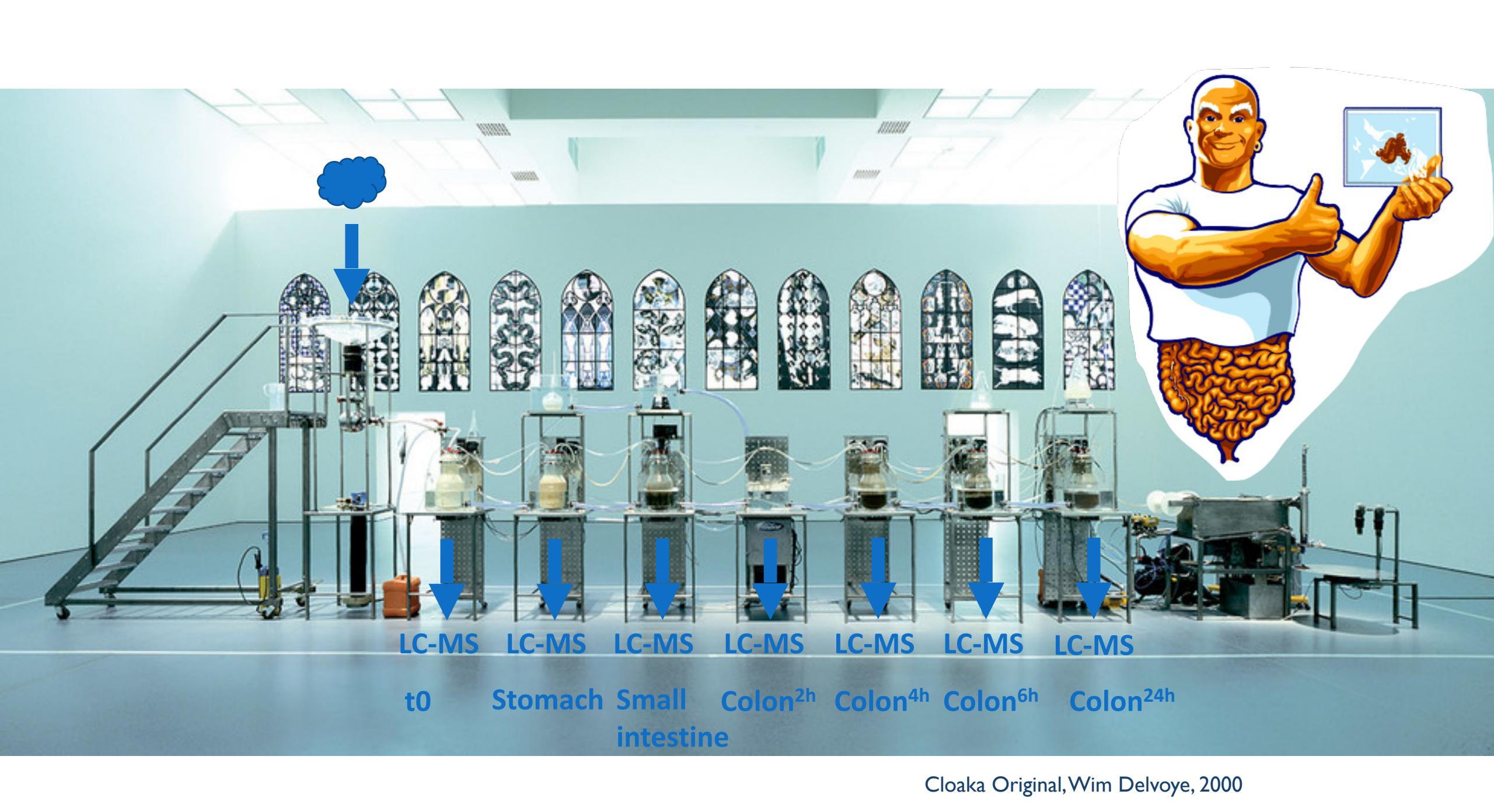


tindeResting:

harvesting expert knowledge in a childlike manner

Charlie Beirnaert

February 23, 2018



• Why this experiment

- Prodrugs

• Why this experiment



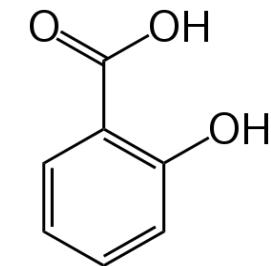
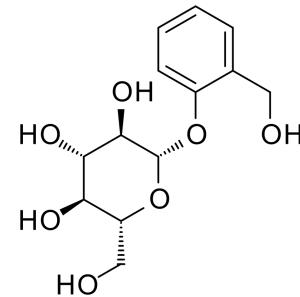
- Prodrugs



• Why this experiment



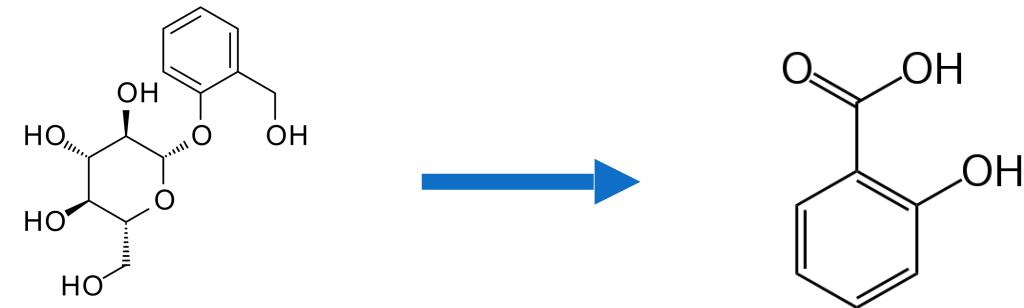
- Prodrugs



• Why this experiment



- Prodrugs



• Why this experiment



- Many more
- Potential unknown lead compounds
 - Malaria
 - Kidney stones
 - Inflammation



• Data analysis



- Longitudinal LC-MS data

- I. XMCS

1. Peak picking
2. Grouping
3. etc.

2. Clean-up & Corrections

3. EDGE^[1,2]

[1] Storey et al., Significance analysis of time course microarray experiments, PNAS 2005
[2] Leek et al., Extraction and analysis of Differential Gene Expression, Bioinformatics 2006

