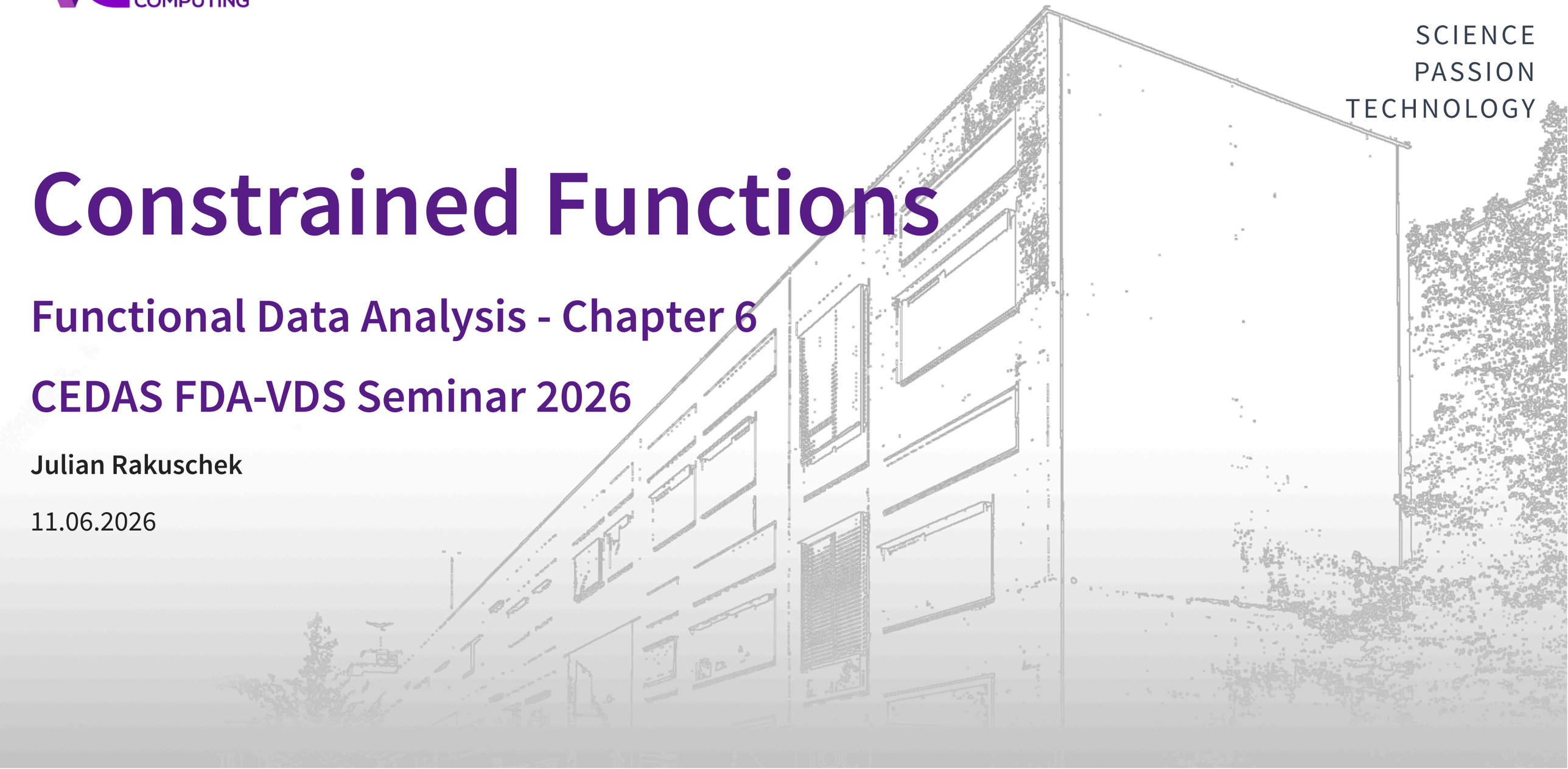
INSTITUTE OF VISUAL COMPUTING

TU Graz

SCIENCE
PASSION
TECHNOLOGY



Constrained Functions

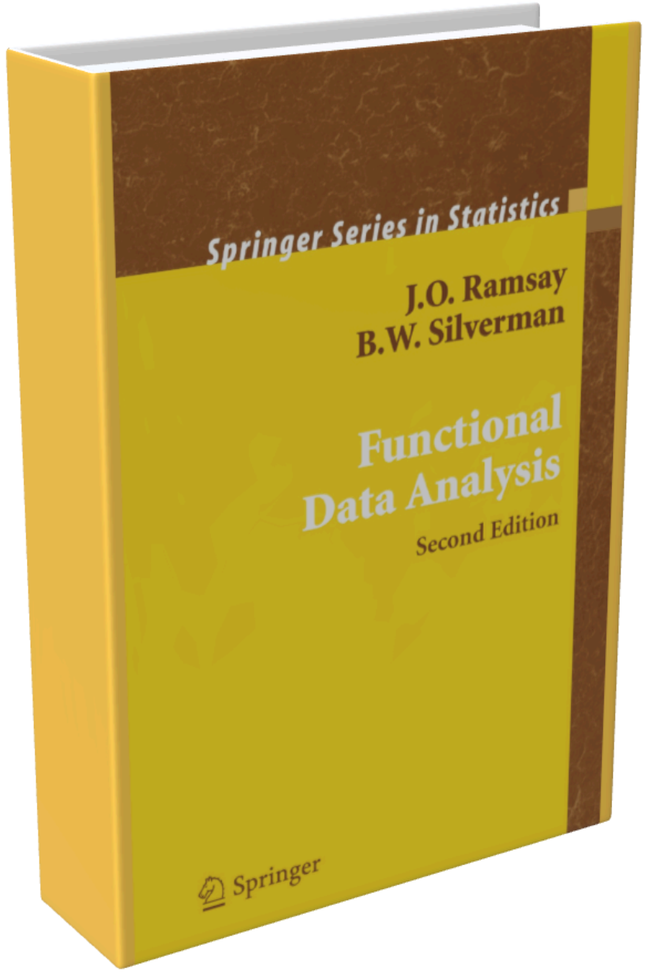
Functional Data Analysis - Chapter 6

CEDAS FDA-VDS Seminar 2026

Julian Rakuschek

11.06.2026

In this lecture

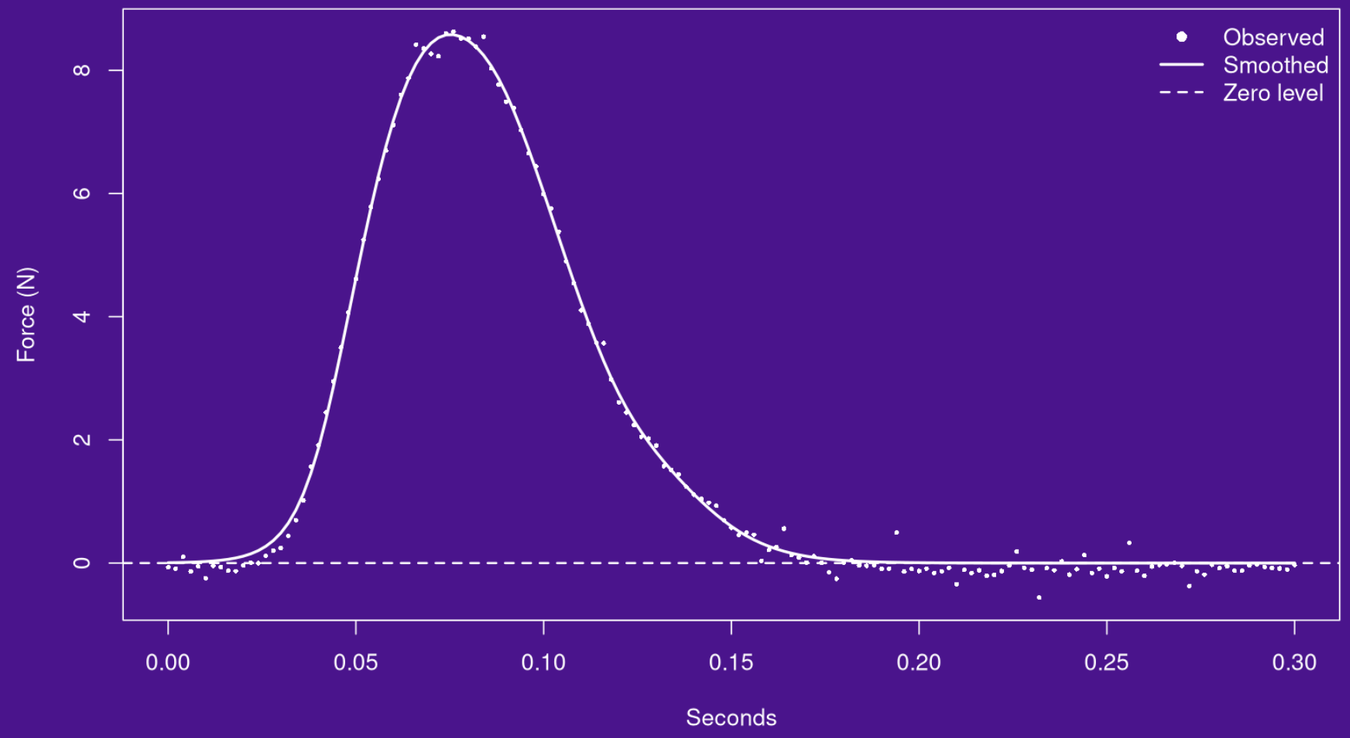


We are going to cover **chapter 6** in *Functional Data Analysis* on *Constrained Functions*

Focus:

