### tidyfun: Tidy Functional Data

# A new framework for representing and working with function-valued data in R

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Let's start at the end...

### This is what we're aiming for:

```
glimpse(dti)
## Observations: 382
   Variables: 5
          <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009, 101...
  $ sex <fct> female, female, male, male, male, male, male, male, male, ...
## $ case <fct> control, control, control, control, control, control, con...
## $ cca <tfd> 1001 1: (0.000,0.49);(0.011,0.52);(0.022,0.54); ..., 1002...
## $ rcst <tfd> 1001_1: (0.000,0.26);(0.018,0.45);(0.037,0.40); ..., 1002...
# group-wise functional medians:
medians = dti %>% group_by(case, sex) %>% summarize(median_rcst = median(rcst))
ggplot(medians) + geom_spaghetti(aes(y = median_rcst, col = sex, linetype = case), ;
                                                                       sex
  0.7
                                                                           male
median_rcst
                                                                            female
  0.6
                                                                       case
                                                                            control
  0.4
                                                                            MS
       0.00
                     0.25
                                   0.50
                                                 0.75
                                                                1.00
```

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### tidyfun

The goal of tidyfun is to provide accessible and well-documented software that makes functional data analysis in R easy, specifically: data wrangling and exploratory analysis.

#### tidyfun provides:

- ▶ new data types for representing functional data: tfd & tfb
- ► arithmetic **operators**, descriptive **statistics** and **graphics** functions for such data
- ▶ tidyverse-verbs for handling functional data **inside** data frames.

tf-Class: Definition

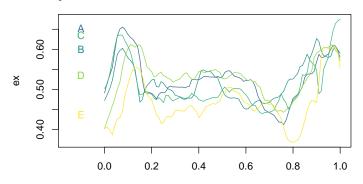
#### tf-class

tf is a new data type for (vectors of) functional data:

- ▶ an abstract superclass for functional data in 2 forms:
  - ► as (argument, value)-tuples: subclass tfd (regular, irregular)
  - ▶ or in basis representation: subclass tfb (splines, FPCs)
- ▶ with additional attributes that define *function-like* behavior:
  - ▶ how to **evaluate** the given "functions" for new arguments
  - ▶ their domain
  - ▶ the **resolution** of the argument values
- ▶ basically, a list of numeric vectors
  (... since lists work well as columns of data frames ...)
  - ▶ evaluations for tfd
  - ▶ basis coefficients for a joint basis for tfb
- ► S3 based

### **Example Data**

ex



```
## tfd[5] on (0,1) based on 93 evaluations each
## interpolation by approx_linear
## A: (0.000,0.49);(0.011,0.52);(0.022,0.54); ...
## B: (0.000,0.47);(0.011,0.49);(0.022,0.50); ...
## C: (0.000,0.50);(0.011,0.51);(0.022,0.54); ...
## D: (0.000,0.40);(0.011,0.42);(0.022,0.44); ...
## E: (0.000,0.40);(0.011,0.41);(0.022,0.40); ...
```

### **Example Data**

```
dti
## # A tibble: 382 x 5
##
         id sex
                   case
                                                 cca
                                                                           rcst
      <dbl> <fct>
##
                   \langle fct. \rangle
                                               <t.fd>
                                                                          <tfd>
##
      1001 female contr~ (0.000,0.49):(0.011,0.52~ (0.0000,0.257):(0.0185,0~
      1002 female contr~ (0.000,0.47); (0.011,0.49~ (0.222,0.443); (0.241,0~
##
##
       1003 male
                   contr~ (0.000,0.50):(0.011,0.51~ (0.222,0.424):(0.241,0~
##
      1004 male
                   contr~ (0.000,0.40);(0.011,0.42~ (0.0000,0.508);(0.0185,0~
##
      1005 male
                   contr~ (0.000.0.40):(0.011.0.41~ (0.222.0.398):(0.241.0~
       1006 male
                   contr~ (0.000,0.45);(0.011,0.45~ (0.0556,0.467);(0.0741,0~
##
##
      1007 male
                   contr~ (0.000,0.55);(0.011,0.56~ (0.0000,0.519);(0.0185,0~
      1008 male
                   contr~ (0.000,0.45);(0.011,0.48~ (0.0000,0.333);(0.0185,0~
##
       1009 male
                   contr~ (0.000.0.50):(0.011.0.51~ (0.0000.0.568):(0.0185.0~
##
##
   10
      1010 male
                   contr~ (0.000,0.46);(0.011,0.47~ (0.222,0.439);(0.241,0~
   # ... with 372 more rows
##
```

