-1}(t_{\min,i}^*)] - [t_{\max,i}^* - t_{\min,i}^*])^2.$$

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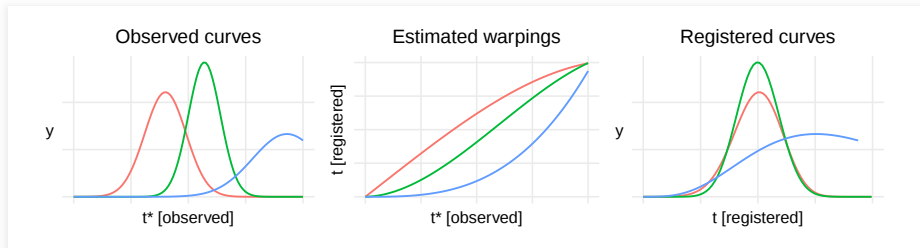
Simplification for trailing incompleteness (with $h_i^{-1}(t_{\min,i}^*) = t_{\min,i}^* \forall i$):

$$\text{pen}(h_i^{-1}) = [h_i^{-1}(t_{\max,i}^*) - t_{\max,i}^*]^2.$$

Incomplete Approach

Manually choose λ based on domain knowledge

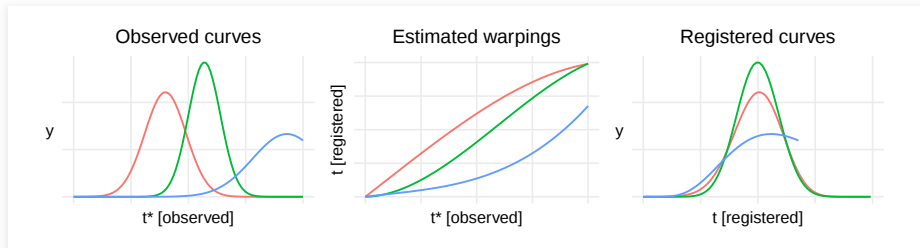
Example: Using a **way too high value**, $\lambda = 10$



Incomplete Approach

Manually choose λ based on domain knowledge

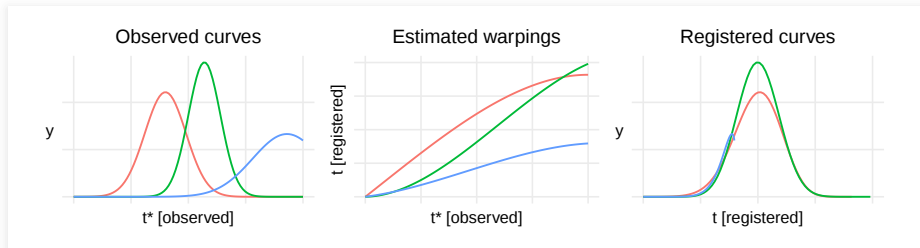
Example: Using a **too high value**, $\lambda = 1$



Incomplete Approach

Manually choose λ based on domain knowledge

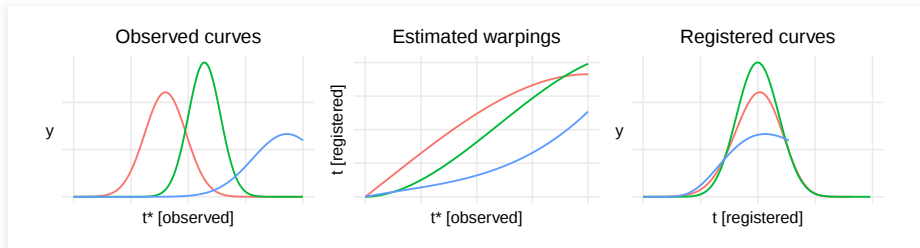
Example: Using a **too low value**, $\lambda = 0$



Incomplete Approach

Manually choose λ based on domain knowledge

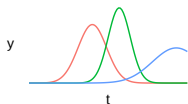
Example: Using a **fitting value**, $\lambda = 0.25$



Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



registr 2.0

Wrobel & Bauer (2021)