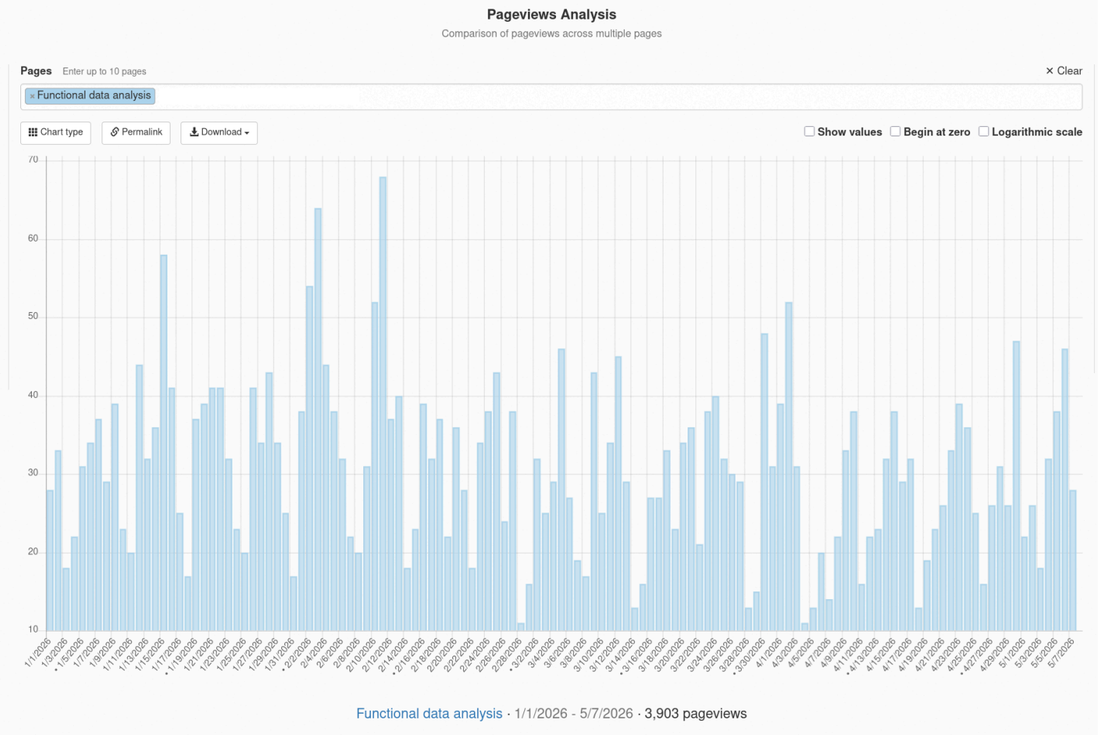
- Positive functions
- Monotonically increasing functions
- Probability density function estimation

Positive Functions



Which functions are positive? (1 / 3)

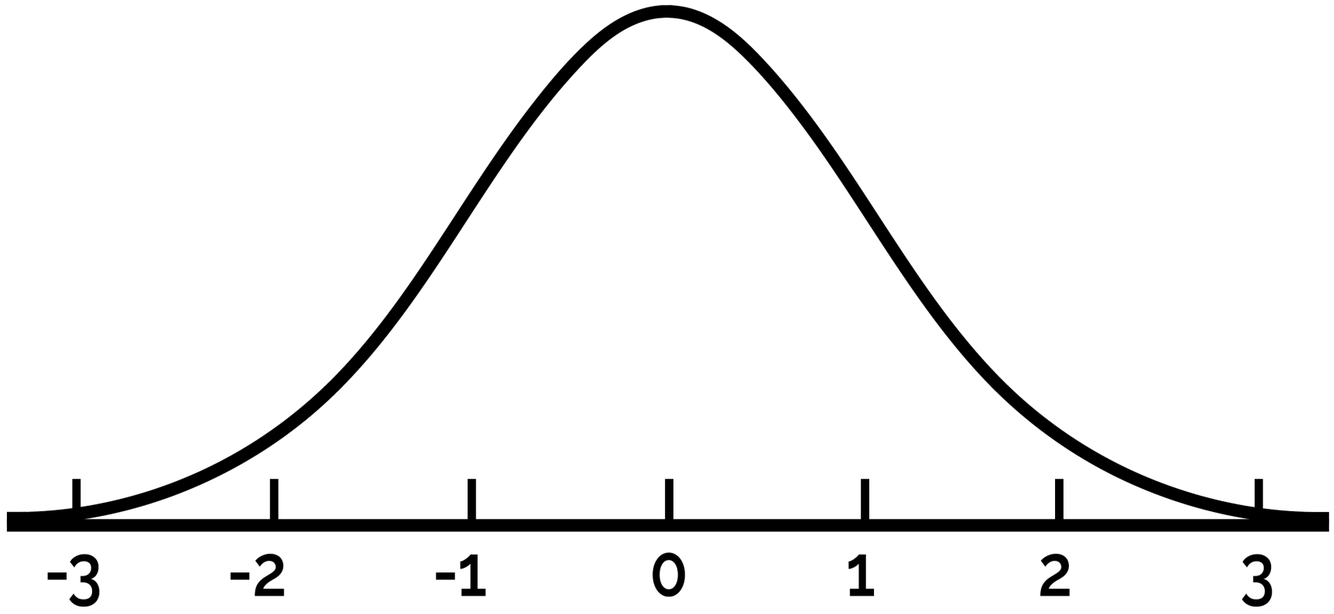
Counts, for example page views



Strictly speaking: This would be non-negative

Which functions are positive? (2 / 3)

Probability functions



Which functions are positive? (3 / 3)

Many quantities can only be positive

Energy

- Kinetic Energy
- Potential Energy

Measures

- Area
- Volume
- Length

Information Theoretic

- Entropy
- Mutual information
- Divergences

Pinch Force

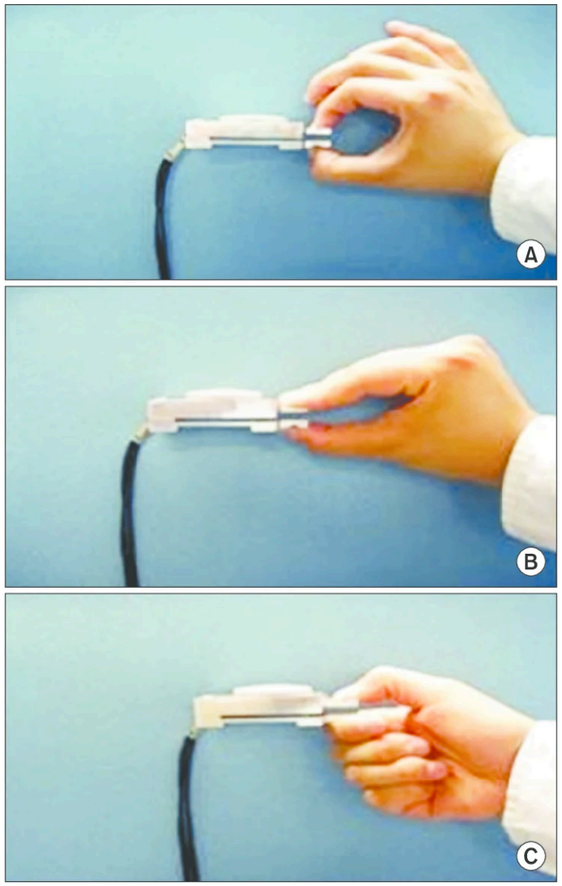
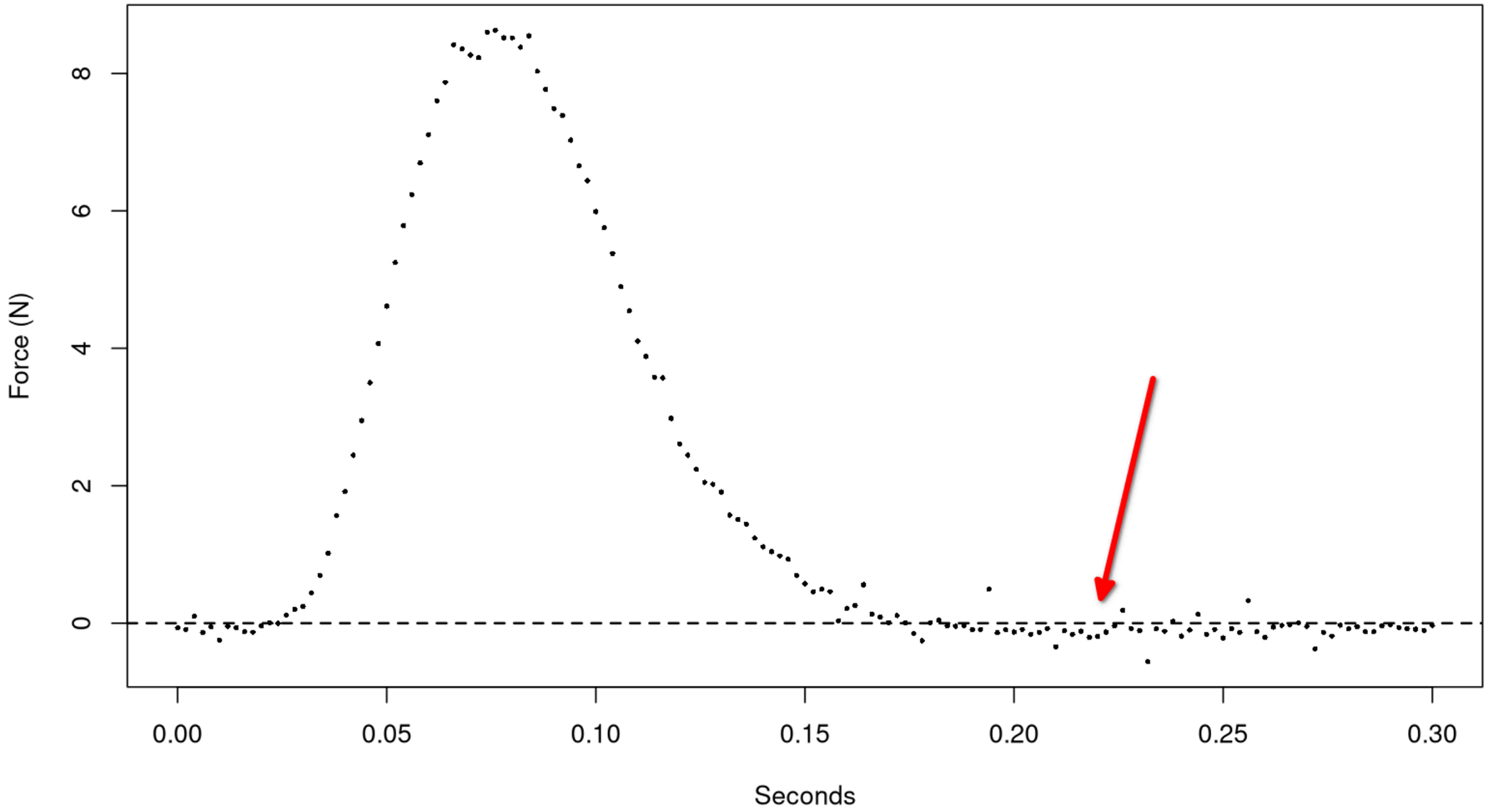


Image Source: Kong, Sangwon & Lee, Kyung & Kim, Junho & Jang, Seong. (2014). The Effect of Two Different Hand Exercises on Grip Strength, Forearm Circumference, and Vascular Maturation in Patients Who Underwent Arteriovenous Fistula Surgery. Annals of Rehabilitation Medicine. 38. 648. 10.5535/arm.2014.38.5.648.