#### tf subclass: tfd

tfd objects contain "raw" functional data:

- subclasses for regular and irregular data
- ▶ represented as a list of evaluations  $f_i(t)|_{t=t'}$  and corresponding argument vector(s) t'

```
ex %>% evaluations() %>% str

## List of 5

## $ : num [1:93] 0.491 0.516 0.535 0.555 0.594 ...

## $ : num [1:93] 0.472 0.487 0.502 0.523 0.554 ...

## $ : num [1:93] 0.502 0.514 0.539 0.573 0.604 ...

## $ : num [1:93] 0.402 0.422 0.439 0.459 0.476 ...

## $ : num [1:93] 0.402 0.406 0.399 0.386 0.41 ...

ex %>% arg() %>% str

## num [1:93] 0 0.011 0.022 0.033 0.043 0.054 0.065 0.076 0.087 0.098 ...

ex %>% domain()

## [1] 0 1
```

#### tf subclass: tfd

► each tfd-vector contains an evaluator function that defines how to inter-/extrapolate evaluations between args (and remembers results of previous calls)

```
evaluator(ex) %>% str
## function (x, arg, evaluations)
## - attr(*, "memoised")= logi TRUE
## - attr(*, "class")= chr [1:2] "memoised" "function"
evaluator(ex) = approx_spline
```

#### tf subclass: tfb

Functional data in basis representation:

- ► represented as a list of coefficients and a common basis\_matrix of basis function evaluations on a vector of arg-values.
- contains a basis function that defines how to compute the basis for new args and how to differentiate/integrate.
- ▶ use either mgcv-spline bases or (F)PCs; wavelets to be added
- ► significant memory and time savings:

```
refund::DTI$cca %>% object.size() %>% print(units = "Kb")
## 304 Kb

dti$cca %>% object.size() %>% print(units = "Kb")
## 354.6 Kb

dti$cca %>% tfb(verbose = FALSE) %>% object.size() %>% print(units = "Kb")
## 169.9 Kb
```

#### tf subclasses: tfb

#### tfb spline basis:

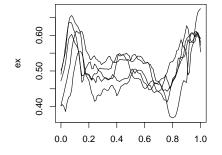
- ▶ accepts all arguments of mgcv's s()-syntax
- ▶ either does a penalized fit with (GCV-based) function-specific smoothing or unpenalized.

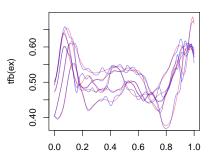
#### tfb FPC-based

- ▶ uses either
  - ► simple unregularized SVD of the data matrix ("smooth = FALSE")
  - ▶ or smoothed covariance estimate from refund::fpca.sc
- ► corresponding FPC basis and mean function saved as tfd-object, observations are linear combinations of those.

### tf subclass: tfb spline basis

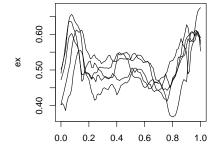
```
ex %>% plot()
ex %>% tfb(k = 20, bs = "ps", m = c(2,1)) %>% plot(col = "red")
ex %>% tfb(k = 45, penalized = FALSE) %>% lines(col = "blue")
```

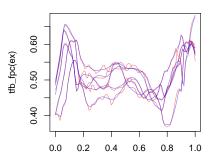




#### tf subclass: tfb FPC-based

```
ex %>% plot()
ex %>% tfb_fpc(smooth = FALSE, pve = .999) %>% plot(col = "red")
ex %>% tfb_fpc(pve = .95) %>% lines(col = "blue")
```





tf-Class: Methods

### Subset, subassign, concatenate

```
ex[1:2]
## tfd[2] on (0.1) based on 93 evaluations each
## interpolation by approx spline
## A: (0.000.0.49):(0.011.0.52):(0.022.0.54): ...
## B: (0.000,0.47);(0.011,0.49);(0.022,0.50); ...
ex[1:2] = ex[2:1]
ex
## tfd[5] on (0,1) based on 93 evaluations each
## interpolation by approx_spline
## B: (0.000,0.47);(0.011,0.49);(0.022,0.50); ...
## A: (0.000.0.49):(0.011.0.52):(0.022.0.54): ...
## C: (0.000.0.50):(0.011.0.51):(0.022.0.54): ...
## D: (0.000,0.40);(0.011,0.42);(0.022,0.44); ...
## E: (0.000,0.40);(0.011,0.41);(0.022,0.40); ...
c(ex["A"], ex[-(1:4)])
## tfd[2] on (0.1) based on 93 evaluations each
## interpolation by approx spline
## A: (0.000,0.49);(0.011,0.52);(0.022,0.54); ...
## E: (0.000.0.40):(0.011.0.41):(0.022.0.40): ...
```