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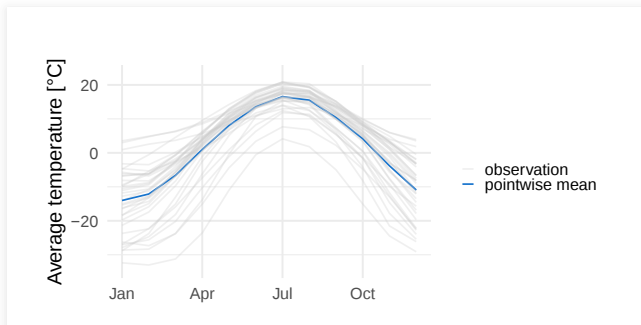
4. Implementation in registr package

Generalized FPCA

Concept of **Functional Principal Component Analysis**

- Estimation of **main modes of variation** around the mean curve
- Can be performed similarly to scalar PCA
taking the eigenvalues of the covariance structure

Example: Canadian weather data Ramsay & Silverman (2005)

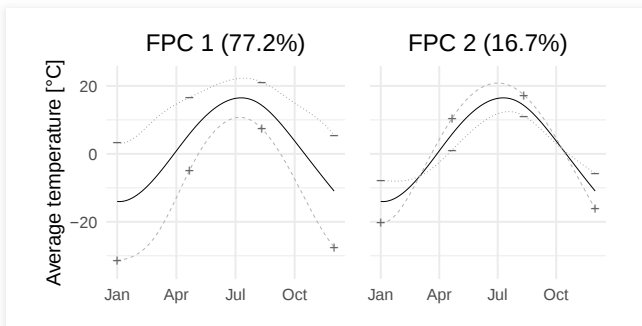


Generalized FPCA

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Example: Canadian weather data Ramsay & Silverman (2005)



Adapt the **two-step approach** of Gertheiss et al. (2017)

Combination of a nonparametric covariance estimator and a Functional Mixed Model

- ✓ Applicable to diverse exponential family settings
- ✓ Availability of efficient, robust software

Central sources of bias for incomplete curves

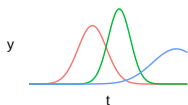
- Poor coverage of the overall domain
- Violation of MCAR assumption

⇒ (Severe) bias of mean and covariance estimators Liebl & Rameseder (2019)

Incomplete Curve Registration

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Bauer et al. (in revision)



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Iterative estimation algorithm Wrobel et al. (2019)

Aim:

- Registration of all observed curves $Y_i(t_i^*)$ to a comparable shape
- Low-rank representation of registered curves $Y_i(t) = Y_i(h_i^{-1}(t_i^*))$

Iterative estimation algorithm Wrobel et al. (2019)

1. Initialize $\hat{h}_i^{-1}(t^*)^{[0]}$: Register curves $y_i(t_i^*)$ to initial template $\mu(t)^{[0]}$

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1. Initialize $\hat{h}_i^{-1}(t^*)^{[0]}$: Register curves $y_i(t_i^*)$ to initial template $\mu(t)^{[0]}$
2. Iterate over index $q = 0, 1, \dots$
while $\sum_{i=1}^N \left(\sum_{j=1}^{n_i} \left[\hat{h}_i^{-1}(t_{i,j}^*)^{[q]} - \hat{h}_i^{-1}(t_{i,j}^*)^{[q-1]} \right]^2 \right) > \Delta_h$
 - (i) Update GFPCA using registered curves $y_i \left(\hat{h}_i^{-1}(t_i^*)^{[q-1]} \right)$
 - (ii) Re-estimate GFPCA representations $\mu_i(t)^{[q]}$
based on first $K^{[q]}$ FPCs explaining a share κ_{var} of the total variance
 - (iii) Update estimates $\hat{h}_i^{-1}(t^*)^{[q]}$ by re-registering curves $y_i(t_i^*)$ to $\mu_i(t)^{[q]}$

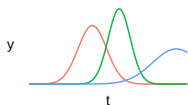
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3. Final GFPCA estimation based on registered curves $y_i \left(\hat{h}_i^{-1}(\mathbf{t}_i^*)^{[q]} \right)$
 $\Rightarrow$ representations $\mu_i(\mathbf{t})$, based on K FPCs explaining a variance share $\geq \kappa_{\text{var}}$

Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



registr 2.0

Wrobel & Bauer (2021)