• Data analysis

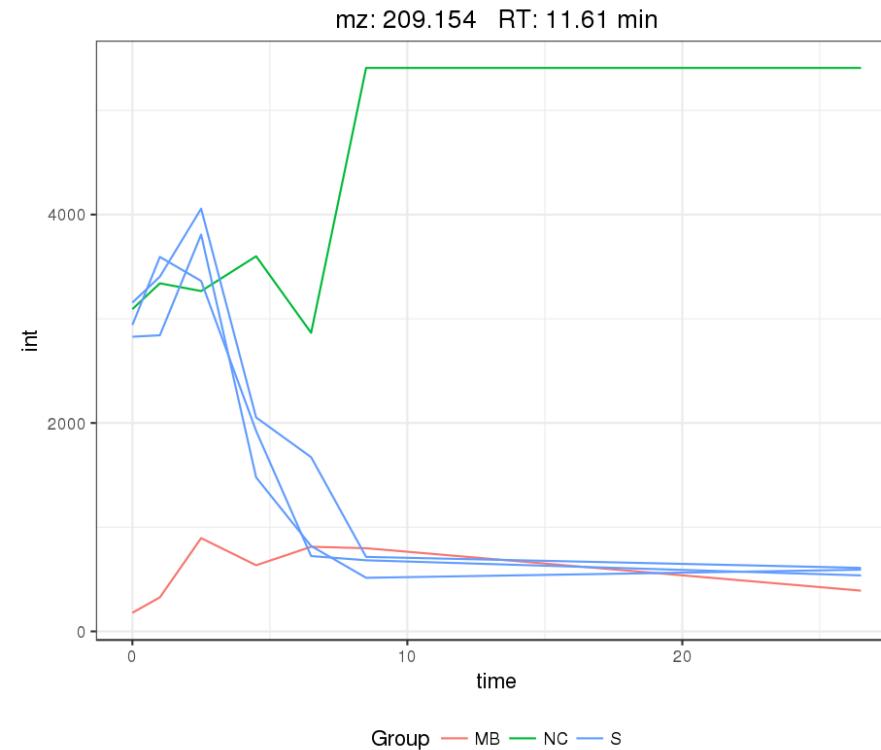


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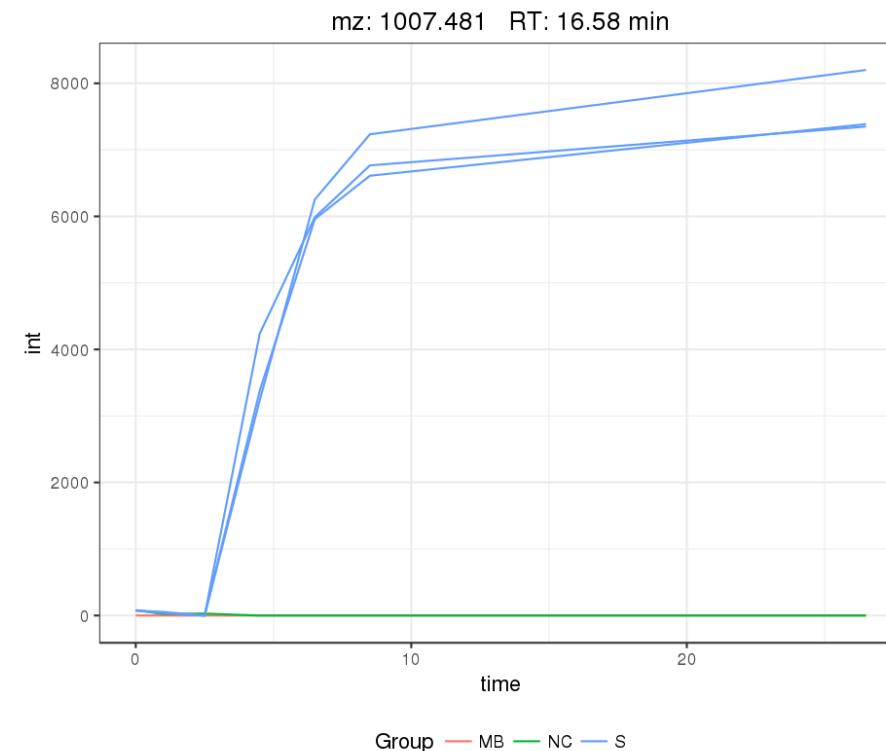
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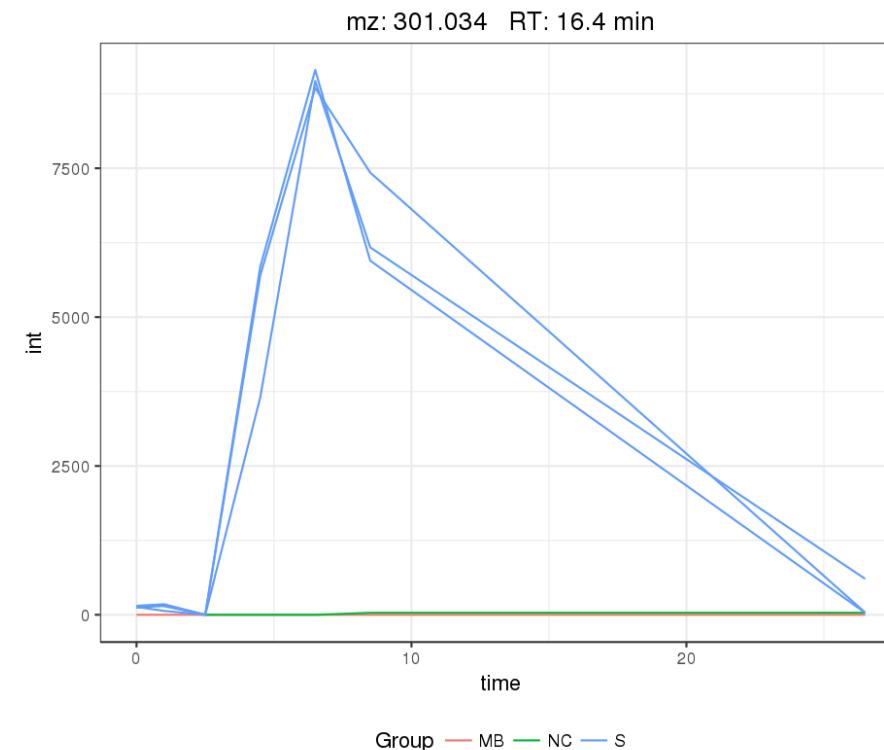
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• EDGE

- Natural cubic splines (flexibility)
- Null-model  Alternative model
- Goodness of fit improvement?
(q values)

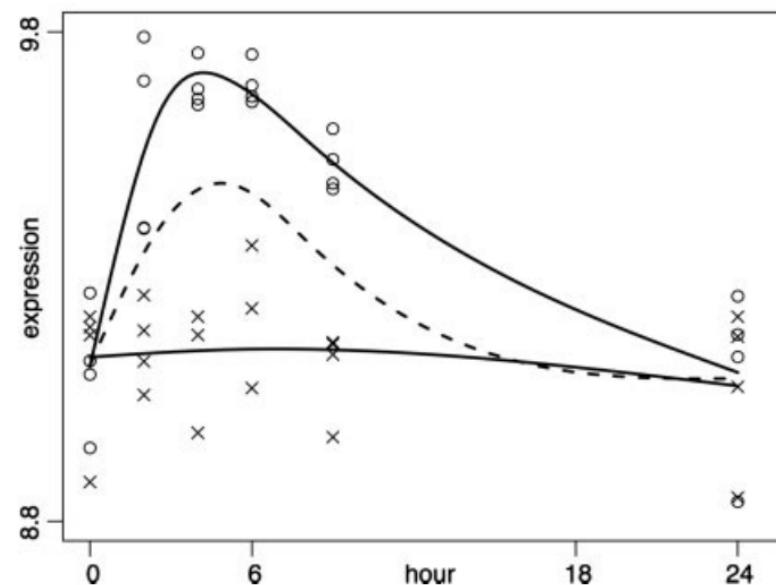


Figure from Storey et al., Significance analysis of time course microarray experiments, PNAS 2005

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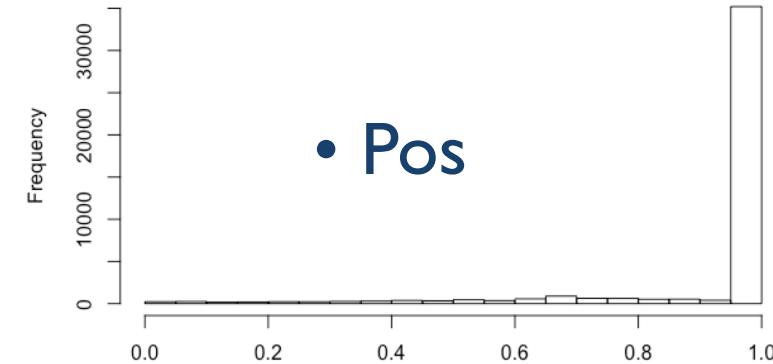
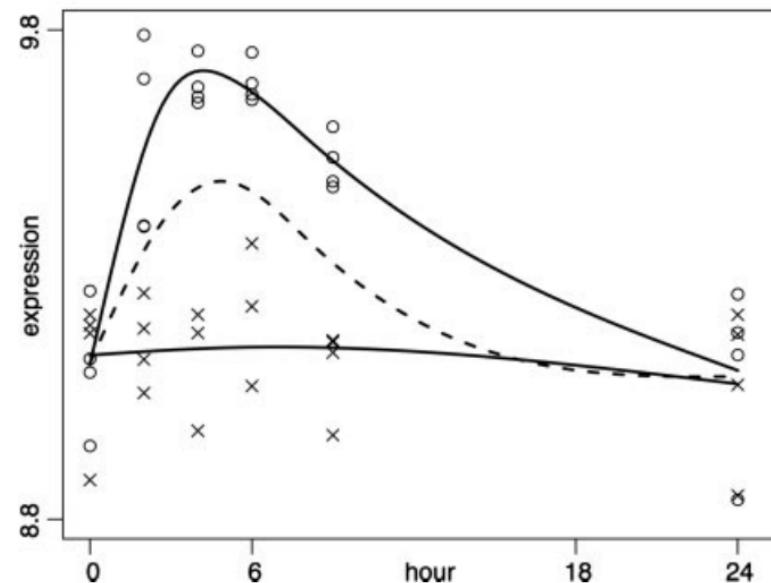