#### **Evaluate**

```
ex[1:2, seq(0, 1, 1 = 3)]
## 0 0.5 1
## B 0.4721627 0.4984125 0.5802742
## A 0.4909345 0.5307563 0.5904773
## attr(, "arg")
## [1] 0.0 0.5 1.0
ex["B", seq(0, .15, l = 3), interpolate = FALSE]
## 0 0.075 0.15
## B 0.4721627 NA 0.4682867
## attr(,"arg")
## [1] 0.000 0.075 0.150
ex[1:2, seq(0, .15, l = 3), matrix = FALSE] %>% str
## List of 2
## $ B:Classes 'tbl_df', 'tbl' and 'data.frame': 3 obs. of 2 variables:
## ..$ arg : num [1:3] 0 0.075 0.15
## ..$ value: num [1:3] 0.472 0.603 0.468
## $ A:Classes 'tbl_df', 'tbl' and 'data.frame': 3 obs. of 2 variables:
## ..$ arg : num [1:3] 0 0.075 0.15
   ..$ value: num [1:3] 0.491 0.656 0.575
##
```

### Compare & compute

ex[1] + ex[1] == 2 \* ex[1]

```
## [1] TRUE
log(exp(ex[2])) == ex[2]
## [1] TRUE
ex - (2:-2) != ex
## [1] TRUE TRUE FALSE TRUE TRUE
```

#### **Summarize**

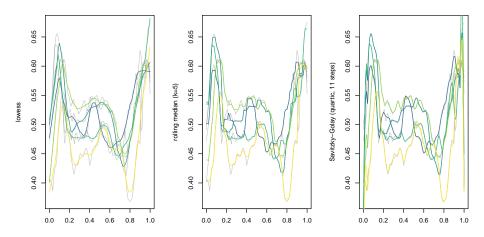
## TRUE

```
c(mean = mean(ex), sd = sd(ex))
## tfd[2] on (0,1) based on 93 evaluations each
## interpolation by approx_spline
## mean: (0.000, 0.45);(0.011, 0.47);(0.022, 0.48); ...
## sd: (0.000,0.049);(0.011,0.052);(0.022,0.062); ...

depth(ex) ## Modified Band-2 Depth (à la Sun/Genton/Nychka, 2012), others to come.
## B A C D E
## 0.60875 0.66005 0.65805 0.55915 0.51400

median(ex) == ex[which.max(depth(ex))]
## A
```

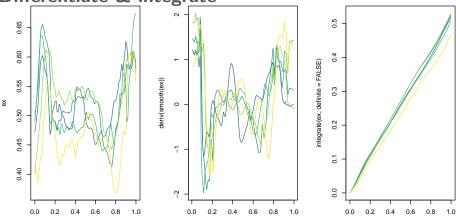
# (Simple, local) smoothing



```
ex %>% smooth("lowess") %>% plot
ex %>% smooth("rollmedian", k = 5) %>% plot
ex %>% smooth("savgol", fl = 11) %>% plot
```

Differentiate & integrate

ex %>% plot



```
ex %>% integrate(definite = FALSE) %>% plot

ex %>% integrate()

## B A C D E

## 0.5201949 0.5260109 0.5082054 0.5305535 0.4668760
```

ex %>% smooth() %>% deriv() %>% plot

### Query & zoom

```
8 00 B D D E 0.0 0.2 0.4 0.6 0.8 1.0
```

```
ex %>% where(value == max(value), "first")

## B A C D E

## 0.900 0.076 1.000 0.110 0.980

ex["A"] %>% zoom(.5, 1) %>% where(value > .6, "range")

## begin end

## A 0.96 0.98

ex %>% zoom(0, 0.1) %>% anywhere(value >= median(ex)[, arg])

## B A C D E

## FALSE TRUE TRUE FALSE FALSE
```