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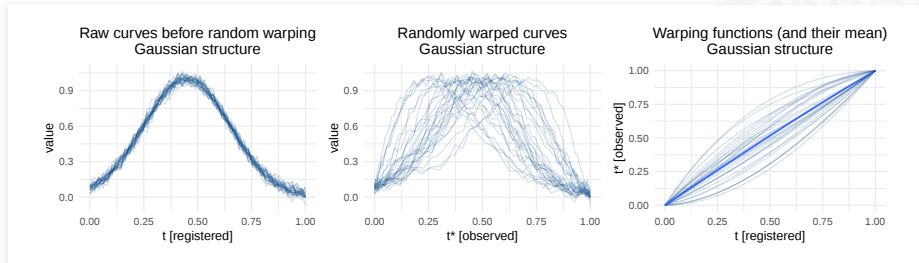
2.3. Joint Approach

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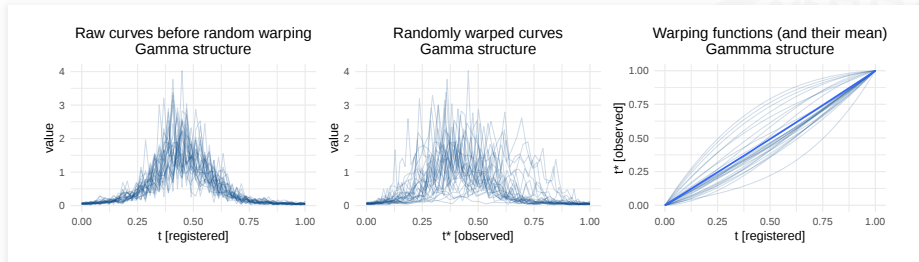
Simulation study

- Basis: Randomly warped (Gamma-transformed) Gaussian density
each setting is run 100 times with 100 curves
- Simulated weak or strong trailing incompleteness
Strong: Cut-off simulated in last 70% of the domain
- Amplitude rank $\in \{1, 2-3, 3-4\}$
also because perfect identifiability is only given for amplitude variation of rank 1

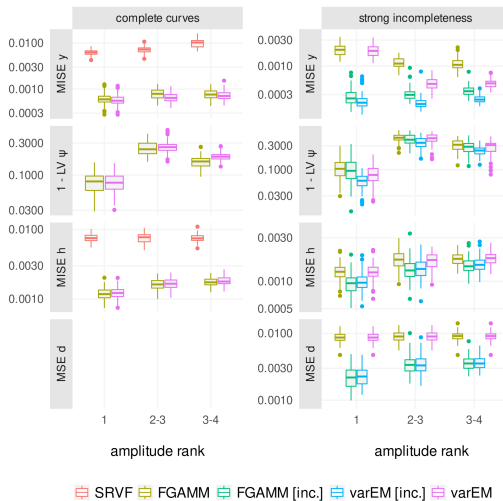


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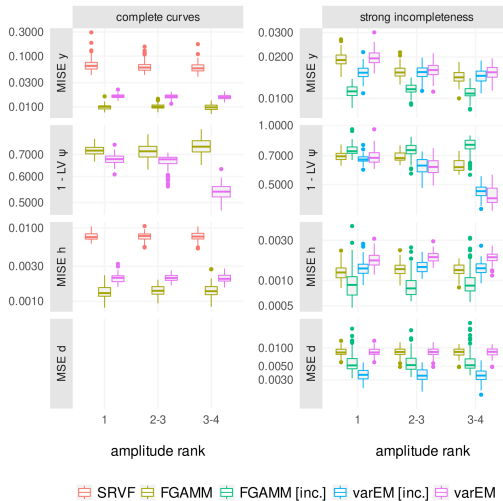


Simulation Study – Gaussian structure



► details on methods and measures

Simulation Study – Gamma structure



Results

- Overall:
Incomplete curve methods better represent the joint variation structure
- Phase:
Incomplete curve methods better estimate the warping structure
- Amplitude:
FGAMM struggles with the estimation of the FPC structure

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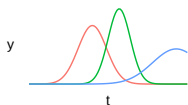
Further results

- Results are similar for weak and strong incompleteness
- Results are similar for settings with correlated amplitude and phase, and correlated amplitude and incompleteness
- FGAMM approach computationally quite inefficient
Gamma runtime on 3000 curves, each with 50 measurements: $\sim 0:27\text{h}$

Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



registr 2.0

Wrobel & Bauer (2021)



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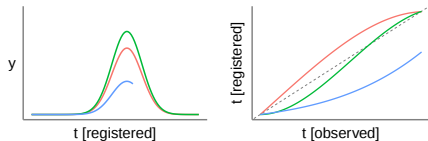
4. Implementation in registr package