Measurements can be noisy and drop below zero



The way we have fitted a function previously

Chapter 5 – smoothing with roughness penalty:

$$\mathrm{PENSSE}_\lambda(x|\mathbf{y}) = \underbrace{[\mathbf{y} - x(\mathbf{t})]^T \mathbf{W} [\mathbf{y} - x(\mathbf{t})]^2}_{\text{Fit of the data}} + \lambda \underbrace{\int (D^2 x(s))^2 ds}_{\text{Function roughness based on curvature}}$$

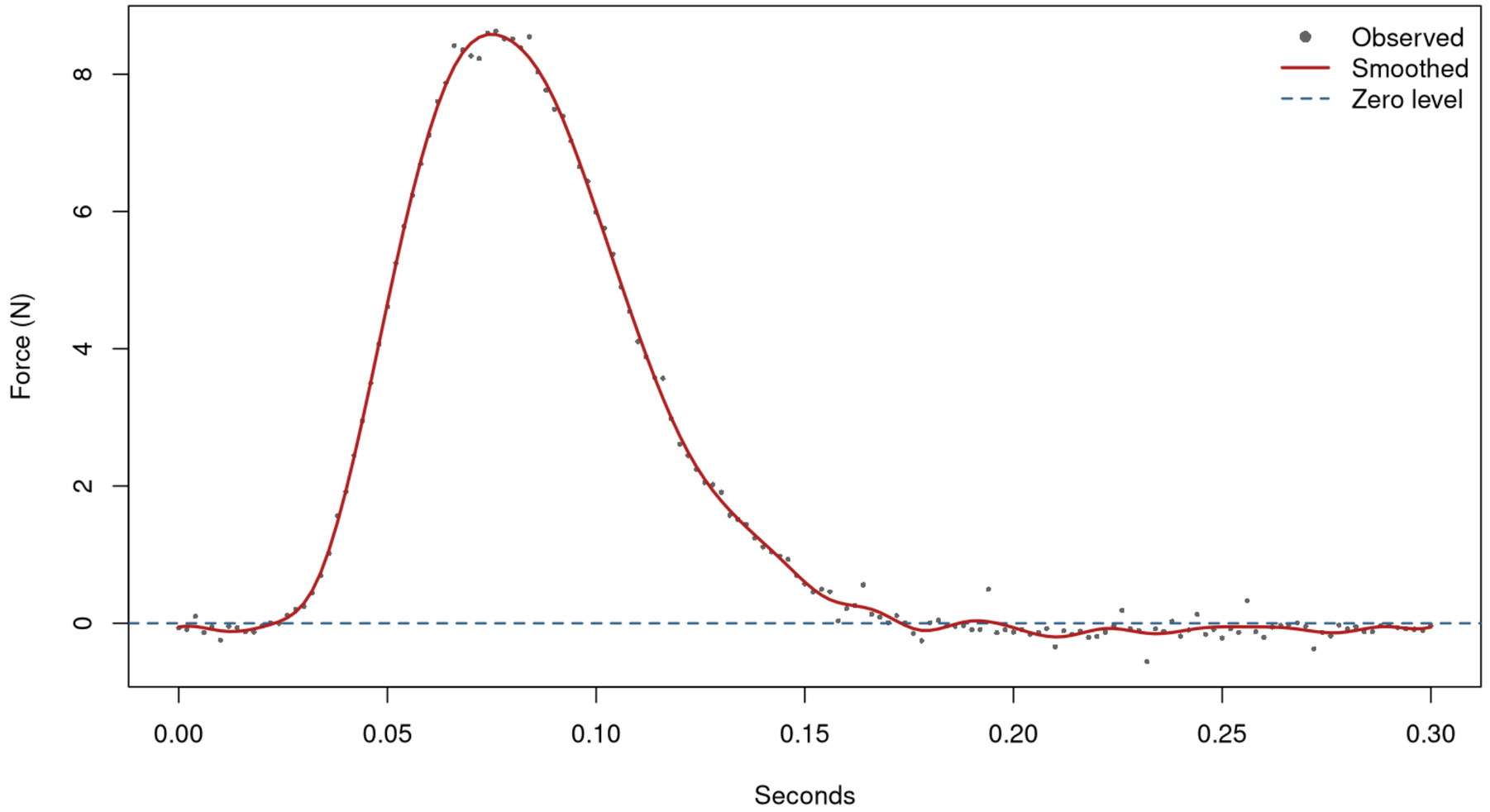
Remember, $x(t)$ is a linear expansion

$$x(t) = \sum_{k=1}^{K} c_k \phi_k(t)$$

In the FDA package

```
fdParobj <- fdPar(
    fdobj = basis,
    Lfdobj = 2,
    lambda = 1e-8
)

fit <- smooth.basis(
    argvals = x_values,
    y = y_values,
    fdParobj = fdParobj
)
```

This creates some noisy tails



Defining positive smoothing functions

Instead of

$$x(t) = \sum_{k=1}^{K} c_k \phi_k(t)$$

we now define

$$x(t) = e^{\sum_{k=1}^{K} c_k \phi_k(t)} = e^{W(t)}$$

Positive smoothing function x can always be defined on the exponential of an unconstrained function W.

Remarks

$$x(t) = e^{W(t)}$$

Any other basis can be used as well!

Nota bene: This function can never be exactly zero. It can only get very close to zero.

The updated optimization criterion

$$\mathrm{PENSSE}_\lambda(x|\mathbf{y}) = [\mathbf{y} - x(\mathbf{t})]^T \mathbf{W} [\mathbf{y} - x(\mathbf{t})]^2 + \lambda \int (D^2 x(s))^2 ds$$

now becomes

$$\mathrm{PENSSE}_\lambda(W|\mathbf{y}) = [\mathbf{y} - e^{W(\mathbf{t})}]^T \mathbf{W} [\mathbf{y} - e^{W(\mathbf{t})}]^2 + \lambda \int (D^2 W(t))^2 dt$$

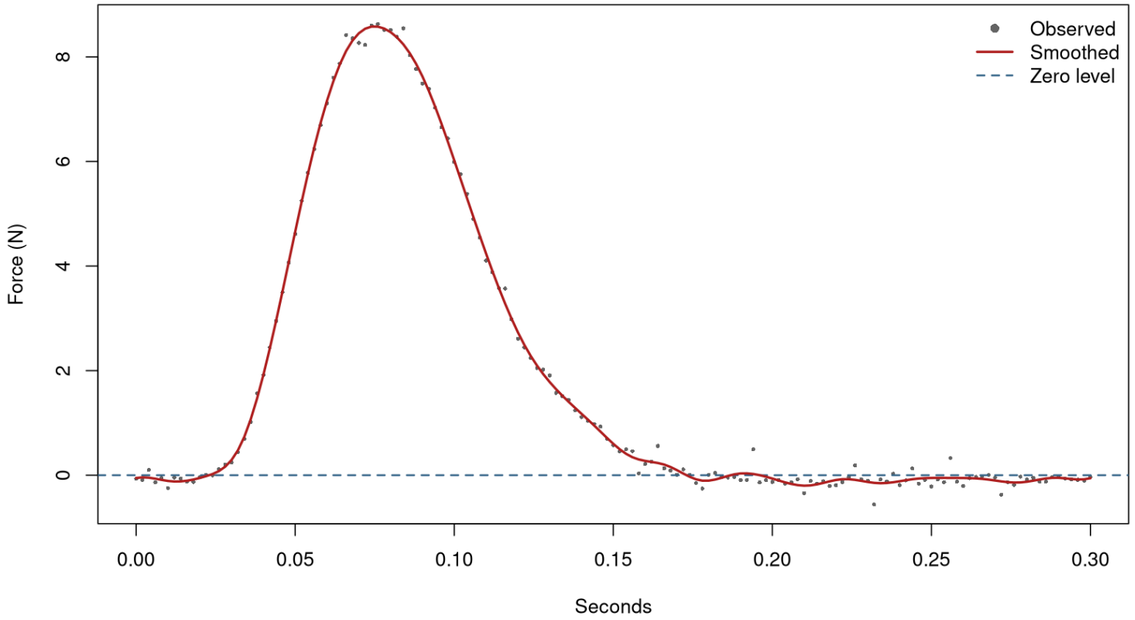
Needs to be solved through numerical methods. But these converge quickly because the expression is only mildly nonlinear.

smooth.basis → smooth.pos

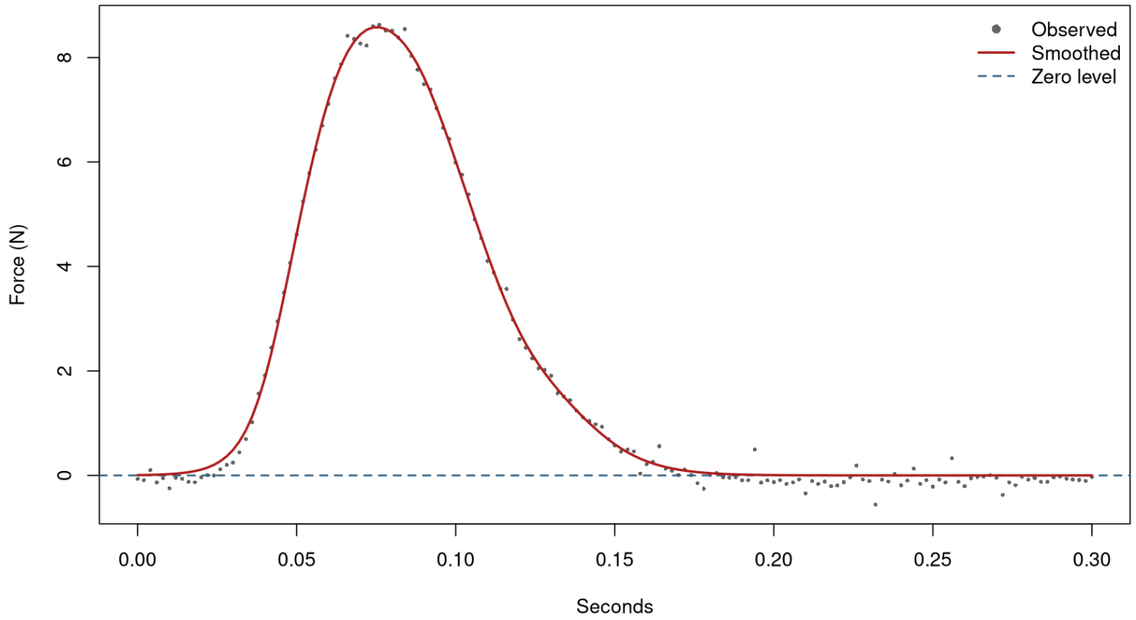
```
fdParobj <- fdPar(
    fdobj = basis,
    Lfdobj = 2,
    lambda = 1e-8
)

fit <- smooth.pos(
    argvals = x_values,
    y = y_values,
    WfdParobj = fdParobj,
    dbglev = 0
)
```