#### Convert & construct

To & from list, matrix or data frame with "id", "arg", "value"-columns:

```
ex matrix = ex %>% as.matrix(); ex matrix[1:2, 1:3]
            0 0.011 0.022
##
## B 0.4721627 0.4866481 0.5018916
## A 0.4909345 0.5164951 0.5352068
ex df = ex %>% as.data.frame(); str(ex df)
## Classes 'tbl_df', 'tbl' and 'data.frame': 465 obs. of 3 variables:
## $ id : Ord.factor w/ 5 levels "B"<"A"<"C"<"D"<..: 1 1 1 1 1 1 1 1 1 1 ...
## $ arg : num 0 0.011 0.022 0.033 0.043 0.054 0.065 0.076 0.087 0.098 ...
## $ value: num 0.472 0.487 0.502 0.523 0.554 ...
ex_matrix[1:2, ] %>% tfd()
## tfd[2] on (0.1) based on 93 evaluations each
## interpolation by approx linear
## B: (0.000,0.47);(0.011,0.49);(0.022,0.50); ...
## A: (0.000,0.49):(0.011,0.52):(0.022,0.54): ...
tfd(ex df) == tfd(ex matrix)
##
## TRUE TRUE TRUE TRUE TRUE
```

#### Visualize: base

```
layout(t(1:2))
plot(ex, type = "spaghetti"); lines(c(median(ex), mean(ex)), col = c(2, 4))
plot(ex, type = "lasagna", col = viridis(50))
   0.60
                                           ∢ -
                                           O -
   0.50
                                           Δ -
   0.40
                                           ш -
       0.0
            0.2
                 0.4
                      0.6
                           0.8
                                1.0
                                              0.0
                                                   0.2
                                                         0.4
                                                              0.6
                                                                    8.0
                                                                         1.0
```

### Visualize: ggplot2

New pasta-themed geoms and plots for functional data:

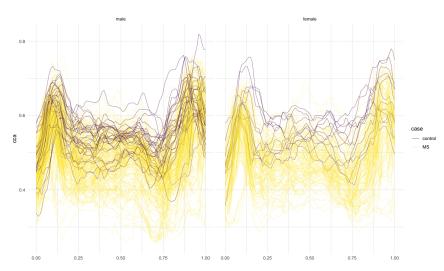
- ► geom\_spaghetti for lines
- ▶ geom\_meatballs for (lines &) points
- ► gglasagna with order-argument to sort the lasagna layers

#### To come:

- ▶ geom\_pappardelle for functional boxplots
- ► geom\_capellini for little sparklines / glyphs on maps etc.

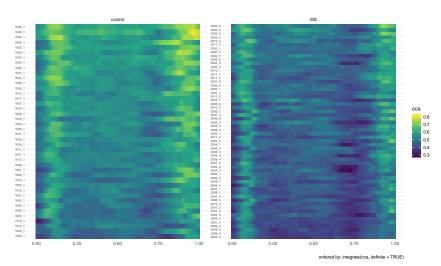
# Visualize: ggplot2

```
ggplot(dti, aes(y = cca, colour = case)) +
geom_spaghetti() + facet_wrap(~ sex)
```



### Visualize: ggplot2

```
gglasagna(dti,cca, order = integrate(cca, definite = TRUE)) +
  facet_wrap(~ case)
```



Wrangling tfs inside data frames

### Wrangling tfs inside data frames: dplyr

dplyr verbs filter, select, mutate, summarize work on tf-columns e.g.:

```
# aroup-wise functional means:
dti %>% group by(case, sex) %>% summarize(mean rcst = mean(rcst, na.rm = TRUE))
## # A tibble: 4 x 3
## case sex
                                        mean rcst
## <fct> <fct>
                                            <tfd>
## 1 control male (0.0000,0.514);(0.0185,0.50...
## 2 control female (0.0000,0.517):(0.0185,0.53...
## 3 MS
            male (0.0000,0.533);(0.0185,0.52...
## 4 MS female (0.0000,0.524):(0.0185,0.51...
# which subjects go below cca = .26:
dti %>% filter(anywhere(cca, value < .26))
## # A tibble: 3 x 5
##
       id sex case
                                              cca
                                                                        rcst
                                            <t.fd>
## <dbl> <fct> <fct>
                                                                       <t.fd>
## 1 2017 male MS
                      (0.000.0.38):(0.011.0.38):~(0.0741.0.519):(0.0926.0.~
## 2 2017 male MS
                      (0.000, 0.34); (0.011, 0.35); (0.0000, 0.616); (0.0185, 0.~
## 3 2083 male MS
                      (0.000,0.39); (0.011,0.43); (0.0000,0.511); (0.0185,0.7)
```