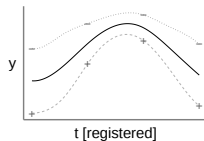
- Joint registration and GFPCA
- Applicable for leading / trailing / full incompleteness

`register_fpca()`

`registr()`



`gfPCA.twoStep()`

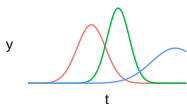


Conclusion

Incomplete Curve Registration

for non-Gaussian data

Bauer et al. (in revision)



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Wrobel & Bauer (2021)

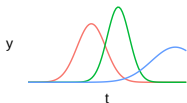


- ✓ Novel approach for incomplete curves
handling leading / trailing / full incompleteness
- ✓ Ability to handle non-Gaussian curves
on irregular, potentially sparse grids
- ✓ **registr package**
applicable to diverse data settings

Incomplete Curve Registration

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Bauer et al. (in revision)



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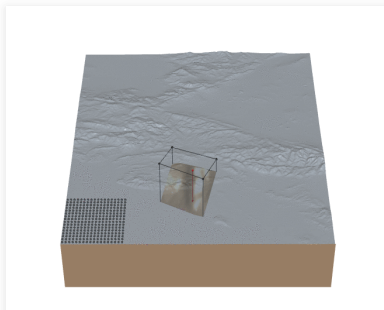


- ✓ Novel approach for incomplete curves
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 - ✓ Ability to handle non-Gaussian curves
on irregular, potentially sparse grids
 - ✓ registr package
applicable to diverse data settings
-
- > Robust & intuitive penalization
 - > Robust & efficient covariance estimation
 - > Analysis of seismic amplitude and phase

Appendix



Application with data on **seismic ground motion propagation**



Research Question

Given the occurrence of a seismic event,
what are the driving forces for its strength?

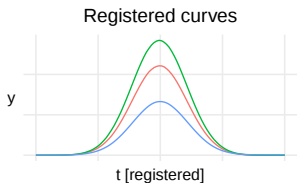
Data

135 simulations of the 1994 Northridge (US) quake,
30s recordings of ground motion at ~ 6000 seismometers

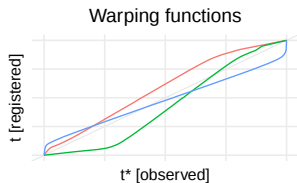
Basic structure of **registration algorithms**

1. Choose a template function
2. Choose a reasonable objective function
3. Optimize wrt. ensuring the well-definedness of warping functions

Amplitude variation



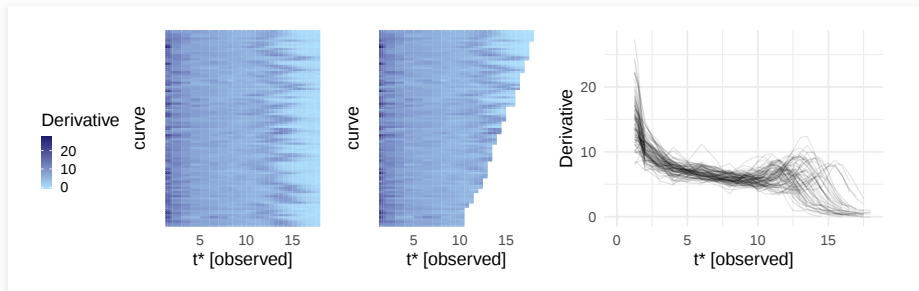
Phase variation



Incomplete Approach

Manually choose λ based on domain knowledge

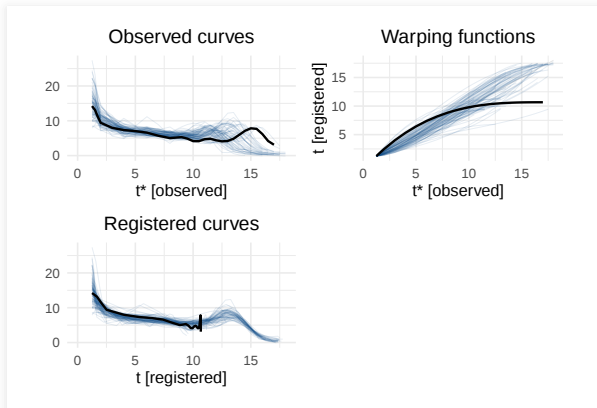
Example: **Berkeley child growth data** with simulated trailing incompleteness



