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:

```
# group-wise functional medians:
medians = dti %>% group_by(case, sex) %>% summarize(median_rcst = median(rcst))
ggplot(medians) + geom_spaghetti(aes(tf = median_rcst, col = sex, linetype = case))
                                                                        sex
                                                                             male
  0.7
                                                                             female
value.
  0.6
                                                                        case
  0.4
                                                                             control

    MS

       0.00
                     0.25
                                    0.50
                                                  0.75
                                                                 1.00
                                    .arg
```

```
glimpse(dti)
## 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, male, male, control, cont
```

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 R 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

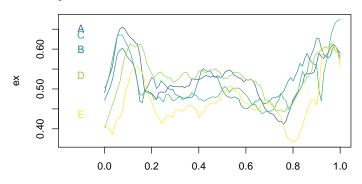
tf-class

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, also irregular or sparse
 - ▶ or in basis representation: subclass tfb
- basically, a list of numeric vectors(... since lists work well as columns of data frames ...)
- ▶ 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
- ► 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

1007 male

1008 male

1009 male

1010 male

... with 372 more rows

dti

7

##

##

10

```
##
  # A tibble: 382 x 5
##
         id sex
                   case
                                                  cca
                                                                            rcst
##
      <dbl> <fct>
                   \langle fct. \rangle
                                                <t.fd>
                                                                           <t.fd>
##
       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~
##
```

contr~ (0.000,0.55);(0.011,0.56~ (0.0000,0.519);(0.0185,0~contr~ (0.000,0.45);(0.011,0.48~ (0.0000,0.333);(0.0185,0~

contr~ (0.000,0.50);(0.011,0.51~ (0.0000,0.568);(0.0185,0~

contr~ (0.000,0.46);(0.011,0.47~ (0.222,0.439);(0.241,0~

tf subclass: tfd

tfd objects contain "raw" functional data:

- ▶ represented as a list of evaluations $f_i(t)|_{t=t'}$ and corresponding argument vector(s) t'
- ▶ has a domain: the range of valid args.

```
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

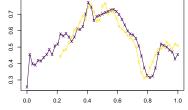
## function (x, arg, evaluations)
## - attr(*, "memoised") = logi TRUE
## - attr(*, "class") = chr [1:2] "memoised" "function"

evaluator(ex) = approx_spline
```

tf subclass: tfd

▶ tfd has subclasses for regular data with a common grid and irregular or sparse data.

```
dti$rcst[1:2]
## tfd[2] on (0.1) based on 43 to 55 (mean: 49) evaluations each
## inter-/extrapolation by approx linear
## 1001_1: (0.000,0.26);(0.018,0.45);(0.037,0.40); ...
## 1002_1: ( 0.22,0.44);( 0.24,0.48);( 0.26,0.48); ...
dti$rcst[1:2] %>% arg() %>% str
## List of 2
  $ 1001 1: num [1:55] 0 0.0185 0.037 0.0556 0.0741 0.0926 0.111 0.13 0.148 0.167
## $ 1002 1: num [1:43] 0.222 0.241 0.259 0.278 0.296 0.315 0.333 0.352 0.37 0.389
dti$rcst[1:2] %>% plot(pch = "x", col = viridis(2))
 0.7
```



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.
- ► (internal) flavors: mgcv-spline bases and FPCs (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 subclass: tfb spline basis