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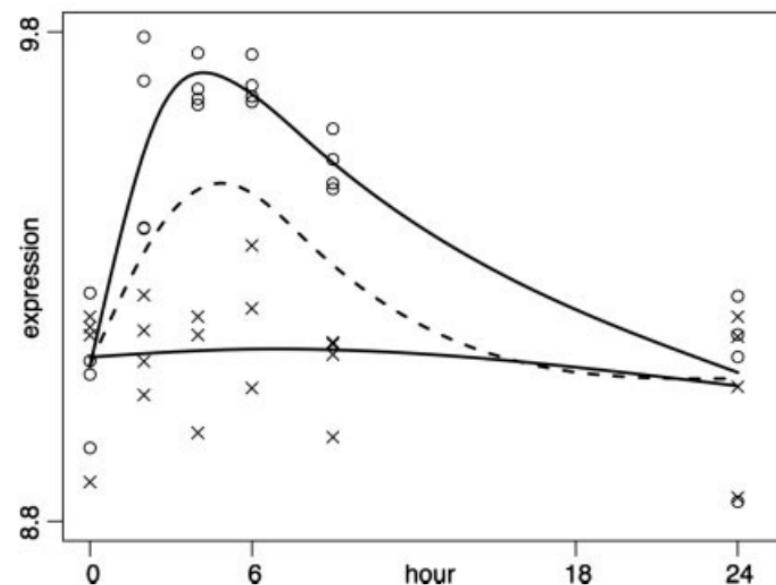
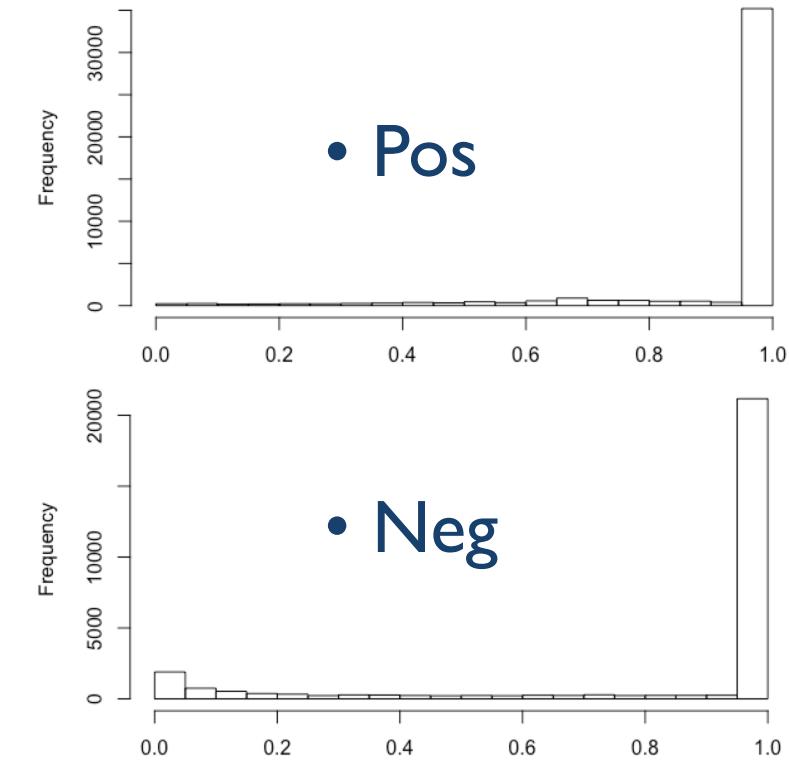
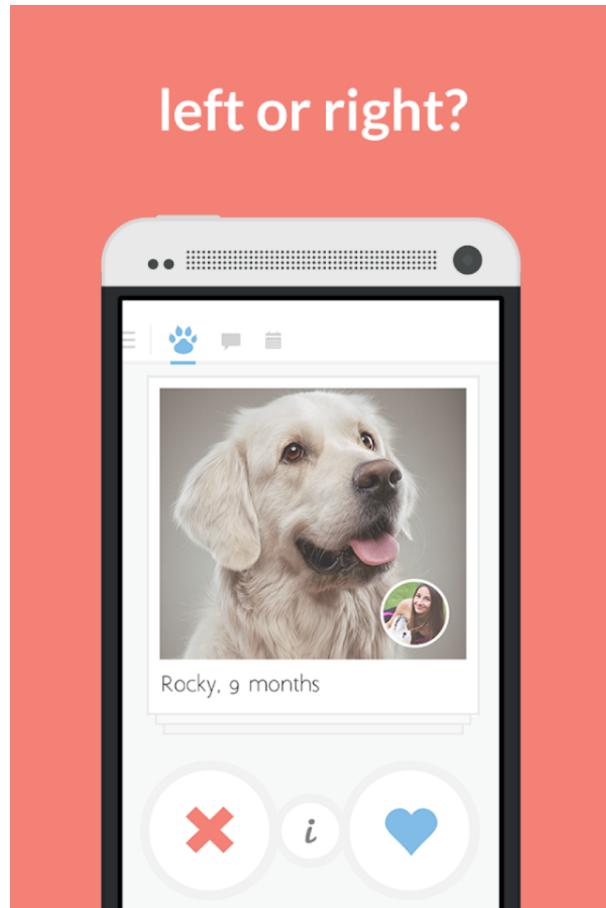


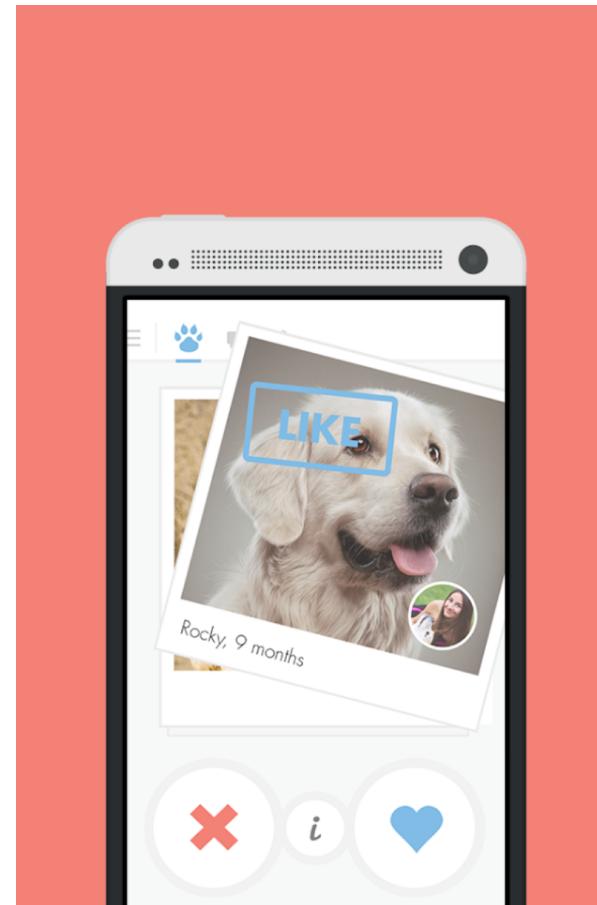
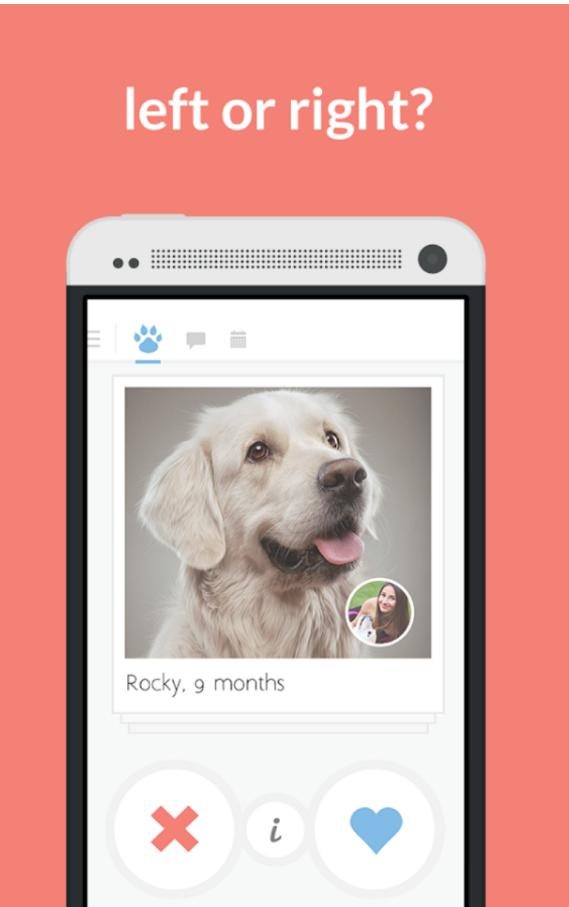
Figure from Storey et al., Significance analysis of time course microarray experiments, PNAS 2005