Incomplete Approach

Manually choose λ based on domain knowledge

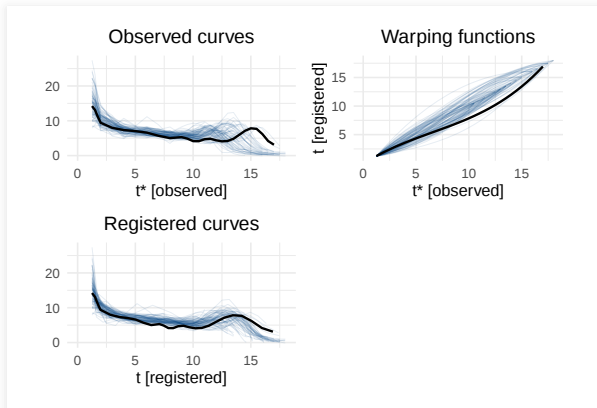
Example: **Berkeley child growth data** with simulated trailing incompleteness, using a **too small value**, $\lambda = 0$.



Incomplete Approach

Manually choose λ based on domain knowledge

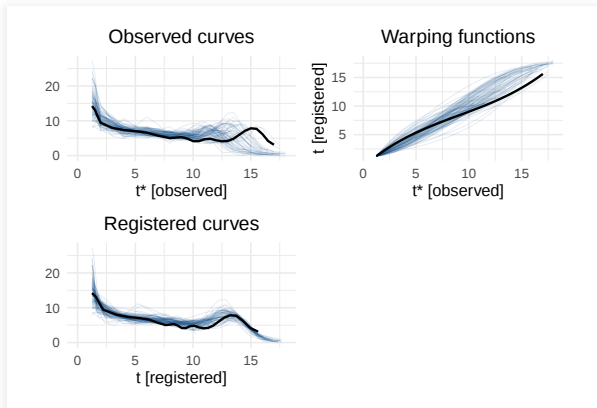
Example: **Berkeley child growth data** with simulated trailing incompleteness, using a **too high value**, $\lambda = 100$.



Incomplete Approach

Manually choose λ based on domain knowledge

Example: **Berkeley child growth data** with simulated trailing incompleteness, using a **reasonable value**, $\lambda = 0.8$.



Two-step approach

applied to the registered curves $Y_i(t) = Y_i(h_i^{-1}(t_i^*))$

1. Estimation of FPCs $\psi_k(t)$ based on a marginal method Hall et al. (2008)
2. Estimation of mean $\alpha(t)$ and FPC scores c_i through a Generalized Functional Additive Mixed Model Gertheiss et al. (2017)

$$E[Y_i(t)] = \mu_i(t) = g[X_i(t)],$$
$$X_i(t) \approx \alpha(t) + \sum_{k=1}^K c_{i,k} \cdot \psi_k(t),$$

Notation

K	number of principal components
$\mu_i(t)$	conditional expected value of $Y_i(t)$
$g[X_i(t)]$	latent Gaussian process transformed with response function $g(\cdot)$

Step 1 – Estimation of FPCs Hall et al. (2008)

based on $E[Y_i(t)] = g[X_i(t)]$

1. Center curves $Y_i(t)$ based on a marginal estimate of $\mu_Y(t) = E[Y_i(t)]$ by smoothing the data in a generalized additive model
2. Marginal estimation of the covariance:

$$\widehat{\text{Cov}}[X_i(s), X_i(t)] \approx \frac{\hat{\sigma}_Y(s, t)}{g^{(1)}[\mu_X(s)] \cdot g^{(1)}[\mu_X(t)]},$$

with

- $\sigma_Y(s, t) = E[Y_{c,i}(s) \cdot Y_{c,i}(t)]$ based on centered curves $Y_{c,i}(t)$, with $\sigma_Y(s_1, s_2)$ the mean of all pairwise products $y_{c,i}(s_1) \cdot y_{c,i}(s_2)$, and $\hat{\sigma}_Y(s, t)$ a smoothed version of $\sigma_Y(s, t)$ using a tensor product P-spline basis
- the marginal mean $\mu_X(t)$ estimated accordingly to $\mu_Y(t)$,
- $g^{(1)}(\cdot)$ the first derivative of the response function.