Comparison

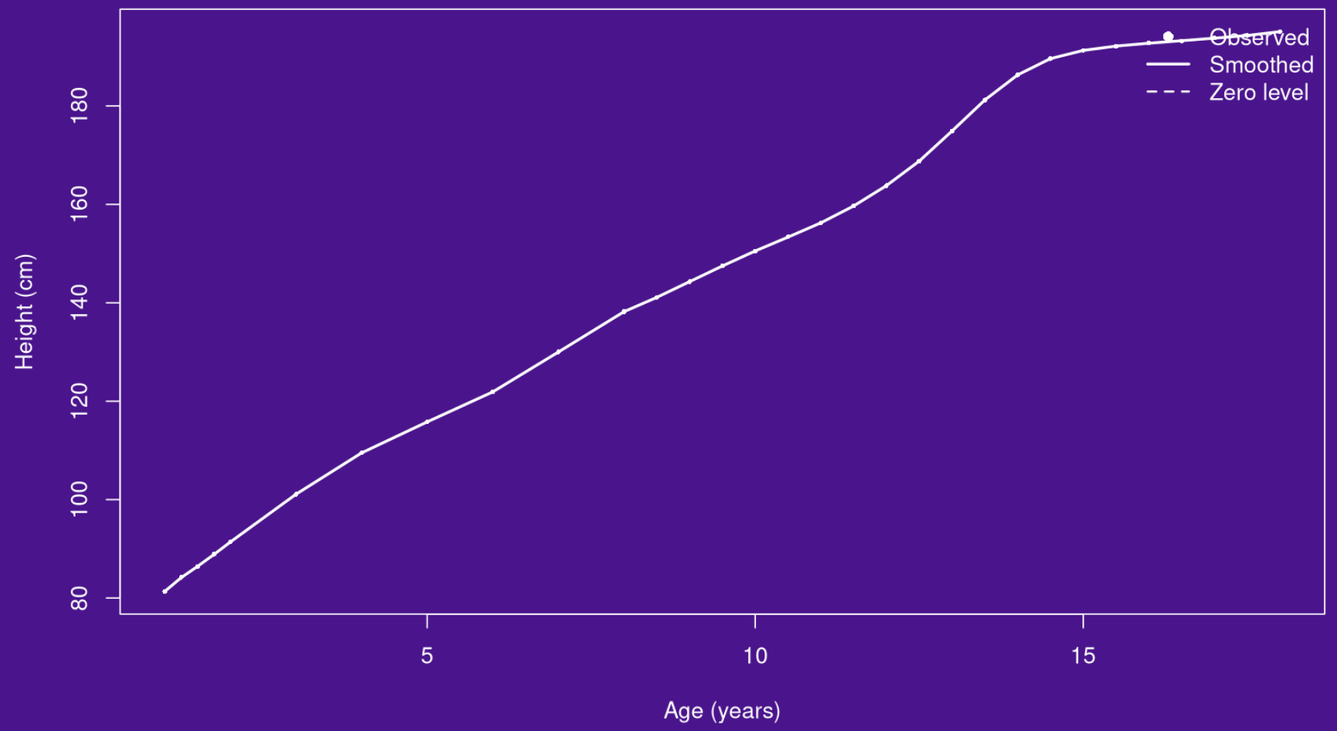
Unconstrained



Constrained

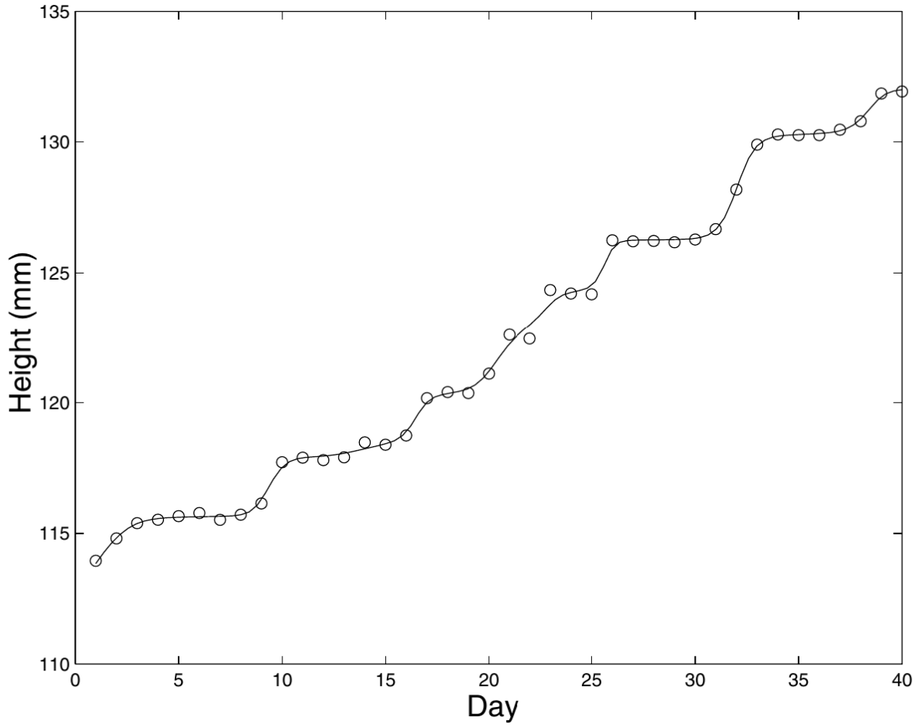


Monotone Functions



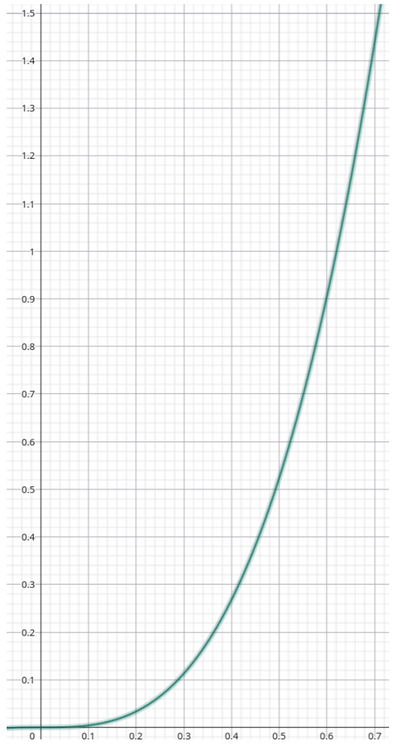
Which functions are monotone? (1 / 3)

Growth



Which functions are monotone? (2 / 3)

Growth

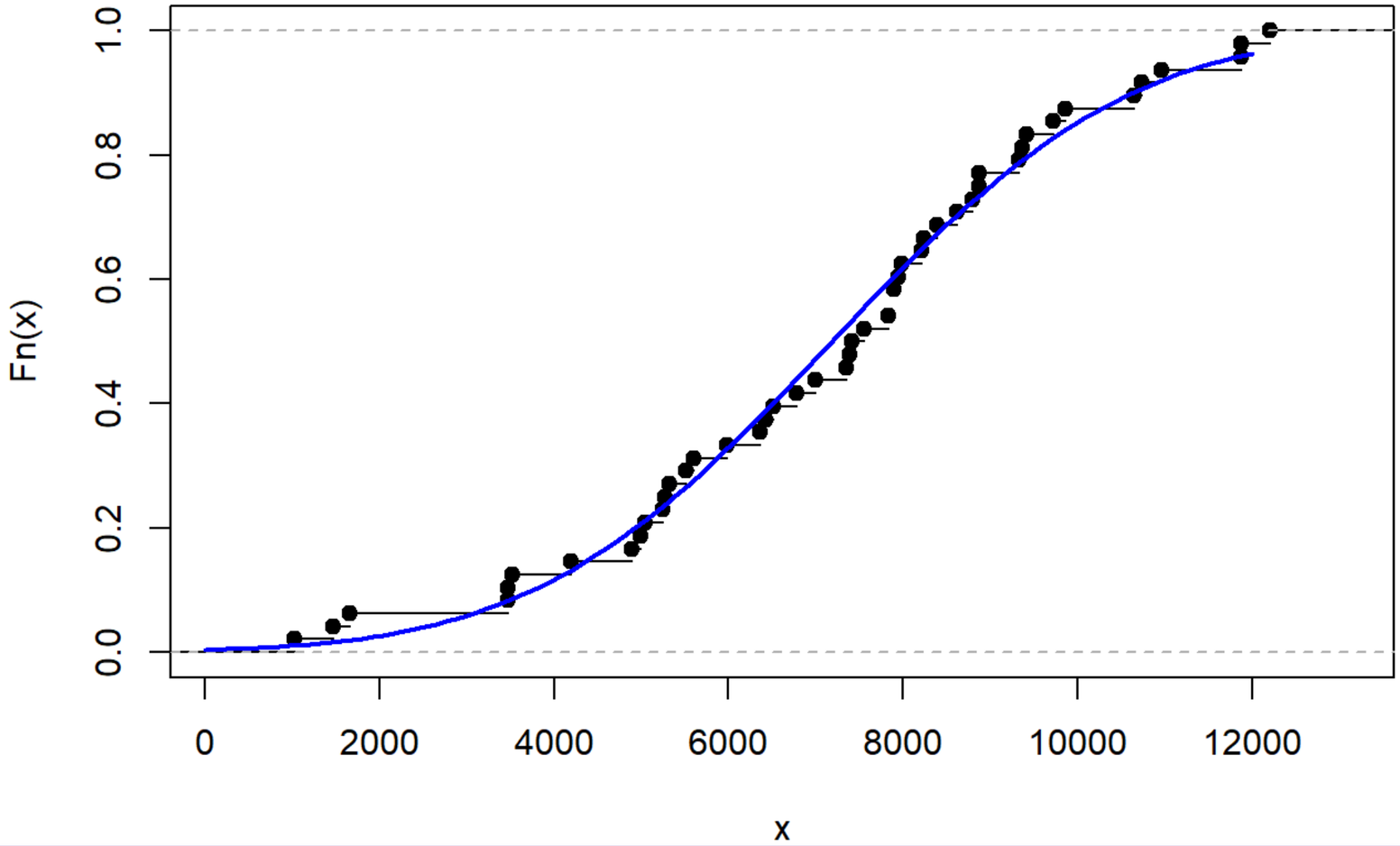


Volume is monotone increasing in the radius.

