`tidyfun`: Tidy Functional Data

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

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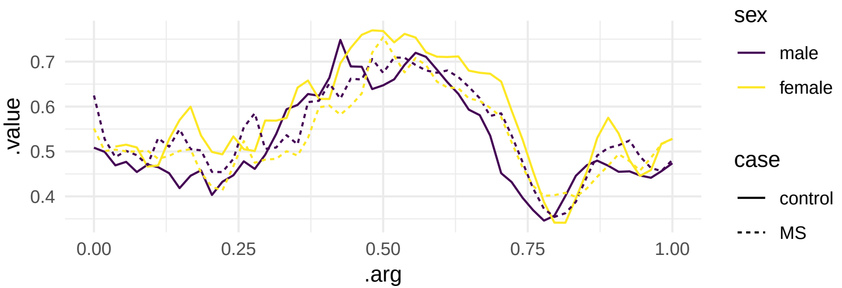
Let's start at the end...

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))
```




```
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,...
## $ 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...
```

`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.

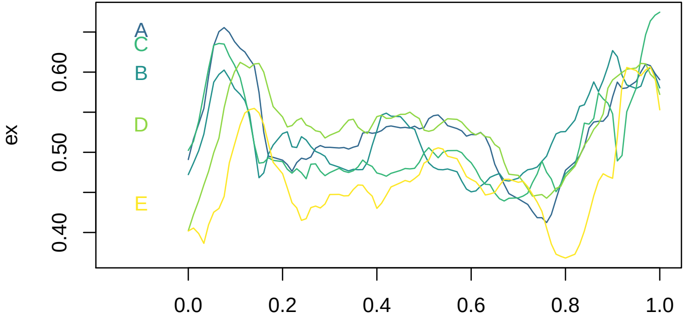
`tf`-Class: Definition

`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`, 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

```
dti
## # A tibble: 382 x 5
##       id sex    case                                cca                          rcst
##    <dbl> <fct>  <fct>                             <tfd>                         <tfd>
##  1  1001 female contr~ (0.000,0.49);(0.011,0.52~ (0.0000,0.257);(0.0185,0~
##  2  1002 female contr~ (0.000,0.47);(0.011,0.49~ ( 0.222,0.443);( 0.241,0~
##  3  1003 male   contr~ (0.000,0.50);(0.011,0.51~ ( 0.222,0.424);( 0.241,0~
##  4  1004 male   contr~ (0.000,0.40);(0.011,0.42~ (0.0000,0.508);(0.0185,0~
##  5  1005 male   contr~ (0.000,0.40);(0.011,0.41~ ( 0.222,0.398);( 0.241,0~
##  6  1006 male   contr~ (0.000,0.45);(0.011,0.45~ (0.0556,0.467);(0.0741,0~
##  7  1007 male   contr~ (0.000,0.55);(0.011,0.56~ (0.0000,0.519);(0.0185,0~
##  8  1008 male   contr~ (0.000,0.45);(0.011,0.48~ (0.0000,0.333);(0.0185,0~
##  9  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:

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

```
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

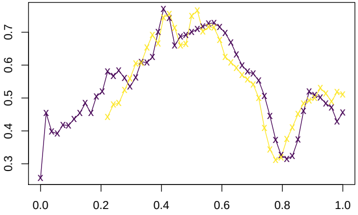
- each **tfd**-vector contains an **evaluator** function that defines how to inter-/extrapolate evaluations between args (and remembers results of previous calls)

```
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))
```



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
```

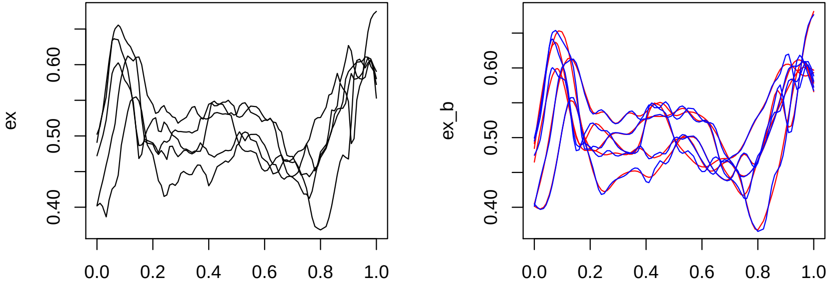
`tf` subclass: `tfb` spline basis

- 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); ...
## B: (0.000,0.47);(0.011,0.49);(0.022,0.50); ...
```

`tf` subclass: `tfb` spline basis

```
ex  %>% plot()
ex_b %>% plot(col = "red")
ex %>% tfb(k = 35, penalized = FALSE) %>% lines(col = "blue")
```



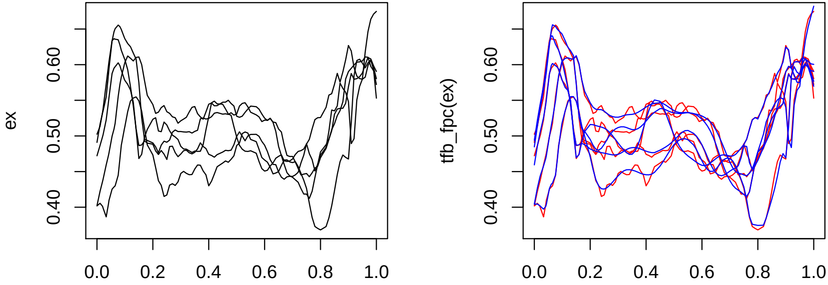
`tf` subclass: `tfb` FPC-based

- 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