3. Spectral decomposition to yield FPCs $\psi_k(t)$ and associated eigenvalues τ_k

Step 2 – Estimation of FPC scores Gertheiss et al. (2017)

Estimation of mean $\alpha(t)$ and FPC scores $\mathbf{c}_i$ conditional on $\psi_k(t)$ in a **Generalized Functional Additive Mixed Model**:

$$g[\mu_i(t)] = \alpha(t) + \sum_{k=1}^K c_{i,k} \cdot \psi_k(t),$$

with the $c_{i,k} \sim N(0, \tau_k)$ random effects in an FPC basis representation.

⇒ Use robust routines (`gamm4` / `lme4`), highly efficient for many random effects

Notation

$\alpha(t) = \Theta_\alpha \alpha$ smooth effect, with P-spline basis Θ_α and parameters α

Approaches for **non-Gaussian FPCA**

Most existing approaches either assume Gaussianity Stefanucci et al. (2018)
or perform a marginal, potentially biased estimation Gertheiss et al. (2017)

Adapt the **two-step approach** of Gertheiss et al. (2017)

Combination of a nonparametric covariance estimator and a Functional Mixed Model

- ✓ Applicable to diverse exponential family settings
- ✓ Availability of efficient, robust software

Practical considerations

- **Central sources of bias**

- Poor coverage of the overall domain
- Violation of MCAR assumption

⇒ (Severe) bias of mean and covariance estimators Liebl & Rameseder (2019)

- **Choosing the number of FPCs** based on explained variance share κ_{var}

- Explained shares of variance refer to the smoothed covariance surface
- Spectral decompositions often yield many subordinate FPCs

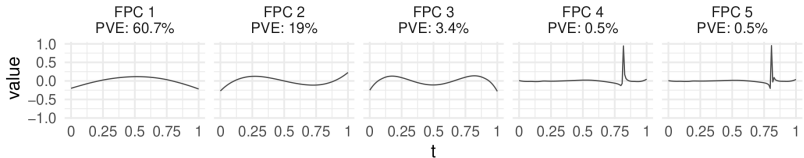
Practical considerations

- **Central sources of bias**

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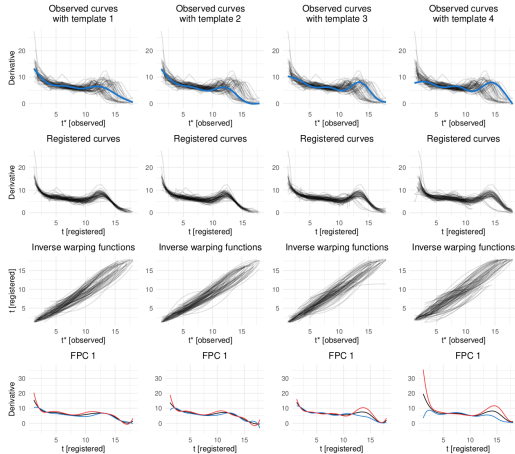
⇒ (Severe) bias of mean and covariance estimators Liebl & Rameseder (2019)

- **Choosing the number of FPCs based on explained variance share κ_{var}**



⇒ Exclude such subordinate FPCs with minor explained shares of variance

Choice of initial template function



Compared methods all performing joint registration and FPCA

SRVF	Complete curve approach of Tucker (2014)
FGAMM	Complete curve approach based on two-step GFPCA
FGAMM [inc.]	$\hookrightarrow$ adapted for incomplete curves
varEM	Complete curve approach of Wrobel et al. (2019)
varEM [inc.]	$\hookrightarrow$ adapted for incomplete curves

Performance metrics based on Mean (Integrated) Squared Errors

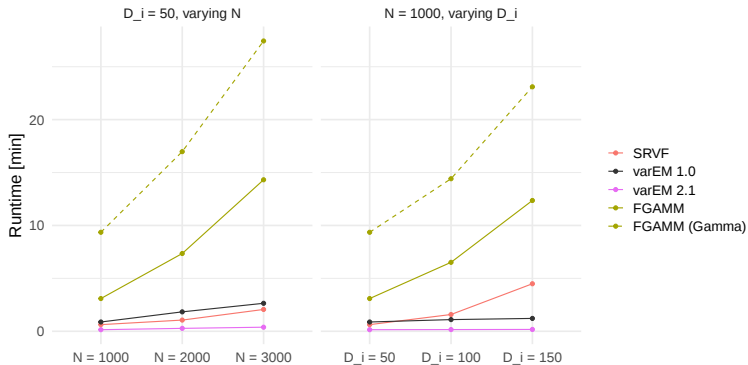
$MISE_y$	Comparison of the simulated mean curves (before adding random noise) and the representations based on the final FPCA solution
LV_ψ	Metric $\in [0, 1]$ quantifying the overlap of the simulated and estimated FPC bases
$MISE_h$	Comparison of the simulated and estimated warping functions
MSE_d	Comparison of the simulated and estimated domain lengths