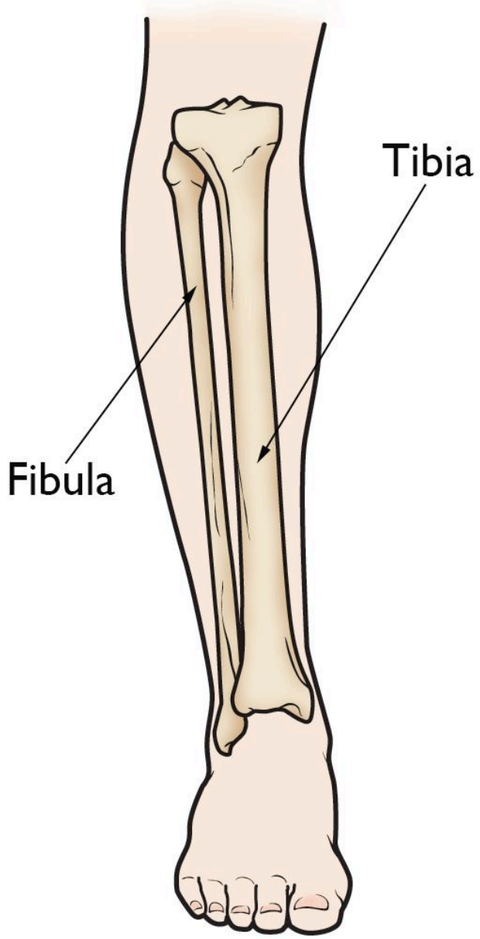
$$V(r) = \frac{4}{3}\pi r^3$$

Which functions are monotone? (3 / 3)

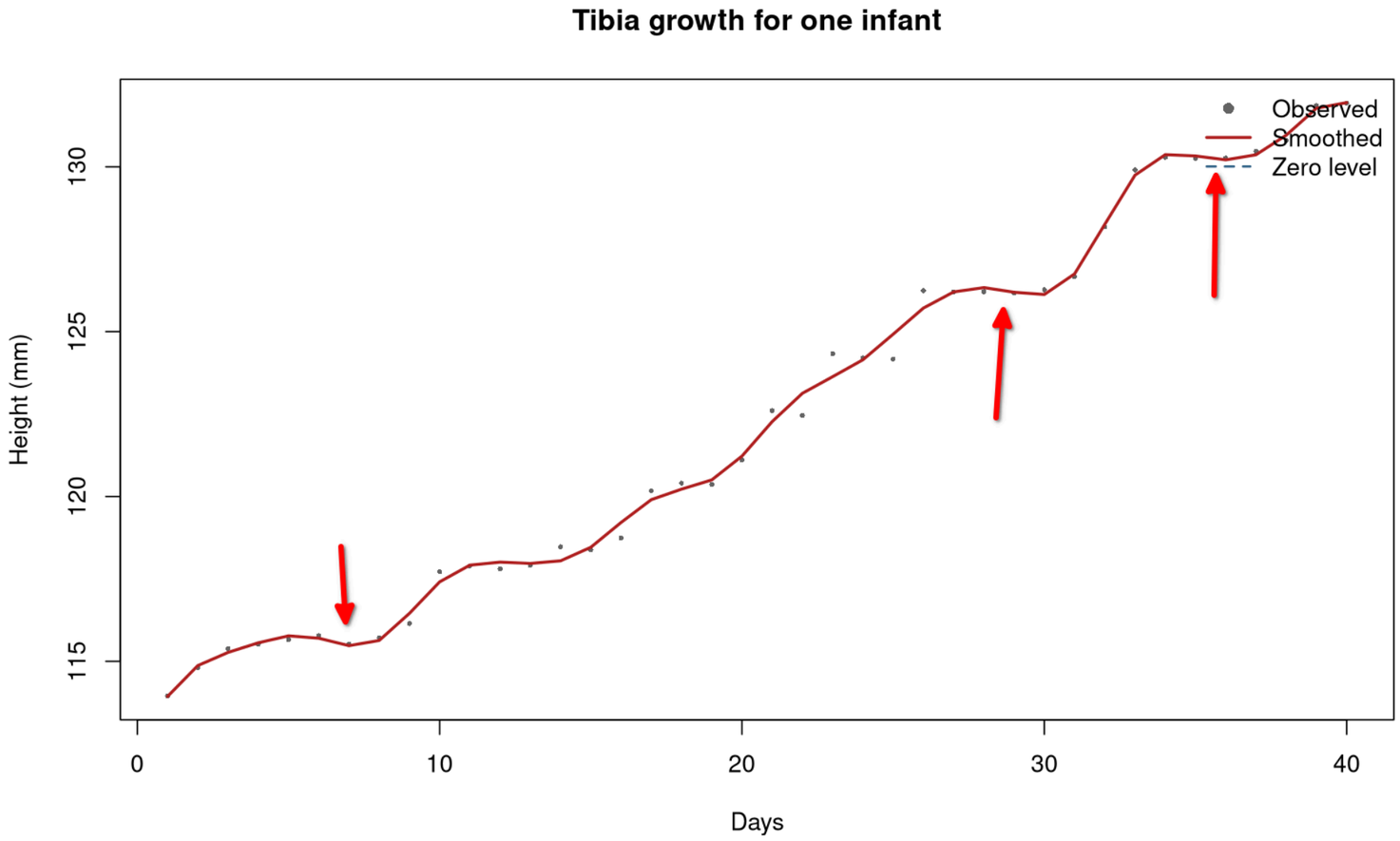
Cumulative Distribution Functions



The Tibia Dataset



Fitting with the previous approach



Ensuring monotone behavior

The first derivative must be positive everywhere.

$$Dx(t) = e^{W(t)}$$

Integrate both sides:

$$x(t) = c + \int_{t_0}^{t} e^{W(u)} du$$

c is a constant estimated from the data.

Depending on c, the function will also be positive everywhere once it crosses the 0-level.

But: A zero increase is not possible, the function is always **strictly** monotone.

The updated optimization criterion

$$\mathrm{PENSSE}_\lambda(x|\mathbf{y}) = [\mathbf{y} - x(\mathbf{t})]^T \mathbf{W} [\mathbf{y} - x(\mathbf{t})]^2 + \lambda \int (D^2 x(s))^2 ds$$

now becomes

$$\mathrm{PENSSE}_\lambda(W|\mathbf{y}) =$$
$$\left[\mathbf{y} - \left(c + \int_{t_0}^{t} e^{W(u)} du\right)\right]^T \mathbf{W} \left[\mathbf{y} - \left(c + \int_{t_0}^{t} e^{W(u)} du\right)\right]^2$$
$$+\lambda \int (D^2 W(t))^2 dt$$

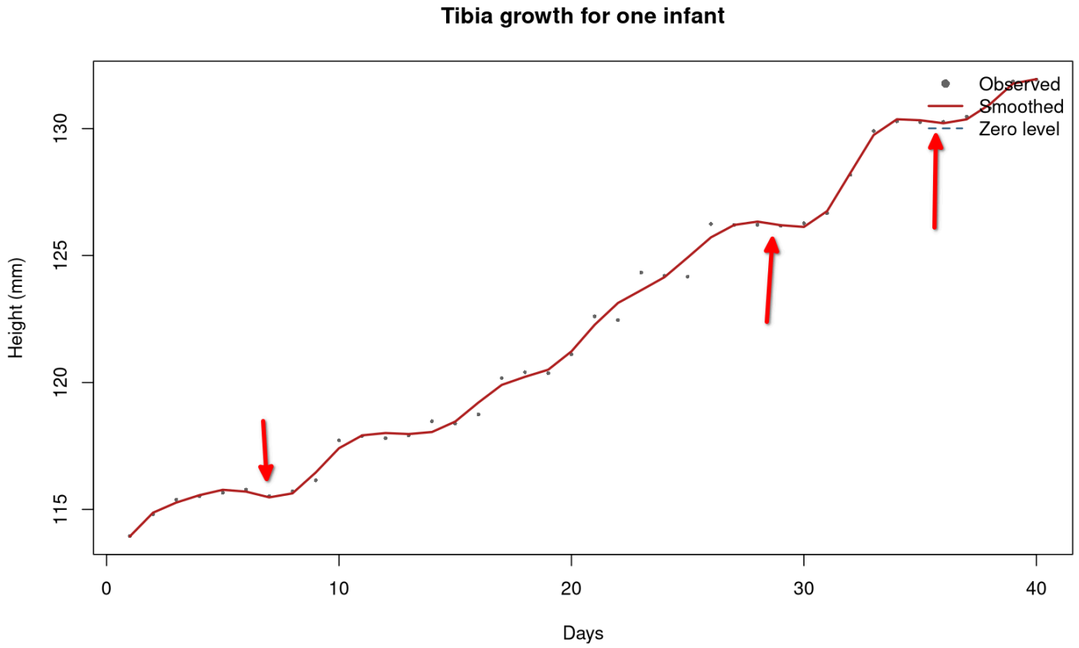
Needs to be solved through numerical methods.

smooth.basis → smooth.monotone

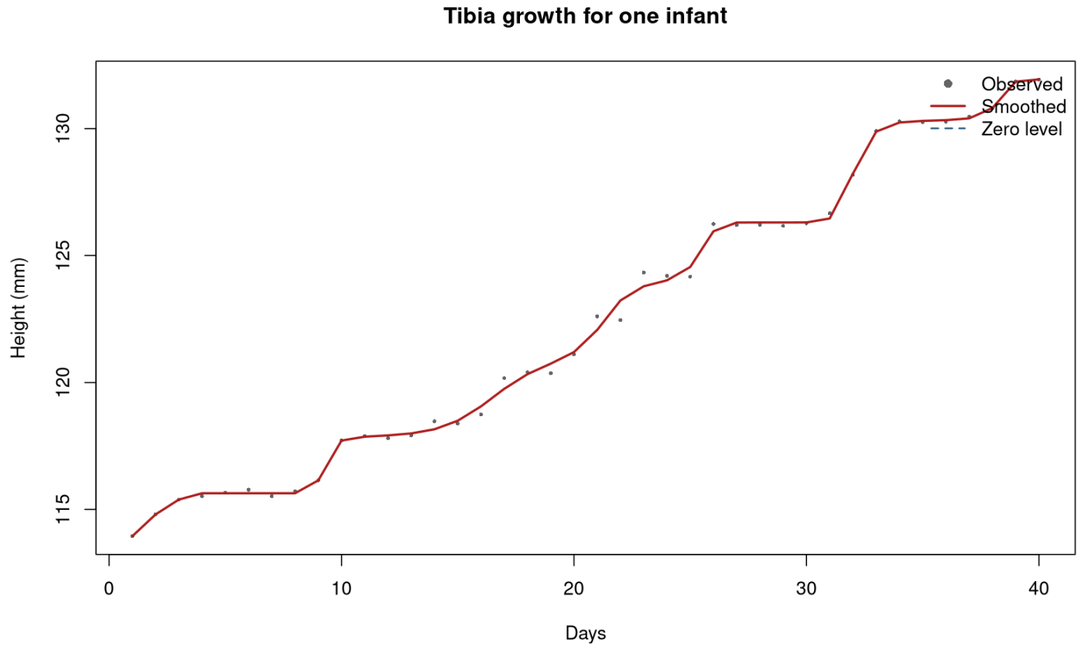
```
fdParobj <- fdPar(
    fdobj = basis,
    Lfdobj = 2,
    lambda = 1e-8
)

fit <- smooth.monotone(
    argvals = x_values,
    y = y_values,
    WfdParobj = fdParobj
)
```