```r
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, l = 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, l = 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
```

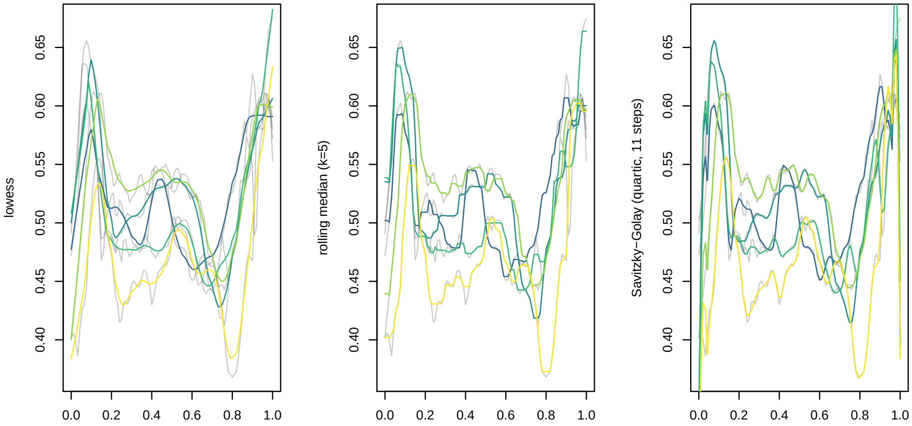
Compare & compute

```
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

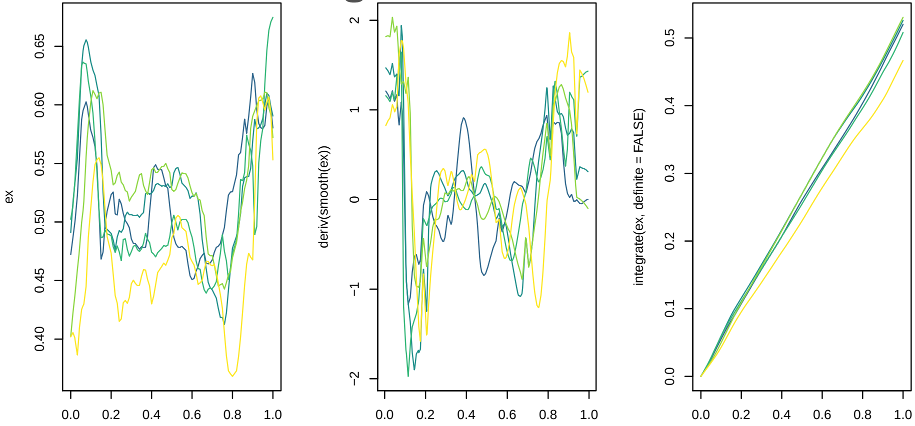
```
c(mean = mean(ex), sd = sd(ex))
## tfd[2] on (0,1) based on 93 evaluations each
## interpolation by approx_spline
## mean: (0.000, 0.45);(0.011, 0.47);(0.022, 0.48); ...
## sd: (0.000,0.049);(0.011,0.052);(0.022,0.062); ...

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
## TRUE
```

(Simple, local) smoothing




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

Differentiate & integrate



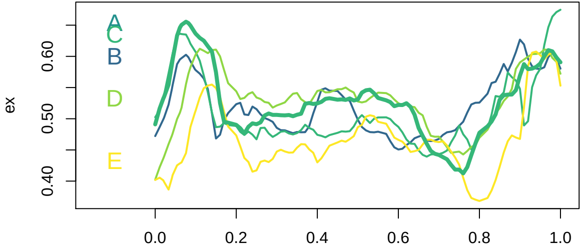

```
ex %>% plot
ex %>% smooth() %>% deriv() %>% plot
ex %>% integrate(definite = FALSE) %>% plot

ex %>% integrate()
##         B         A         C         D         E
## 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)
##     B     A     C     D     E
## 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")
##    B    A    C    D    E
## 0.89 0.96 0.96 0.93 0.93
```

Zoom & query




```
ex %>% where(value == max(value), "first")
##     B     A     C     D     E
## 0.900 0.076 1.000 0.110 0.980

ex[c("A", "D")] %>% zoom(.5, 1) %>% where(value == max(value), "first")
##    A    D
## 0.97 0.96

ex %>% zoom(0.2, 0.6) %>% anywhere(value <= median(ex)[, arg])
##    B    A    C    D    E
## TRUE TRUE TRUE TRUE TRUE
```

