

registr 2.0: Incomplete Curve Registration for Exponential Family Functional Data

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Introduction

Functional data are observed in many different fields. Typical examples are longer-term panel studies where a sequence of measurements is observed for each subject. Compared to classical longitudinal studies, functional data analysis focuses more on the shapes of the (time-dependent) processes by analyzing the observed curve per subject. E.g., one can analyze the speed of growth of children until adulthood in the Berkeley child growth study (see left pane of Figure 1).

Functional data comprise different modes of variation. In the Berkeley study, not only can growth spurts be more or less pronounced regarding the actual growth (i.e., *amplitude variation* along the y-axis), but each spurt can also be shifted for some months / years for individual subjects (i.e., *phase variation* along the x-axis). Observed curves often have to be preprocessed with a *registration method* in order to separate phase and amplitude variation before analysis.

Most registration methods can only handle continuous data or data with a Gaussian structure. However, functional data are often non-Gaussian or even categorical. E.g., function values could be binary indicators representing physical (in)activity of patients over time (Wrobel et al., 2019). Moreover, most registration approaches are only applicable to completely observed curves that comprise the underlying process from its very start to its very end.

Basic routines for registering (Gaussian) data are implemented in R package Ramsay et al. (2020). Performing joint registration and clustering is possible with Parodi et al. (2015). The popular square-root velocity function (SRVF) framework for curve registration is implemented in Tucker (2020) for completely observed curves on a regular grid. Similar to our approach the package allows for registering all curves to similar shapes which can be well represented by some low-rank basis.

Exponential Family-based Registration

The registr package is based on the methods outlined in Wrobel et al. (2019). Registration is performed using a likelihood-based approach and estimates *inverse warping functions* $h_i^{-1}: t_i^* \mapsto t$ that map the observed time domain t_i^* for subject i to the common time domain t_i^* . The overall model is

$$\begin{split} E\left[Y_i\left(h_i^{-1}(t_i^*)\right)|h_i^{-1},\alpha(t),\boldsymbol{c}_i,\boldsymbol{\psi}(t)\right] &= \mu_i(t),\\ g\left[\mu_i(t)\right] &= \alpha(t) + \sum_{k=1}^K c_{ik}\psi_k(t), \end{split}$$



with $Y_i\left(t_i^*\right)$ and $Y_i\left(h_i^{-1}(t_i^*)\right)$ the unregistered and registered curves, respectively, and $\mu_i(t)$ the estimated subject-specific means serving as template functions, i.e., the target for the registration. The assumed distribution with link function $g(\cdot)$ and this conditional expectation allow us to define a log-likelihood $\ell(i)$ for each observed function (see Wrobel et al., 2019). The subject-specific means $\mu_i(t)$ are expressed through a low-rank representation based on a population-level mean $\alpha(t)$ and a linear combination of population-level basis functions $\psi_k(t)$ and subject-specific scores c_i , composed with a fixed link function $g(\cdot)$. We estimate this representation using a likelihood-based approach for generalized functional principal component analysis (GFPCA).

The overall model is estimated with function register_fpca(), which iterates between the estimation of warping functions (implemented in function registr()) and GFPCA estimation (functions fpca_gauss() or bfpca() for Gaussian or binomial data, respectively). This approach is consistent with earlier versions of the registr package (compare Wrobel, 2018).

In version 2.0, the package now includes the *two-step GFPCA* approach of Gertheiss et al. (2017) to handle further exponential family distributions. The respective implementation is based on the gfpca package of Goldsmith (2016). New distributions are supported both for registration and GFPCA. Furthermore, for the registration step, the individual template functions (to which each curve is mapped) can now be flexibly defined by the user with the argument Y_template in registr() and register_fpca(). This is of relevance since in many settings the overall mean of the unregistered curves is no reasonable template.

Incomplete Curve Registration

We extend the approach of Wrobel et al. (2019) to incomplete curves where the underlying process was either not observed from its very beginning (i.e., *leading incompleteness*) or until its very end (*trailing incompleteness*), or both (*full incompleteness*).

Since the underlying process is fully contained in the observed interval for complete curves, the first and last value of complete-curve warping functions lie on the diagonal line so that they preserve the overall domain. For incomplete curves, warping functions are estimated without this starting point and / or endpoint constraint.

However, fully removing these constraints can lead to extreme distortions of the time domain. We include a regularization term λ that penalizes the amount of domain dilation or compression performed by the inverse warping functions. Mathematically speaking, we add a penalization term to the log likelihood $\ell(i)$ for curve i. For a setting with full incompleteness this results in

$$\begin{split} \ell_{\mathrm{pen}}(i) &= \ell(i) - \lambda \cdot n_i \cdot \mathrm{pen}(i), \\ \text{with} \quad \mathrm{pen}(i) &= \left([\hat{h}_i^{-1}(t^*_{max,i}) - \hat{h}_i^{-1}(t^*_{min,i})] - [t^*_{max,i} - t^*_{min,i}] \right)^2, \end{split}$$

where $t_{min,i}^*, t_{max,i}^*$ are the minimum / maximum of the observed time domain of curve i and $\hat{h}_i^{-1}(t_{min,i}^*), \hat{h}_i^{-1}(t_{max,i}^*)$ the inverse warping function evaluated at this minimum / maximum. For leading incompleteness with $h_i^{-1}(t_{max,i}^*) = t_{max,i}^* \forall i$ this simplifies to $\text{pen}(i) = \left(\hat{h}_i^{-1}(t_{min,i}^*) - t_{min,i}^*\right)^2$, and for trailing incompleteness with $h_i^{-1}(t_{min,i}^*) = t_{min,i}^* \forall i$ to $\text{pen}(i) = \left(\hat{h}_i^{-1}(t_{max,i}^*) - t_{max,i}^*\right)^2$. The penalization term is scaled by the number of measurements n_i of curve i to ensure a similar impact of the penalization for curves with different numbers of measurements. In practical settings, λ has to be set manually to specify which kinds of warpings are deemed unrealistic and should be prevented. The choice of λ should be based on subject knowledge by comparing the registration results given different λ values.



In registr() and register_fpca() the type of incompleteness can be defined by argument incompleteness. Further details are given in the package vignette *incomplete_curves*. When applied to the Berkeley data with simulated full incompleteness, our approach leads to a reasonable registration as shown in Figure 1.

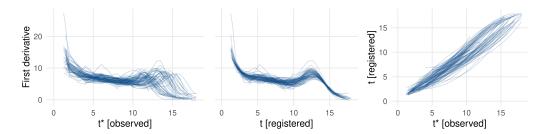


Figure 1: Left pane: Berkeley child growth data with simulated incompleteness; center: curves after registration; right: estimated inverse warping functions.

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