Comparison

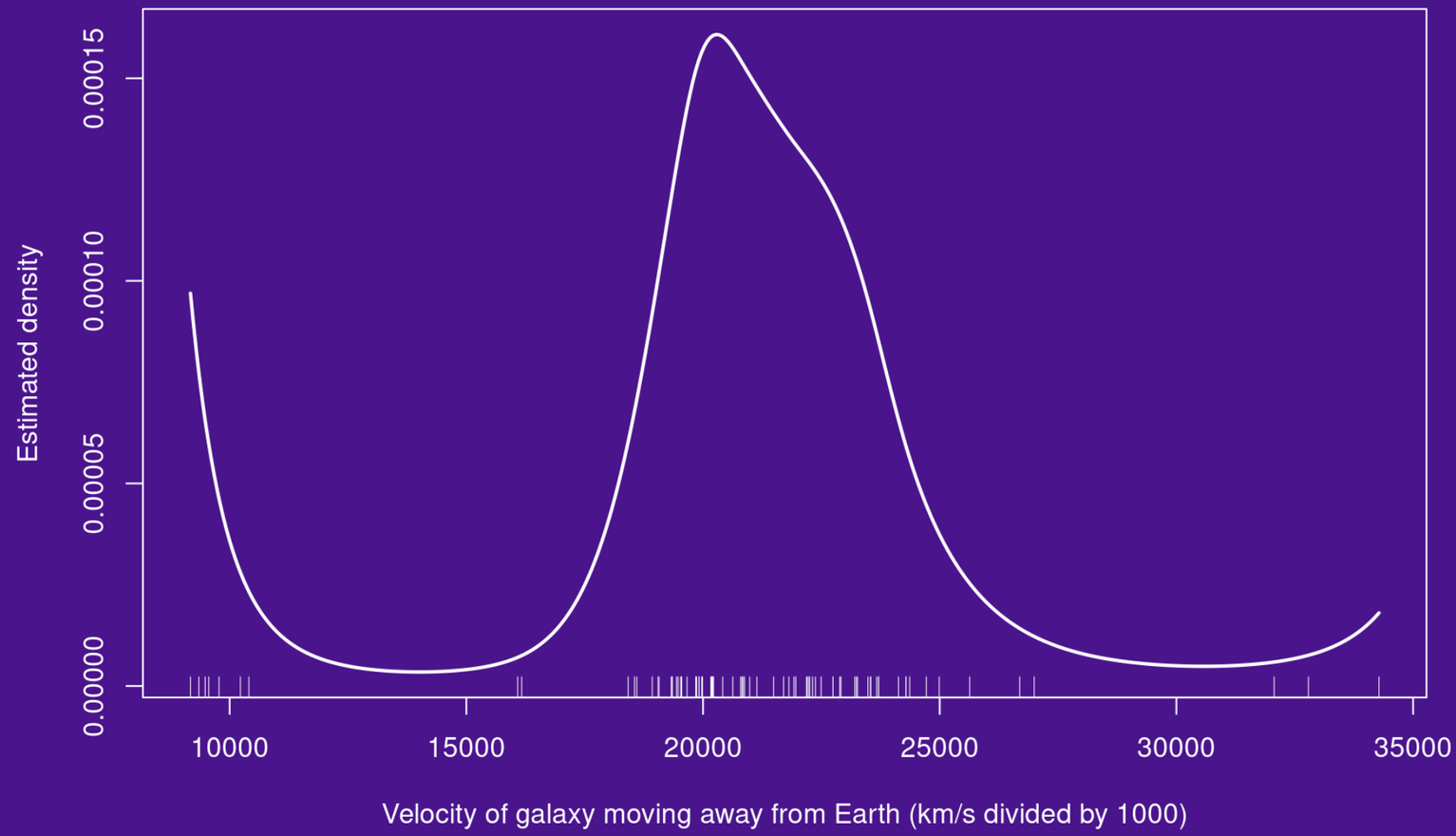
Unconstrained



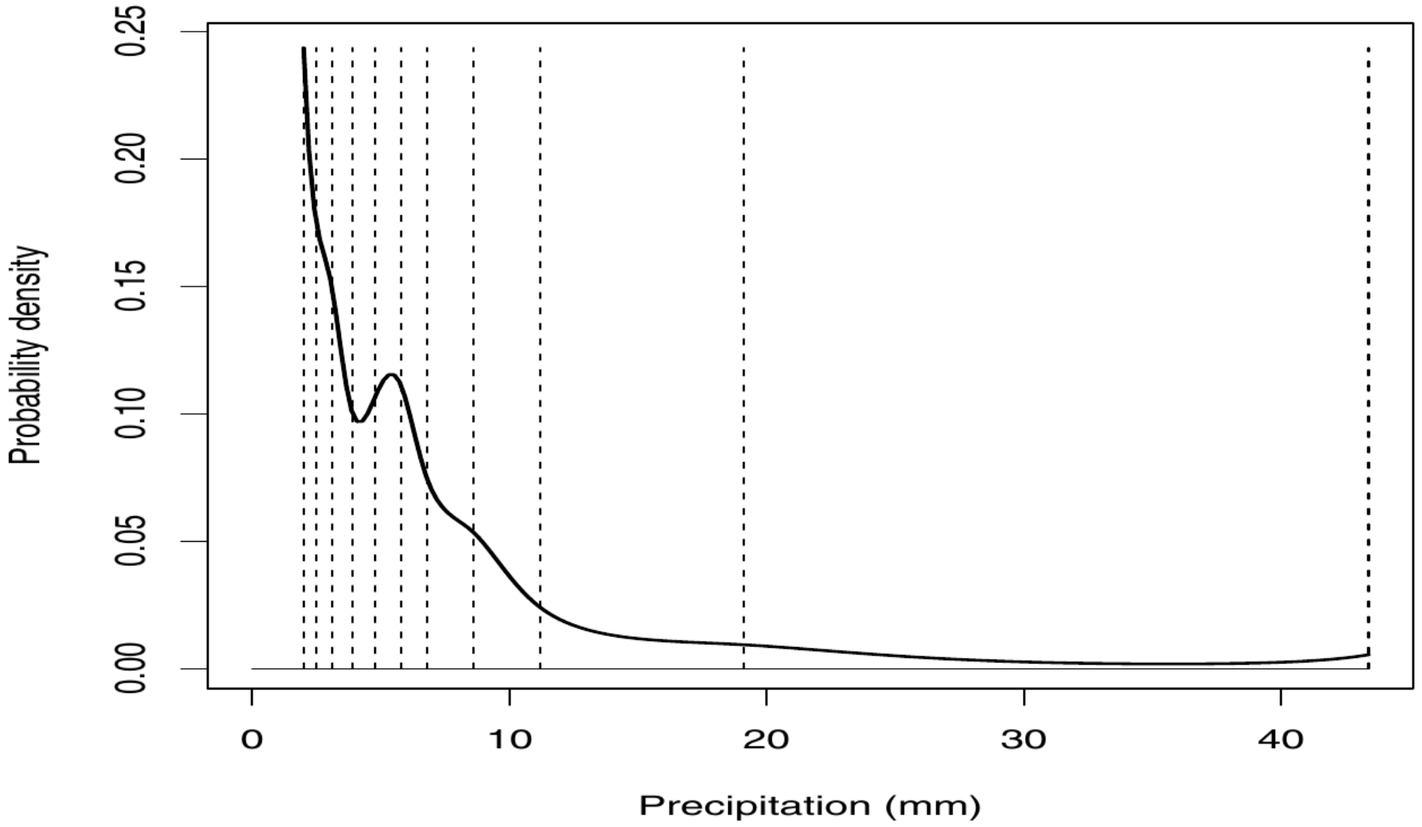
Constrained



Probability Density Functions



We now want to fit a probability density function



Each t has a probability of $p(t)$ to occur.

Two constraints for this function

$$p(t) > 0$$

$$\int p(t)dt = 1$$

$p(t)$ therefore looks like this:

$$p(t) = \frac{\overbrace{e^{W(t)}}^{\text{positive function, } p(t)>0}}{\underbrace{\int e^{W(t)} dt}_{\text{normalizing constant, } \int p(t)dt=1}}$$

This is our density model.

Remember our basis expansion

$$W(t) = \sum_{k=1}^{K} c_k \phi_k(t)$$

The goal is to find an optimal coefficient vector c for the model $p(t) = \frac{e^{W(t)}}{\int e^{W(t)} dt}$

Using **maximum likelihood estimation** is the way to go!

Likelihood Refresher

Likelihood for all N observations $t_1, \ldots, t_N$:

$$L(W|c) = \prod_{i=1}^{N} p(t_i)$$

Maximum likelihood means finding a density that assigns high probability density to the observed samples.