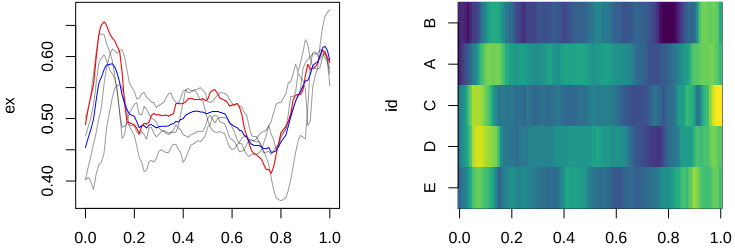
Convert & construct

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)
##    B    A    C    D    E
## TRUE TRUE TRUE TRUE TRUE
```

Visualize: base

```r
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))
```



Visualize: `ggplot2`

New **pasta-themed** geoms with a `tf`-aesthetic for functional data:

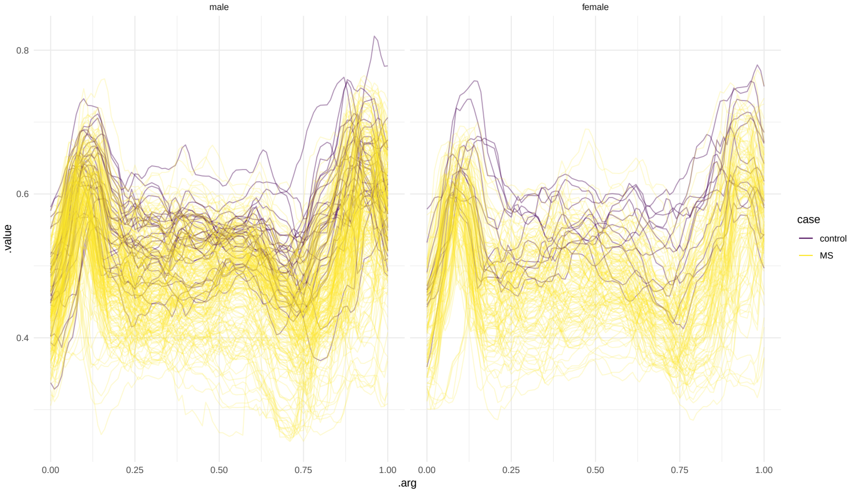
- **`geom_spaghetti`** for lines
- **`geom_meatballs`** for (lines &) points
- **`geom_lasagna`** with an `order`-aesthetic to sort the lasagna layers

To come:

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

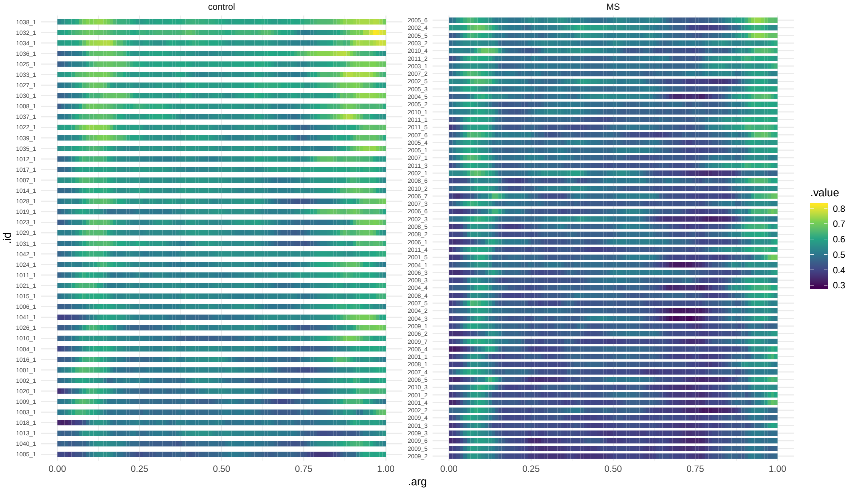
Visualize: `ggplot2`

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



Visualize: `ggplot2`

```r
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>                           <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
##   <dbl> <fct> <fct>                      <tfd>                         <tfd>
## 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.~
```

Wrangling tfs inside data frames: dplyr

```
# center & scale functional data:
dti %>%
  mutate(cca = tfb(cca, verbose = FALSE),
    cca_z = (cca - mean(cca))/sd(cca)) %>% glimpse
## Observations: 382
## Variables: 6
## $ id    <dbl> 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009, 10...
## $ sex   <fct> female, female, male, male, male, male, male, male, male...
## $ case  <fct> control, control, control, control, control, control, co...
## $ cca   <tf> 1001_1: (0.000,0.48);(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); ..., 100...
## $ cca_z <tf> [1]: (0.000,  0.84);(0.011,  0.98);(0.022,  1.10); ..., [...
```

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:

- `tf_spread`: `tf` → columns for each `arg`
- `tf_gather`: columns for each `arg` → `tf`

- `tf_nest`   : data in long format (`id`, `arg`, `value`) → `tf`
- `tf_unnest`: `tf` → 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     <dbl> 0.4909345, 0.4721627, 0.5023738, 0.4021894, 0.401874...
## $ 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, fema...
## $ 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...
## $ 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> [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![1]

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

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

[1] *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.)