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

```
ex_b = ex \% \% tfb(); ex_b[1:2]
## Percentage of raw input data variance preserved in basis representation:
## (per functional observation, approx.):
     Min. 1st Qu. Median Mean 3rd Qu.
##
                                            Max.
##
    96.00 96.70 97.60 97.42 98.00 98.80
## tf[2] on (0,1) in basis representation:
   using basis s(arg, bs = "cr", k = 25)
## A: (0.000,0.48);(0.011,0.52);(0.022,0.54); ...
## B: (0.000,0.46);(0.011,0.49);(0.022,0.51); ...
ex[1:2] \%\% tfb(bs = "tp", k = 55)
## Percentage of raw input data variance preserved in basis representation:
## (per functional observation, approx.):
##
     Min. 1st Qu. Median Mean 3rd Qu.
                                         Max.
##
    99.50 99.58 99.65 99.65 99.72 99.80
## tf[2] on (0,1) in basis representation:
## using basis s(arg, bs = "tp", k = 55)
## A: (0.000,0.49);(0.011,0.51);(0.022,0.53); ...
```

tf subclass: tfb spline basis

```
%>% plot()
ex_b %>% plot(col = "red")
ex %>% tfb(k = 35, penalized = FALSE) %>% lines(col = "blue")
    0.60
    0.50
                                                   0.50
    0.40
              0.2
        0.0
                    0.4
                          0.6
                                0.8
                                      1.0
                                                       0.0
                                                             0.2
                                                                   0.4
                                                                         0.6
                                                                              0.8
                                                                                    1.0
```

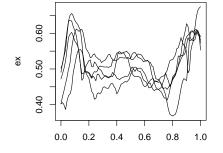
tf subclass: tfb FPC-based

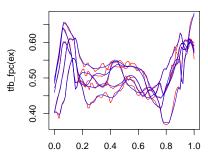
- uses either
 - ► simple unregularized SVD of the data matrix ("smooth = FALSE")
 - ▶ or smoothed covariance estimate from refund::fpca.sc
- corresponding FPC basis and mean function saved as tfd-object
- observed functions are linear combinations of those.

```
(ex %>% tfb_fpc(smooth = FALSE, pve = .999))
## tfb[5] on (0,1) in basis representation:
  using basis FPC: 4 components.
## 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); ...
(ex \%\% tfb_fpc(pve = .95))
## tfb[5] on (0,1) in basis representation:
   using basis FPC: 21 components.
## A: (0.000,0.48);(0.011,0.51);(0.022,0.54); ...
## B: (0.000,0.46);(0.011,0.49);(0.022,0.51); ...
## C: (0.000,0.49);(0.011,0.52);(0.022,0.55); ...
## D: (0.000,0.40);(0.011,0.43);(0.022,0.45); ...
## E: (0.000, 0.4);(0.011, 0.4);(0.022, 0.4); ...
```

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

```
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); ...
```

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, 1, 1 = 2), matrix = FALSE] %>% str
## List of 2
## $ B:Classes 'tbl_df', 'tbl' and 'data.frame': 2 obs. of 2 variables:
## ..$ arg : num [1:2] 0 1
## ..$ value: num [1:2] 0.472 0.58
   $ A:Classes 'tbl df', 'tbl' and 'data.frame': 2 obs. of 2 variables:
##
## ..$ arg : num [1:2] 0 1
   ..$ value: num [1:2] 0.491 0.59
##
```

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

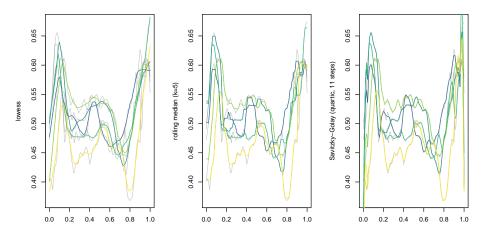
A ## TRUE

```
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

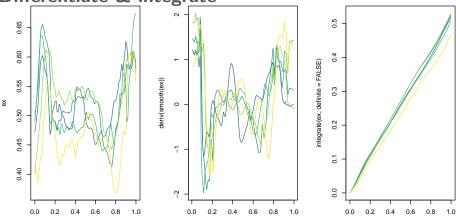
median(ex) == ex[which.max(depth(ex))]
```

(Simple, local) smoothing



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

Differentiate & integrate



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

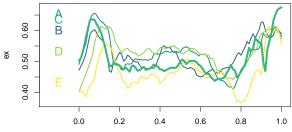
0.5201949 0.5260109 0.5082054 0.5305535 0.4668760

Query

Find arguments t satisfying a condition on value f(t) (and argument t):