Products are annoying

Therefore we apply the log to convert it to a sum:

$$\log L(W|c) = \sum_{i=1}^{N} \log p(t_i)$$

Insert our density model

$$\log L(W|c) = \sum_{i=1}^{N} \log p(t_i) = \sum_{i=1}^{N} \log \left(\frac{e^{W(t)}}{\int e^{W(t)} dt} \right)$$

$$\text{Apply } \log \left(\frac{A}{B} \right) = \log A - \log B$$

$$= \sum_{i=1}^{N} \left[\log \left(e^{W(t)} \right) - \log \left(\int e^{W(t)} dt \right) \right]$$

$$= \sum_{i=1}^{N} [W(t)] - N \log \left(\int e^{W(t)} dt \right)$$

Insert basis expansion

$$\log L(W|c) = \sum_{i=1}^{N} \left[\mathbf{c}^T \phi(t_i)\right] - N \ln \left(\int e^{\mathbf{c}^T \phi(t_i)} dt \right)$$

So what do the terms mean?

$$\log L(W|c) = \sum_{i=1}^{N} \left[\mathbf{c}^T \phi(t_i)\right] - N \ln \left(\int e^{\mathbf{c}^T \phi(t_i)} dt \right)$$

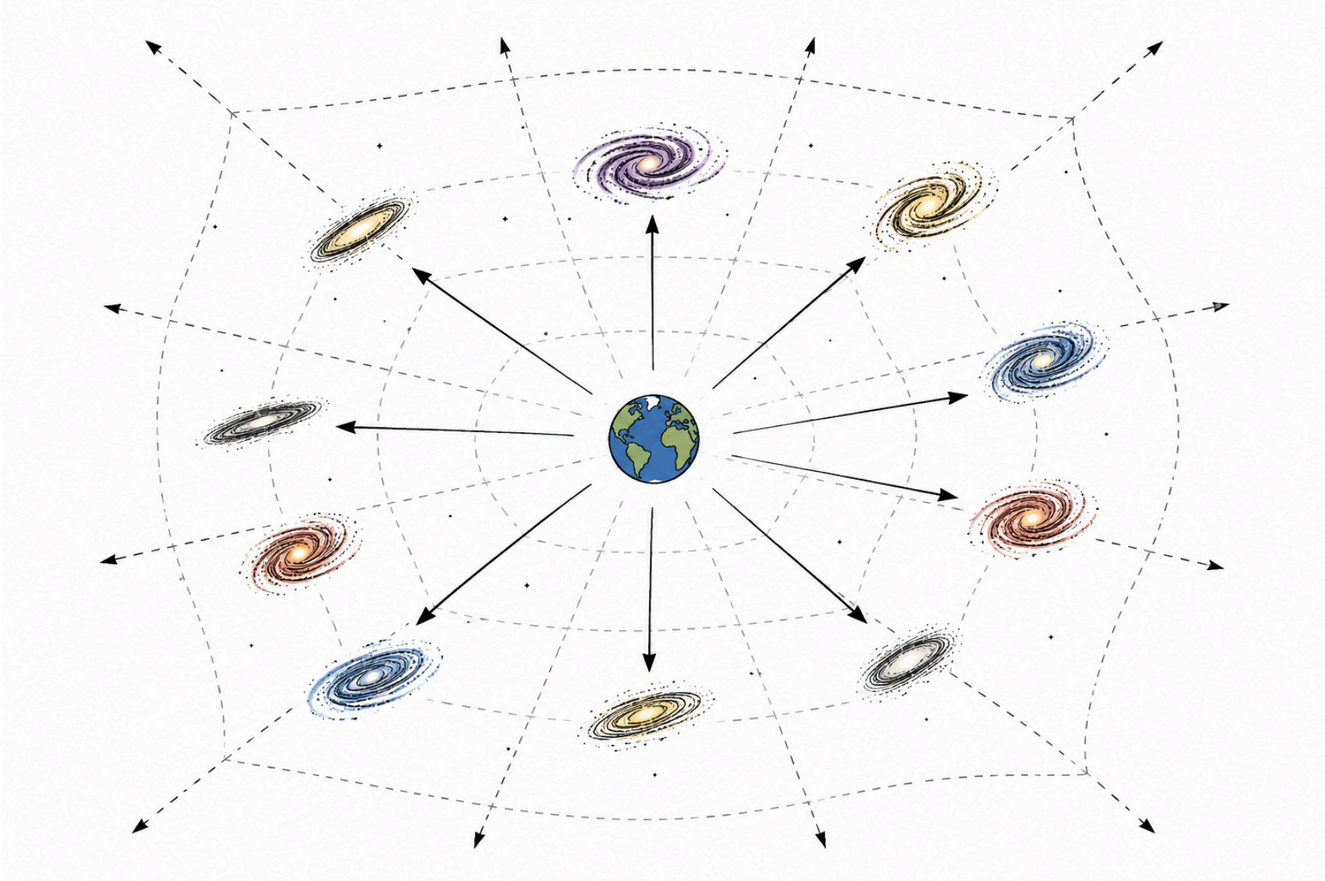
$$\sum_{i=1}^{N} \left[\mathbf{c}^T \phi(t_i)\right]$$

Rewards making W large where data points occur.

$$N \ln \left(\int e^{\mathbf{c}^T \phi(t_i)} dt \right)$$

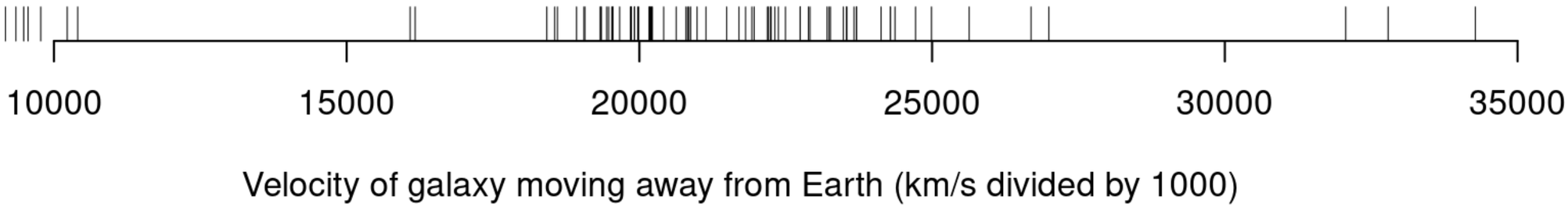
Normalization penalty; without it, $W \to \infty$ everywhere, the term forces the density to integrate to 1.

Let's apply this to the R galaxies dataset!



82 observatons of the velocities (in 1000 km/second) of distant galaxies diverging from our own

The dataset is a simple list of velocities



Constructing the R script (1)

Preliminaries

```r
library(fda)
library(MASS)
data(galaxies)
dataset <- galaxies
N <- length(dataset)
```

Constructing the R script (2)

Construct a B-Spline basis

```
Wknots <- dataset[round(N * seq(1 / N, 1, length.out = 11), 0)]
Wnbasis <- length(Wknots) + 2
Wbasis <- create.bspline.basis(
  rangeval = range(dataset),
  nbasis   = Wnbasis,
  norder   = 4,
  breaks   = Wknots
)
```

Constructing the R script (3)

Then we compute the fit using **density.fd**

```
Wlambda <- 0
Wfd0 <- fd(matrix(0, Wnbasis, 1), Wbasis)
WfdPar <- fdPar(Wfd0, Lfdobj = 2, lambda = Wlambda)

# Fit the density with density.fd.
# The result contains:
# - Wfdobj: fitted log-density component W(x)
# - C: normalizing constant
densityList <- density.fd(dataset, WfdPar)
```

Attention: density.fd is only available up until version 6.2.0. It has been removed in version 6.3.0.

Constructing the R script (4)

Evaluate the fitted fda density on a fine grid.

```
Wfd <- densityList$Wfdobj
Cconst <- densityList$C
Zfine <- seq(min(dataset), max(dataset), length.out = 401)
Wfine <- eval.fd(Zfine, Wfd)
Pfine <- exp(Wfine) / Cconst
```

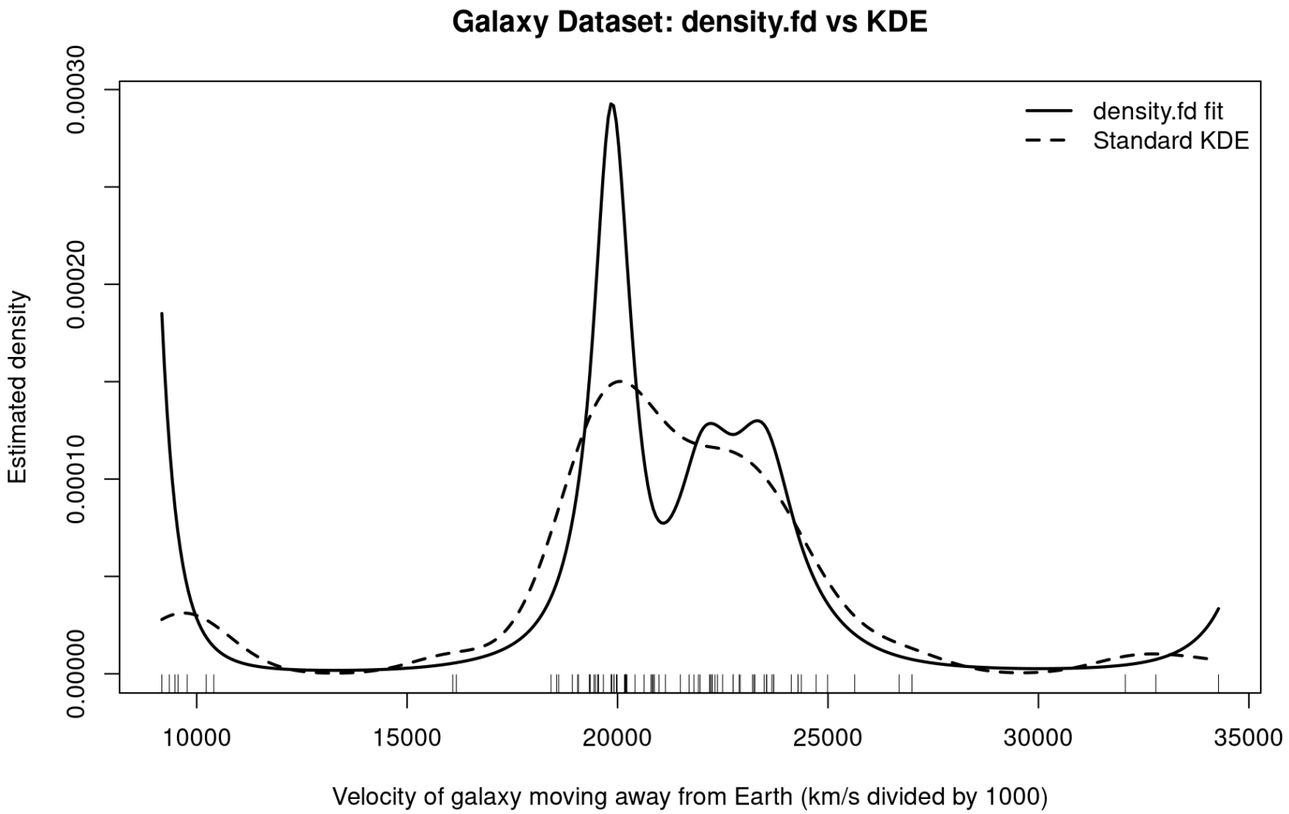
densityList only gives you $W(t)$ and the normalization constant, but not $p(t)$, so you need to stitch it together yourself.

Constructing the R script (5)

Finally plot it.

```r
plot(
  Zfine, Pfine,
  type = "l",
  lwd = 2,
  xlab = "Velocity of galaxy moving away from Earth (km/s divided by 1000)",
  ylab = "Estimated density",
  main = "Galaxy Dataset: density.fd vs KDE"
)

lines(kde_fit$x, kde_fit$y, lwd = 2, lty = 2)
```

The initial approach overfits badly!



No smoothness control!