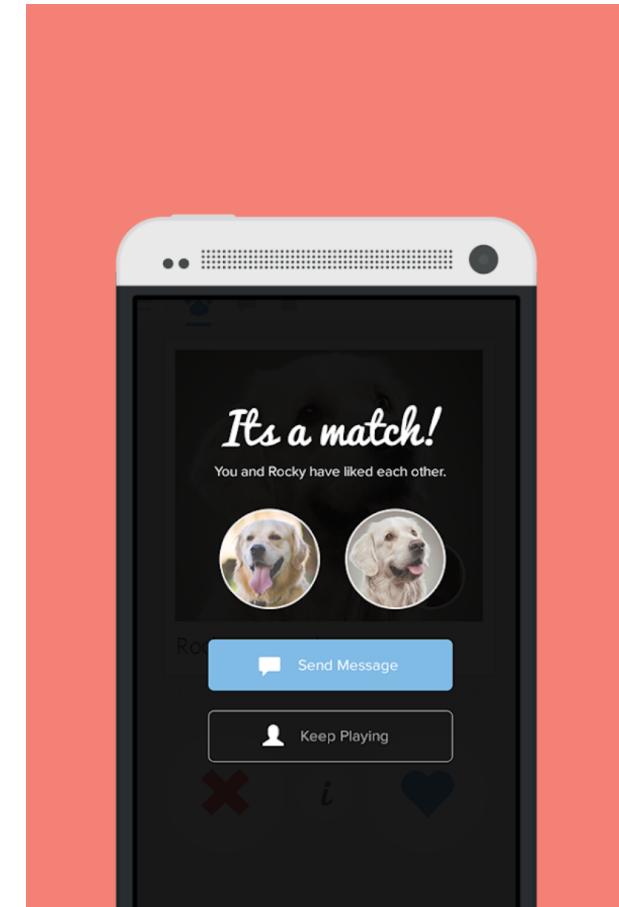
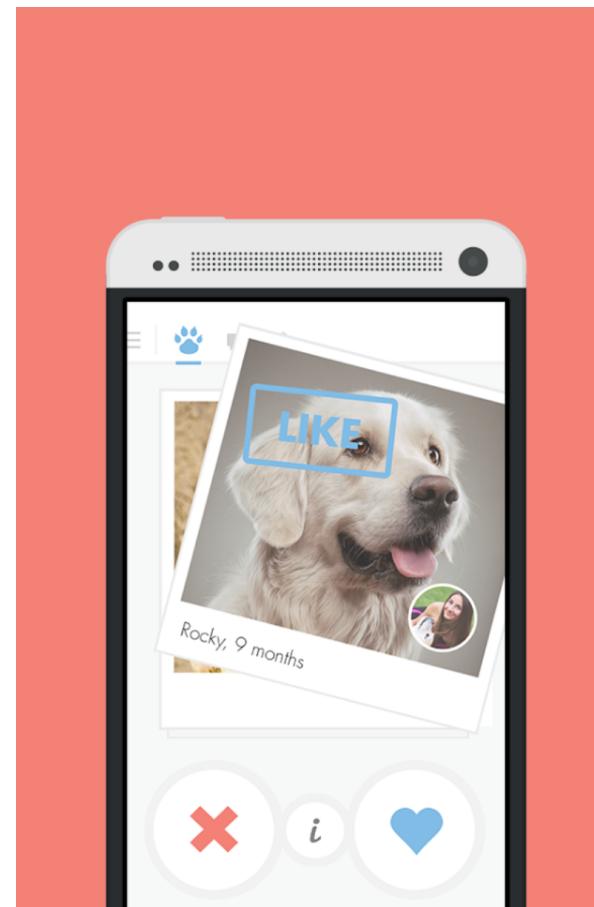
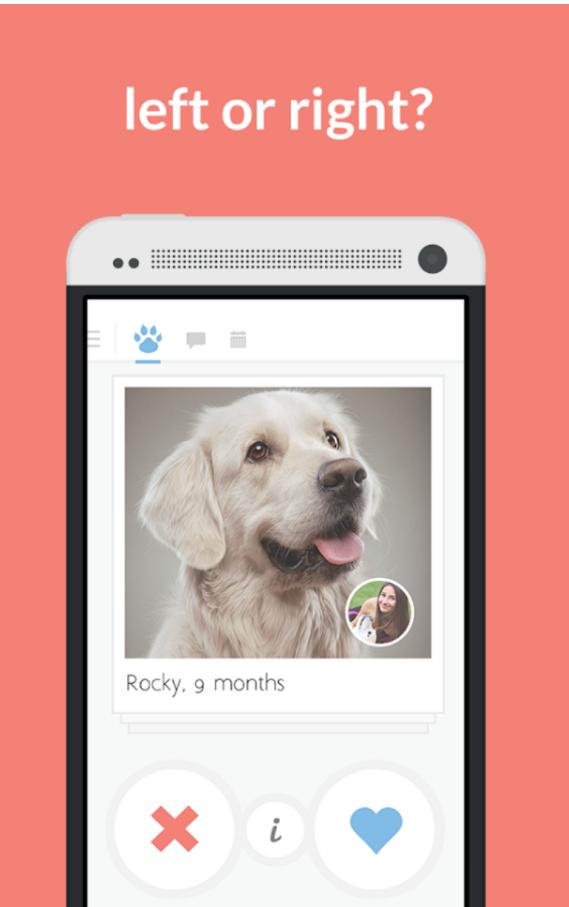
• Tinder



• Tinder



• Tinder



• What is Shiny?



Shiny

from  Studio

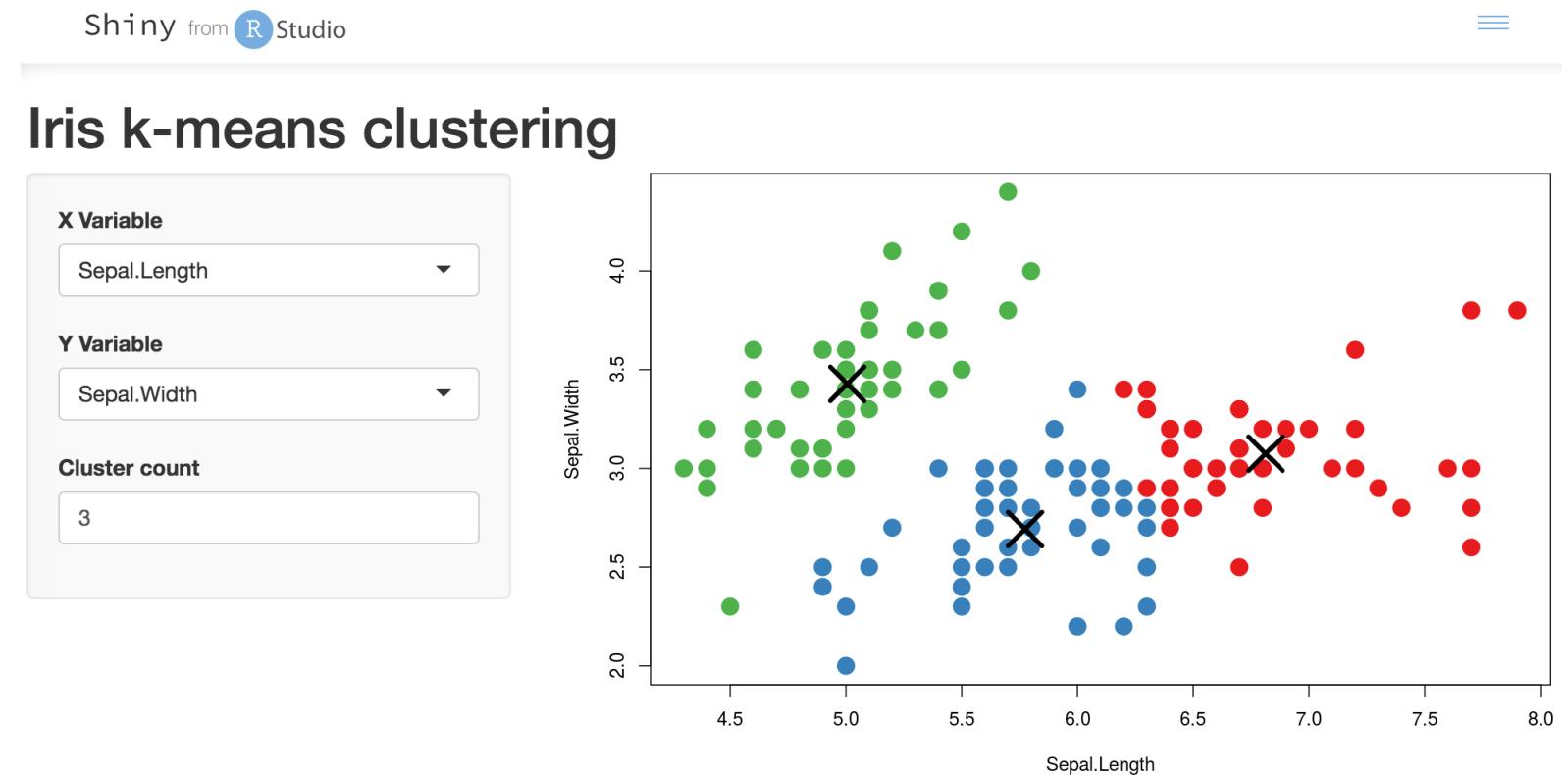
- R package
- Easy to build
- Interactive web apps