```
ex %>% anywhere(value > .65)
##
## FALSE TRUE TRUE FALSE FALSE
ex[1:2] \%\% where(value > .6, "all")
## $B
## [1] 0.076 0.890 0.900 0.910 0.980
##
## $A
  [1] 0.054 0.065 0.076 0.087 0.098 0.110 0.120 0.130 0.140 0.960 0.970
## [12] 0.980
ex[2] %>% where(value > .6, "range")
##
    begin end
## A 0.054 0.98
ex %>% where(value > .6 & arg > .5, "first")
        A C D
## 0.89 0.96 0.96 0.93 0.93
```

Zoom & query



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]
##
              0.011 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 with a tf-aesthetic for functional data:

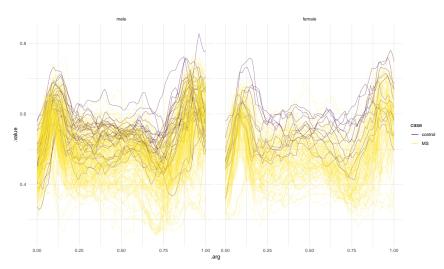
- ▶ geom_spaghetti for lines
- ▶ geom_meatballs for (lines &) points
- ▶ geom_lasagna with an order-aesthetic to sort the lasagna layers

To come:

- geom_pappardelle for functional boxplots
- ► geom_capellini for little sparklines / glyphs on maps etc.

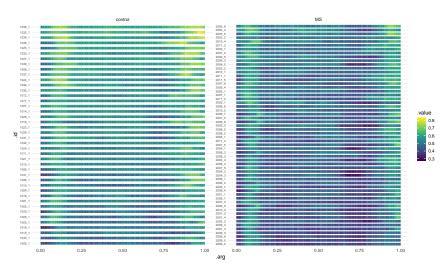
Visualize: ggplot2

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



Visualize: ggplot2

```
ggplot(dti, aes(tf = cca, order = integrate(cca, definite = TRUE))) +
  geom_lasagna() + 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.:

```
# group-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>
##
                                              <t.fd>
## 1 control male (0.0000,0.514);(0.0185,0.50...
## 2 control female (0.0000,0.517):(0.0185,0.53...
            male (0.0000,0.533):(0.0185,0.52...
## 3 MS
## 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
   <dbl> <fct> <fct>
##
                                              <tfd>
                                                                         <tfd>
                       (0.000,0.38); (0.011,0.38); (0.0741,0.519); (0.0926,0.741,0.519);
## 1 2017 male MS
## 2 2017 male MS
                       (0.000, 0.34); (0.011, 0.35); (0.0000, 0.616); (0.0185, 0.~
                       (0.000, 0.39); (0.011, 0.43); (0.0000, 0.511); (0.0185, 0.~
## 3 2083 male MS
```

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
- lacktriangledown tf_gather: columns for each arg ightarrow tf
- ▶ tf_nest : data in long format (id, arg, value) → 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 ara
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, male, ...
## $ case <fct> control. control. control. control. control. control. control.
## $ 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, 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...
             <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009...
## $ id
## $ sex
             <fct> female. female. male. male. male. male. male. male. ...
## $ case <fct> control, control, control, control, control...
             <tfd> [1]: (0.000.0.26):(0.018.0.45):(0.037.0.40): .... [2...
## $ rcst
## $ cca value <tfd> 1001 1: (0.000,0.49);(0.011,0.52);(0.022,0.54); ...,...
```

Fin

Summary

... I like it. You might, too, give it a spin!¹

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

Get it: devtools::install_github("fabian-s/tidyfun")

¹Currently a moving target. Still early β , some kinks need to be worked out.

Outlook

Next up:

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

Version 1.0:

- extensions for multivariate functions
- ▶ 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.