Let's extend it with a roughness penalty

$$\log L(W|c) = \sum_{i=1}^{N} \left[\mathbf{c}^T \phi(t_i)\right] - N \ln \left(\int e^{\mathbf{c}^T \phi(t_i)} dt \right) - \underbrace{\lambda \int \left[D^3(\mathbf{c}^T \phi(t_i))\right]^2 dt}_{\mathrm{PEN}_3(W)}$$

$\mathrm{PEN}_3(W)$ penalizes changes in curvature:

- less wiggles
- less oscillations
- less rapid shape changes

λ is the smoothing parameter (similar to bandwidth in KDE).

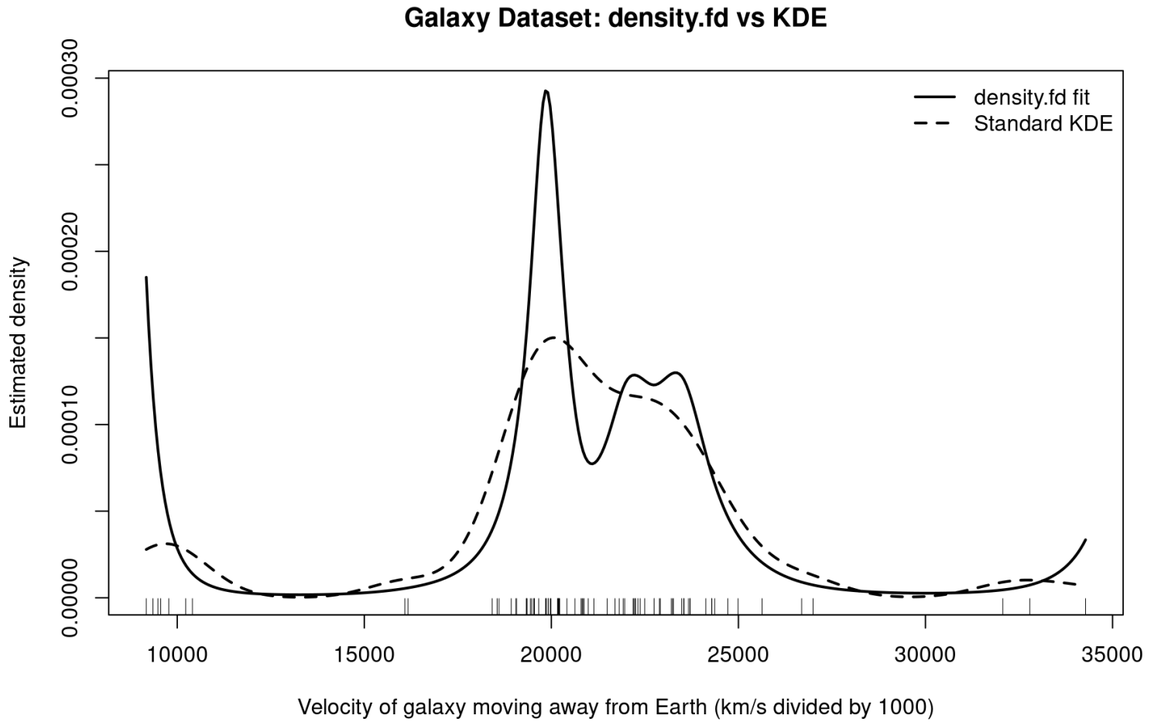
Find coefficient vector $\mathbf{c}$ via numerical optimization.

The density.fd function accepts λ as a parameter.

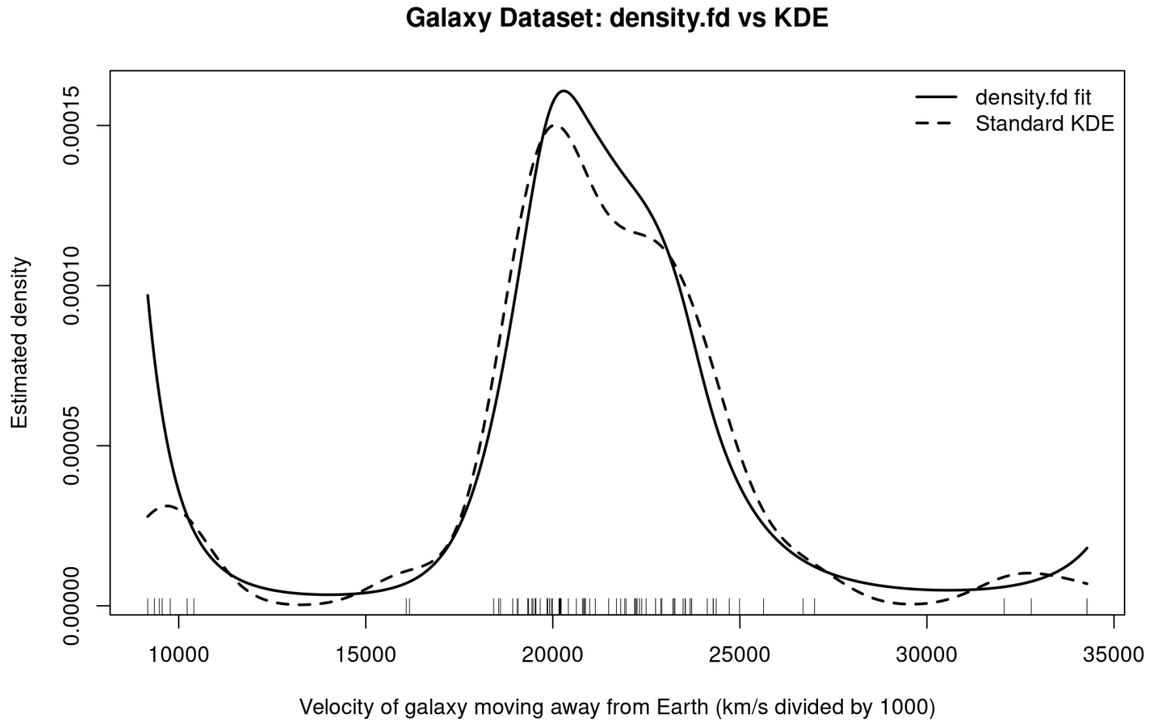
Adjust **Wlambda** accordingly

```r
Wlambda <- 3e+9
Wfd0 <- fd(matrix(0, Wnbasis, 1), Wbasis)
WfdPar <- fdPar(Wfd0, Lfdobj = 2, lambda = Wlambda)

# Fit the density with density.fd.
# The result contains:
# - Wfdobj: fitted log-density component W(x)
# - C: normalizing constant
densityList <- density.fd(dataset, WfdPar)
```

The effect of λ



$\lambda = 0$



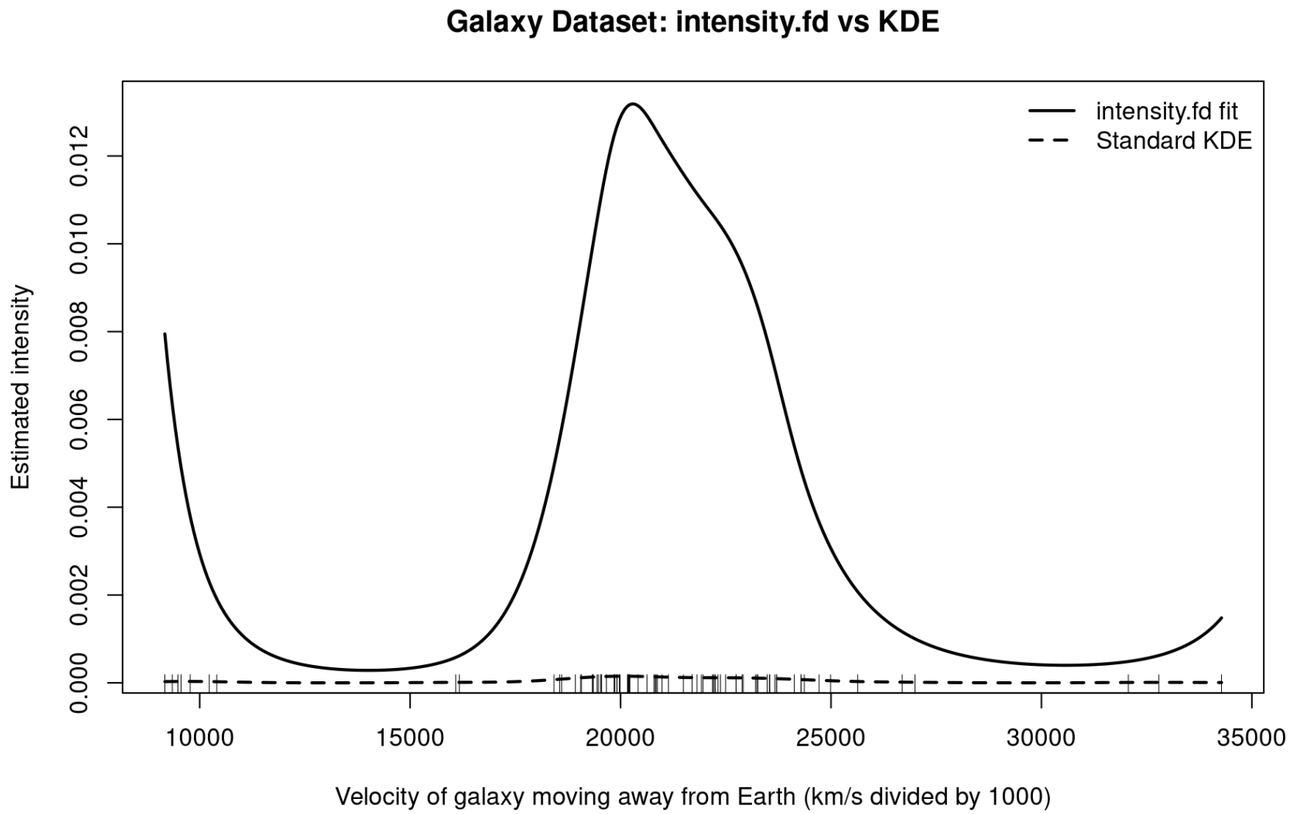
$\lambda = 3 \times 10^9$

For the fda package version 6.3.0, intensity.fd can be used

intensity.fd is essentially the same as density.fd, but does not normalize.

```
# Fit the intensity with intensity.fd.
# The result contains:
# - Wfdobj: fitted log-intensity component W(x)
densityList <- intensity.fd(dataset, WfdPar)

Wfd <- densityList$Wfdobj

# Evaluate the fitted intensity on a fine grid.
Zfine <- seq(min(dataset), max(dataset), length.out = 401)
Wfine <- eval.fd(Zfine, Wfd)
Ifine <- as.numeric(exp(Wfine))
```

Same curve, but not normalized.



intensity.fd does not provide us a normalization constant.

Question to the experts here:

Why would we use this method instead of simply computing the usual KDE?

Exercise

Task 1

Task 2

Task 3

Questions?