• What is Shiny?

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The app

This is the GOA tindeResting! app.

Your name: Louise

Preference: ♂

Ion mode: Positive

Model based filter: no

max q value: 0.2

minimal RT (min): 0

Time profiles: New to me

Swipe Order: Significance

474 Features Selected

Selected: FALSE (red), TRUE (blue)

Oopsie daisy

Update Predictions

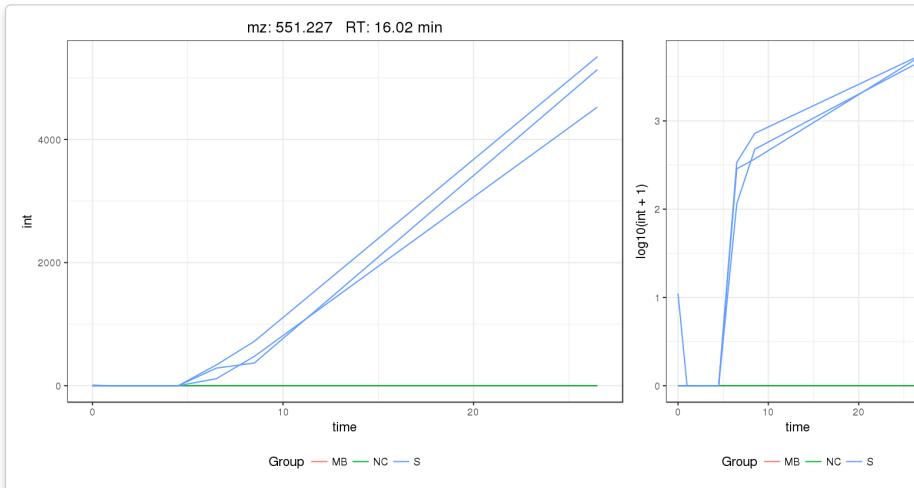
Swipe Me! Or use the arrows

Swipe the plot to the right if the time profile is interesting. Left if not.

◀ boring

↑ other

→ interesting



Swipe History

index	mz	rt	swipe
9121	281.98165	520.1005	Right

The app

This is the GOA tindeResting! app.

Your name: Louise

Preference: Cat ♀ ♂

Ion mode: Positive

Model based filter: no yes

max q value: 0.2

minimal RT (min): 0

Time profiles: New to me

Swipe Order: Significance

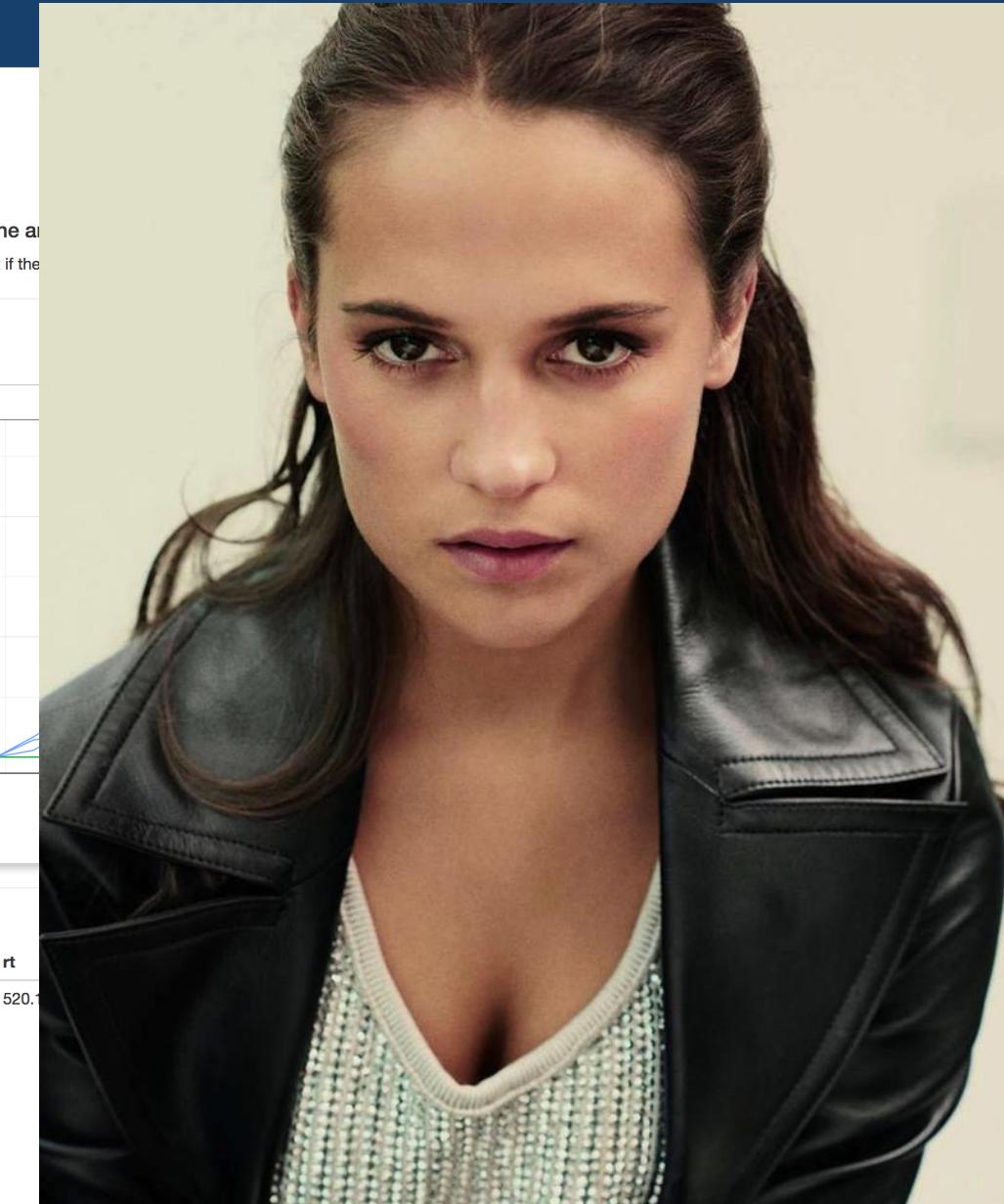
474 Features Selected

Swipe History:

index	mz	rt
9121	281.98165	520.1

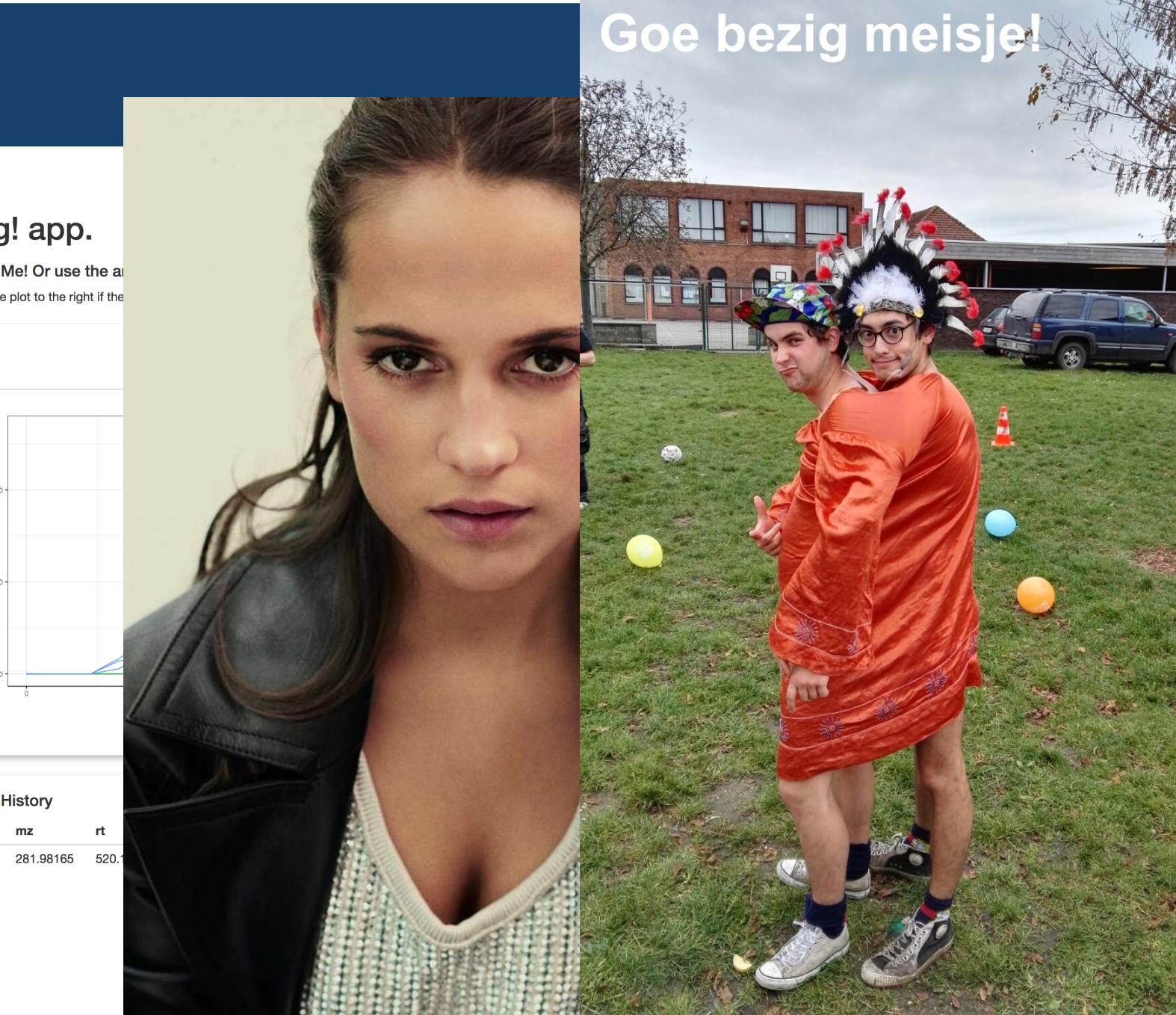
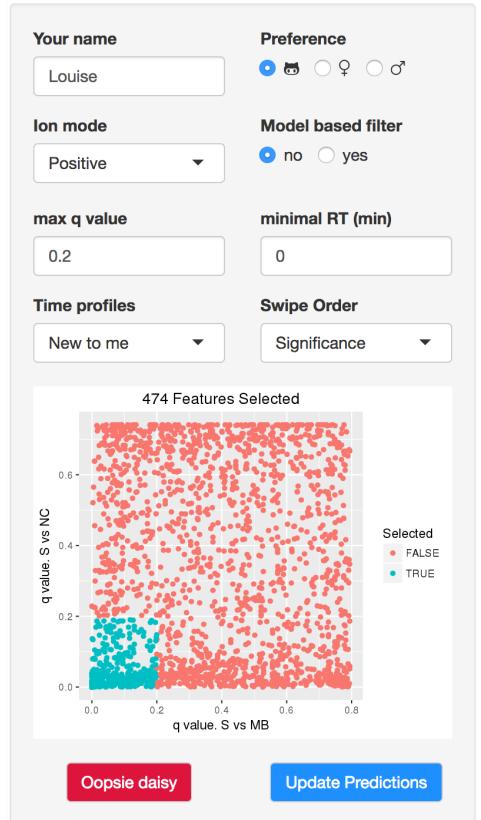
Oopsie daisy

Update Predictions



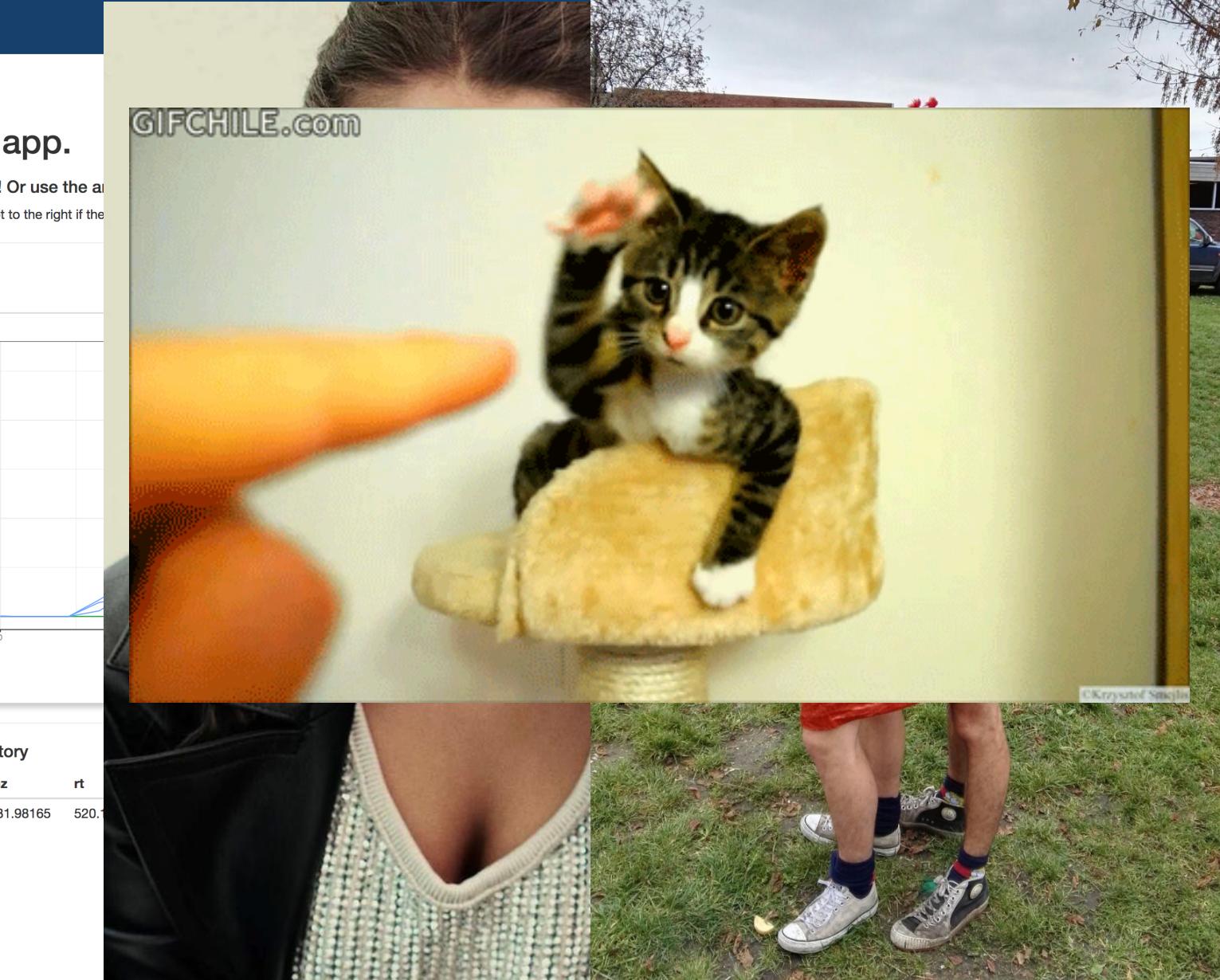
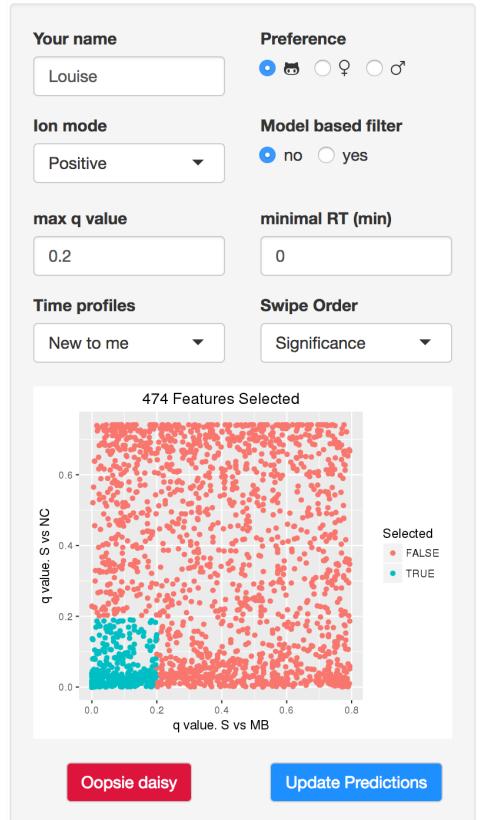
The app

This is the GOA tindeResting! app.

