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Art of Automation

Bringing data, automation and modelling together with Kotlin

A data-science journey from scripting to simulation

Dr. Holger Brandl
Analytics Solution Architect
2. November 2021

About Me

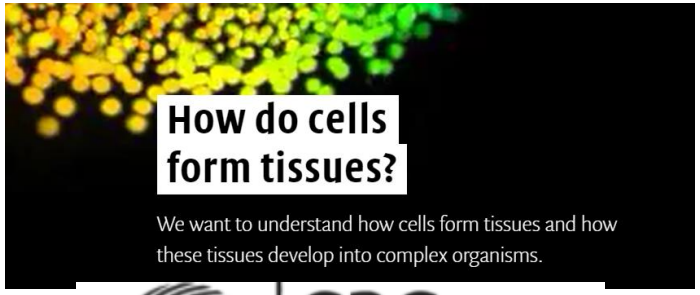
GitHub

`kscript` `krangl` `kravis` `kalasim`

2010 — 2015 — 2020

HONDA

Universität Bielefeld



CBG
Max Planck Institute of Molecular Cell Biology and Genetics

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INDUSTRY 4.0

A modern programming language that makes developers happier.

Get started | Why Kotlin

Developed by JetBrains & Open-source Contributors

Multiplatform Mobile

The natural way to share code between mobile platforms

Server-side

Modern development experience with familiar JVM technology

Web Frontend

Extend your projects to web

Android

Recommended by Google for building Android apps

February 2016: A new language was born

Kotlin v1.0 released

Type Inference

Extension Functions

Data Classes

DSLs in Mind

Default Parameters

Lives in JVM

Scripting Support

Data Science Requirements

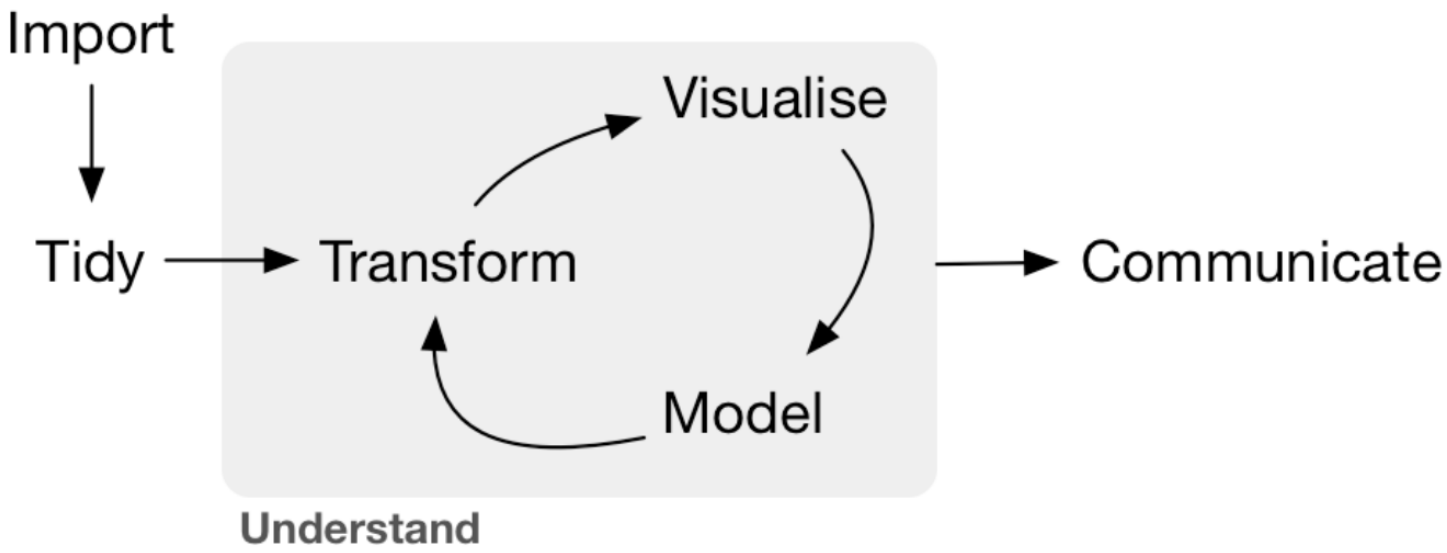
Proper Dependency Model ✓

Scales from idea to product ✓

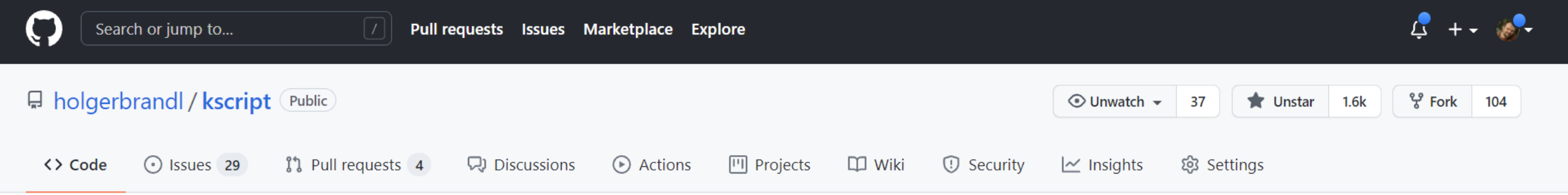
Teachable ✓

Rapid Prototyping ✓

The data-science life cycle



- Python: `pandas + scikit-learn + matplotlib/seaborn + jupyter`
- R: `readr + tidyr + dplyr + ggplot2 + caret/broom + knitr`
- JVM, and Kotlin in particular?