### Wrangling tfs inside data frames: dplyr

### Wrangling tfs inside data frames: tidyr

tidyfun provides tf\_ variants of tidyr-verbs to reshape and reformat functional data while keeping it in sync with other covariates:

- ightharpoonup tf\_spread: tf ightharpoonup columns for each arg
- $\blacktriangleright$  tf\_gather: columns for each arg  $\rightarrow$  tf
- ▶  $tf_nest$  : data in long format (id, arg, value)  $\rightarrow$  tf
- ▶ tf\_unnest: tf  $\rightarrow$  data in long format (id, arg, value)

### Wrangling tfs inside data frames: tidyr

```
# spread tf out into columns for each arg
dti_wide = dti %>% tf_spread(cca); dti_wide[, 1:7] %>% glimpse()
## Observations: 382
## Variables: 7
## $ id <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009...
## $ sex <fct> female, female, male, male, male, male, male, male, ...
## $ case <fct> control, control, control, control, control, control...
## $ rcst <tfd> 1001_1: (0.000,0.26);(0.018,0.45);(0.037,0.40); ...,...
## $ cca 0.011 <dbl> 0.5164951, 0.4866481, 0.5135178, 0.4222717, 0.405536...
## $ cca 0.022 <dbl> 0.5352068, 0.5018916, 0.5386470, 0.4394859, 0.398715...
# collect all columns into a single tf-column
# (... will try to guess arg from column names, name of tf from their prefix)
dti_wide %>% tf_gather(matches("cca_")) %>% glimpse()
## Observations: 382
## Variables: 5
## $ id <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009, 101...
## $ sex <fct> female, female, male, male, male, male, male, male, male,...
## $ case <fct> control, control, control, control, control, control, con...
## $ rcst <tfd> 1001 1: (0.000.0.26):(0.018.0.45):(0.037.0.40): .... 1002...
## $ cca <tfd>[1]: (0.000,0.49);(0.011,0.52);(0.022,0.54); ..., [2]: (0...
```

### Wrangling tfs inside data frames: tidyr

```
# unnest tf by writing 3 loong columns id, arg, value:
# (will try to avoid unnecessary duplication of columns)
dti long = dti %>% tf unnest(cca); dti long %>% glimpse()
## Observations: 35.526
## Variables: 7
## $ id <dbl> 1001, 1001, 1001, 1001, 1001, 1001, 1001, 1001, 1001...
## $ sex
             <fct> female, female, female, female, female, female, female...
## $ case <fct> control, control, control, control, control...
## $ rcst <tfd> 1001 1: (0.000,0.26);(0.018,0.45);(0.037,0.40); ...,...
## $ cca_id <chr> "1001_1", "1001_1", "1001_1", "1001_1", "1001_1", "1...
## $ cca arg <dbl> 0.000, 0.011, 0.022, 0.033, 0.043, 0.054, 0.065, 0.0...
## $ cca value <dbl> 0.4909345, 0.5164951, 0.5352068, 0.5546577, 0.594497...
# nest tf by writing 3 loong columns id, arg, value:
dti_long %>% tf_nest(cca_value, .id = cca_id, .arg = cca_arg) %>% glimpse()
## Observations: 382
## Variables: 6
## $ cca_id <chr> "1001_1", "1002_1", "1003_1", "1004_1", "1005_1", "1...
## $ id
         <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009...
             <fct> female, female, male, male, male, male, male, male, ...
## $ sex
## $ case <fct> control, control, control, control, control, control...
## $ rcst
          <tfd>[1]: (0.000,0.26);(0.018,0.45);(0.037,0.40); ..., [2...
## $ cca value <tfd> 1001_1: (0.000,0.49);(0.011,0.52);(0.022,0.54); ...,...
```

# Wrap-Up

### ... I like it. You might, too, give it a spin!<sup>1</sup>

https://github.com/fabian-s/tidyfun

Get it: devtools::install\_github("fabian-s/tidyfun")

<sup>&</sup>lt;sup>1</sup>Caveat emptor. Currently a moving target, still fairly early Beta.

### Outlook

#### Next up:

- ▶ integrate fda bases & penalties, wavelet bases
- ▶ improve & extend ggplot2 interface
- ► functions for registering & warping
- validate & improve

#### Version 1.0:

- ▶ extensions for multivariable functions (small images, too...?)
- ▶ much more extensive documentation & tests
- ▶ integration with refund for modeling and inference

#### Thanks.

https://github.com/fabian-s/tidyfun

(I don't even have references.)