[▶ back to sim study results](#)

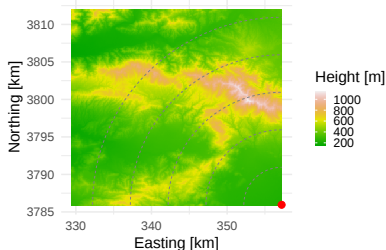
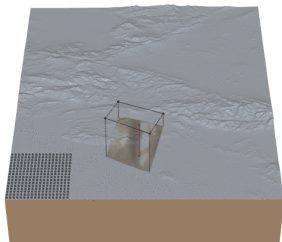
Simulation Study

Median runtimes

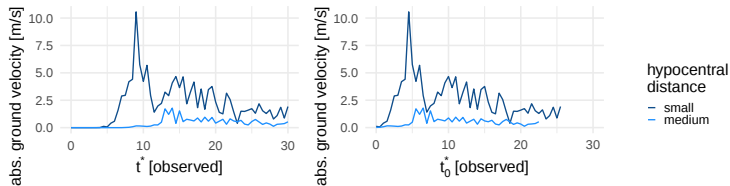
for one setting of the simulation study with amplitude rank 2-3 and no incompleteness, based on 20 runs for each parameter combination.



[▶ back to sim study results](#)



- Focus on wave propagation in northwest direction and close to the hypocenter
 - Focus on t_0^* as the *time since the arrival of seismic P-waves*
- ⇒ Joint approach with **Gamma distribution** and **trailing incompleteness**



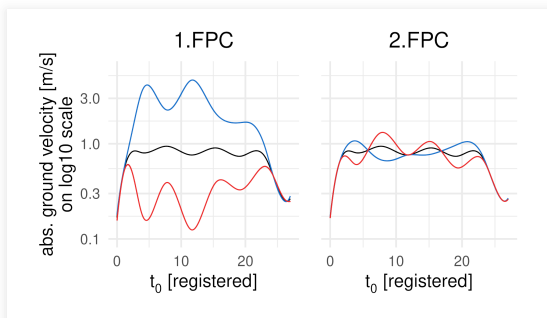
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 - Focus on t_0^* as the *time since the arrival of seismic P-waves*
- ⇒ Joint approach with **Gamma distribution** and **trailing incompleteness**

Seismic application – Estimation details

- Used penalization parameter $\lambda = 0.004$
- 10 joint iterations, taking overall 3:31h, using a parallelized call for the registration steps with 5 cores
- The FPCs were chosen to explain 95% of amplitude variation

Curves and FPCs

with the first two FPCs visualized by the mean curve $\pm 2 \cdot \sqrt{\hat{\tau}_k} \cdot \psi_k(t)$

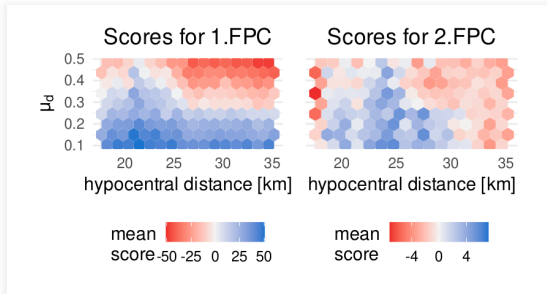


⇒ FPC 1 $\hat{=}$ overall magnitude with two peaks caused by surface waves

⇒ FPC 2 $\hat{=}$ salience of the initial peak

Heatmaps of estimated phase and amplitude variation

conditional on hypocentral distance and the dynamic coefficient of friction μ_d



- ⇒ Overall ground motion shows strong association with μ_d
- ⇒ Initial peaks are most pronounced at hypocentral distances $\sim 25\text{km}$