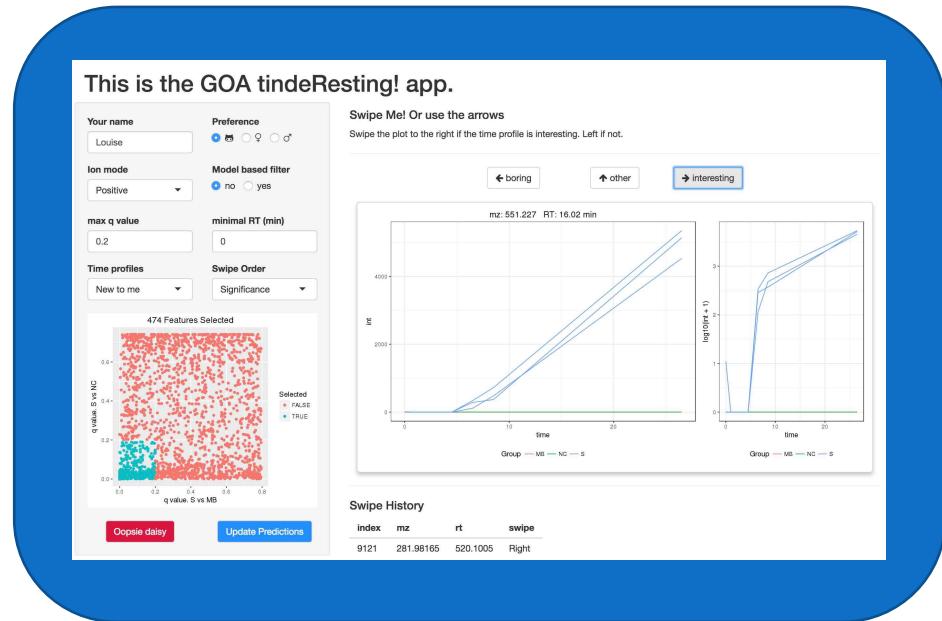


The app

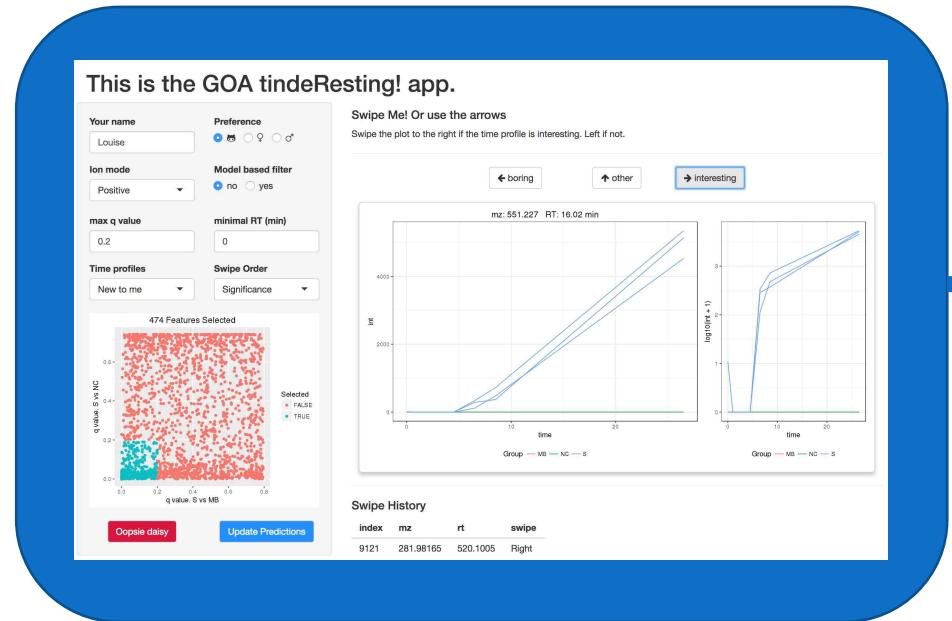
This is the GOA tindeResting! app.



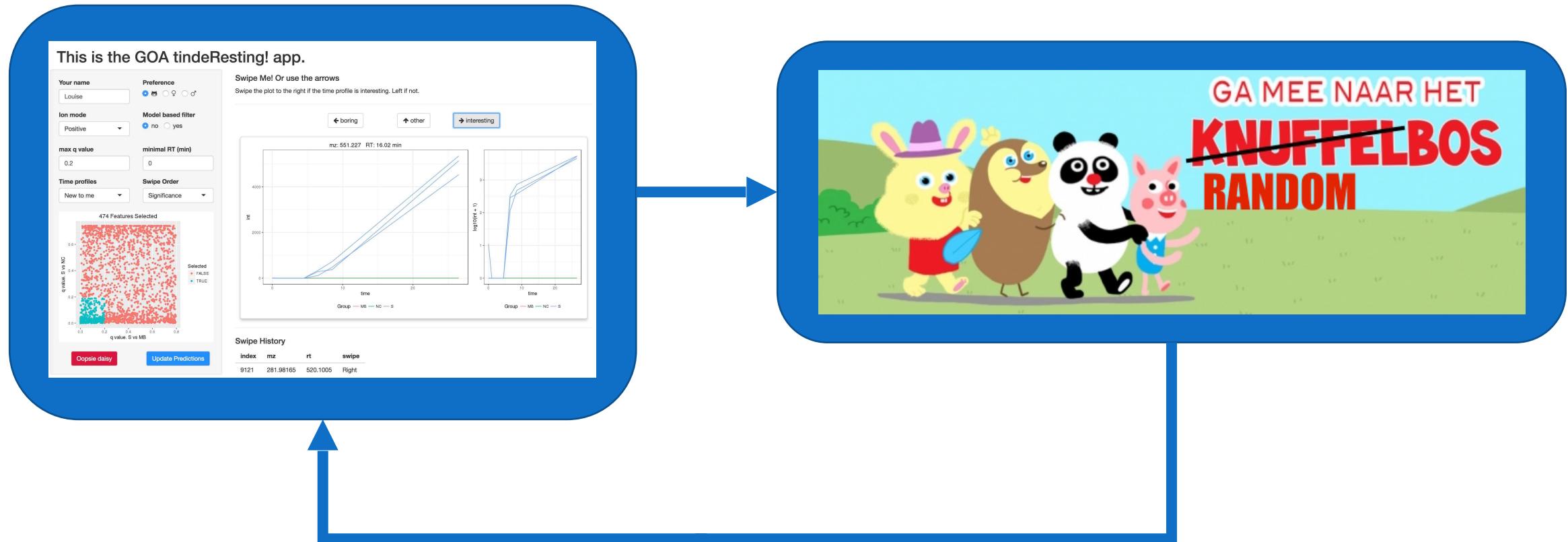
• Active Learning



● Active Learning



• Active Learning

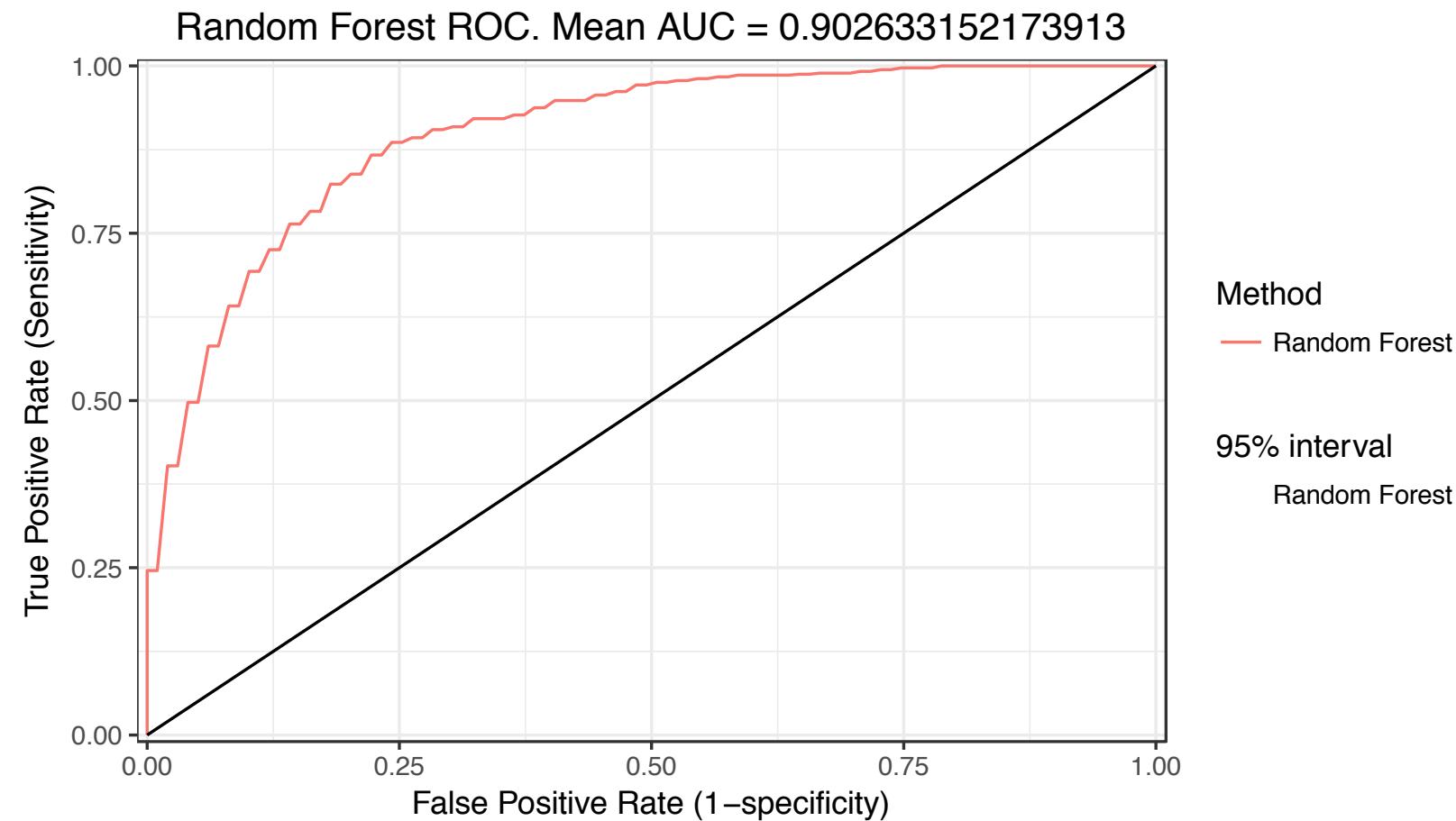


● Machine learning performance

- Use already reviewed time profiles
- 10 fold CV

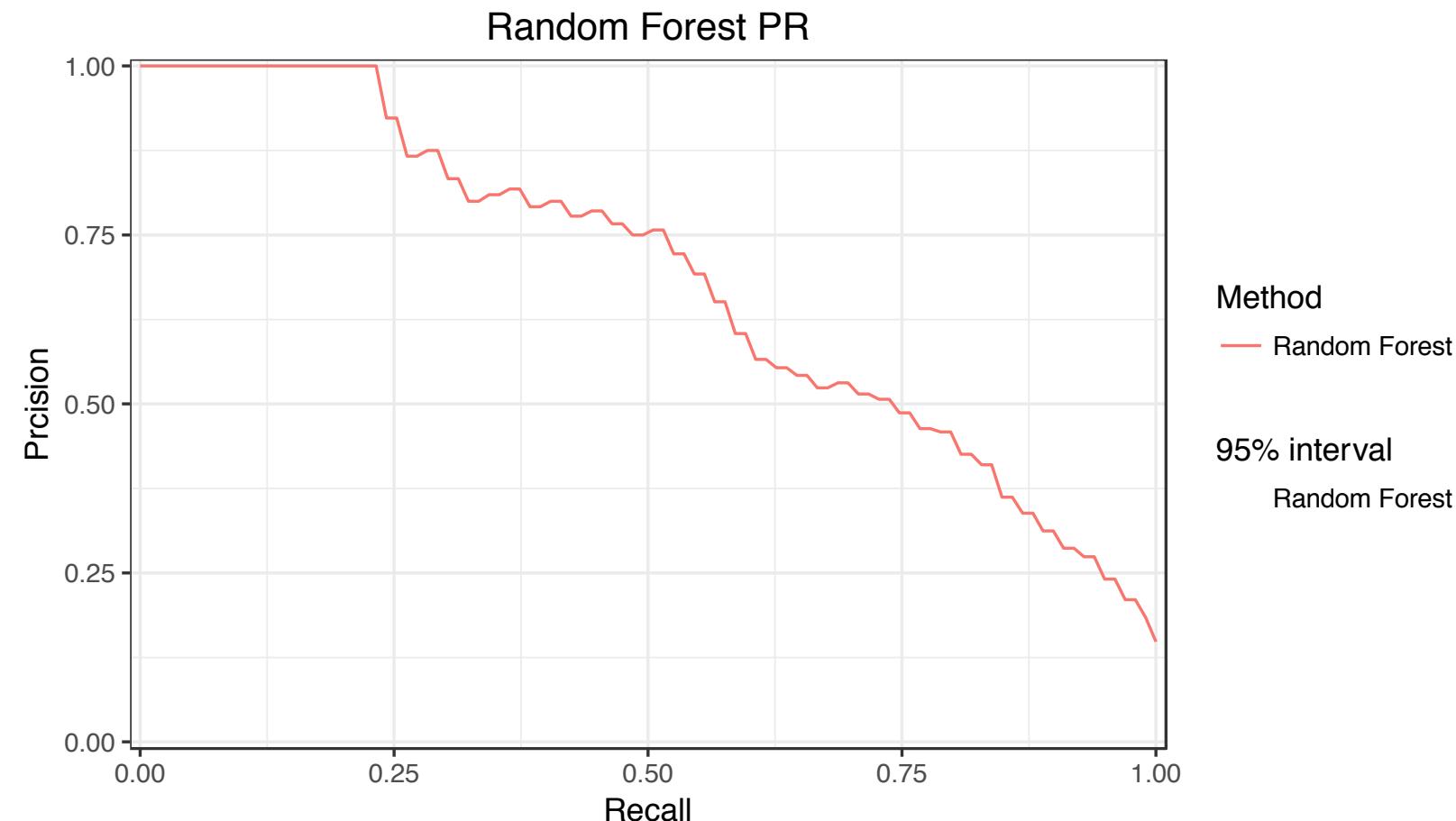
Machine learning performance

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Machine learning performance

- Use already reviewed time profiles
- 10 fold CV



• Try it yourself



- tindeResting lite:



GitHub

Beirnaert/tindeResting-template

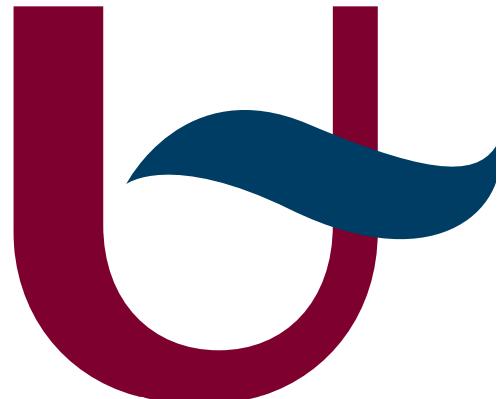
- Full app:



GitHub

Beirnaert/tindeResting

• Acknowledgements



biominq

- Kris Laukens
- Adrian Covaci
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- Kenne Fouquet
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- Anastasia Van der Auwera
- Many more