Enhanced scripting support for Kotlin on *nix-based systems.

Kotlin has some built-in support for scripting already but it is not yet feature-rich enough to be a viable alternative in the shell.

In particular this wrapper around kotlinc adds

- Compiled script caching (using md5 checksums)
- Dependency declarations using gradle-style resource locators More options to provide scripts including interpreter mode, reading from stdin, local files or URLs
- Embedded configuration for Kotlin runtime options
- Support library to ease the writing of Kotlin scriptlets
- Deploy scripts as stand-alone binaries

Use just the linux shell for data-driven science?

> But it's faster and way shorter to do it bash! (unknown colleague)

Do *magical* things in the terminal without dependencies

```
removeMultiMappers(){
perl -ne 'unless((!($_=~/^@.*/)&&!(m/AS:i:/))||(m/AS:i:(\S+).+XS:i:(\S+)/ && $1-$2<1)){print;}'
}

bowtie2 $fastqFile | samtools view -SF 4 -  | removeMultiMappers | samtools sort - result.bam
```

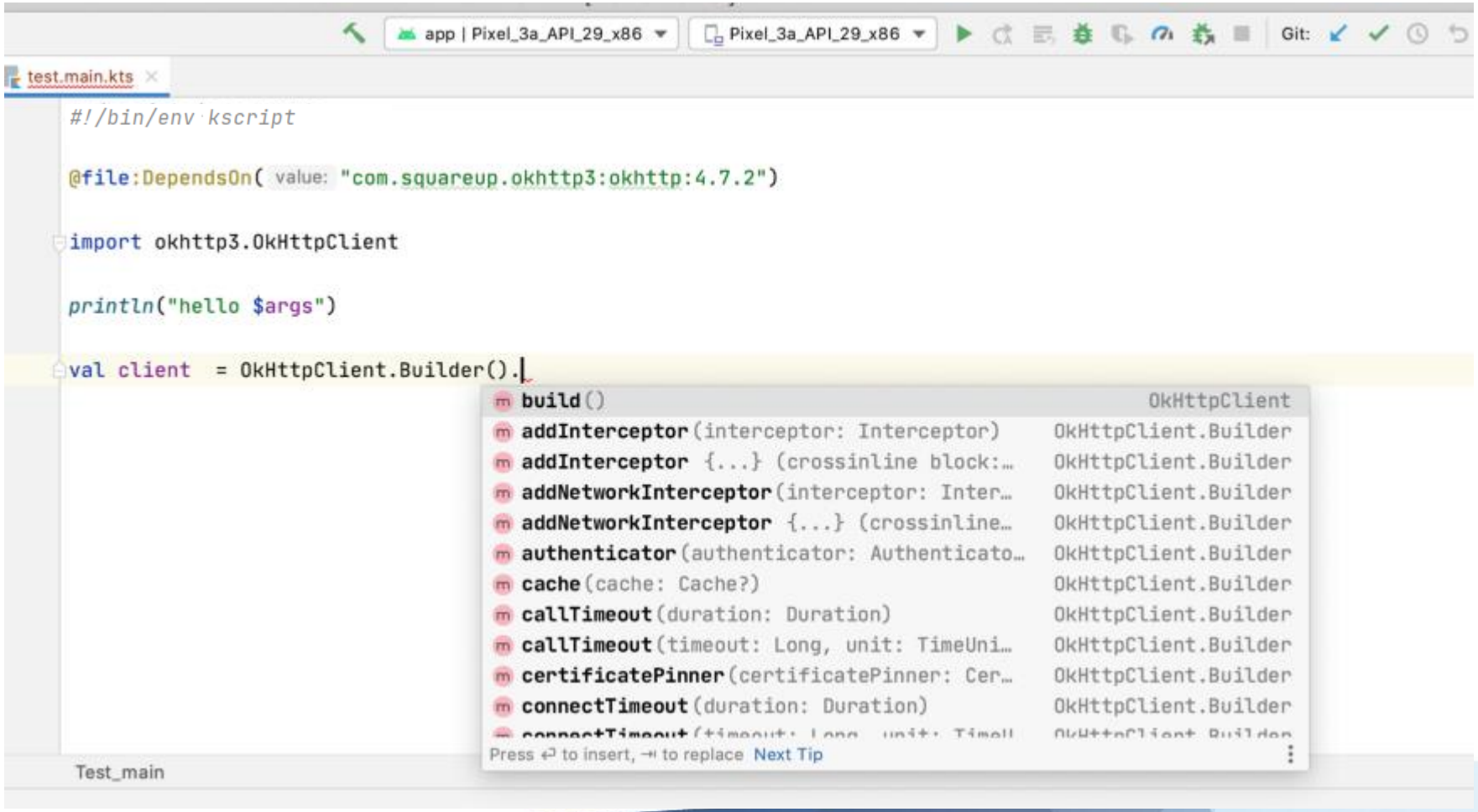
> Marta Florio, Mareike Albert, Elena Taverna, Takashi Namba, **Holger Brandl**, Eric Lewitus, Christiane Haffner, Alex Sykes, Fong Kuan Wong, Jula Peters, E. Guhr, Sylvia Klemroth, Kay Prüfer, Janet Kelso, Ronald Naumann, Ina Nüsslein, Andreas Dahl, Robert Lachmann, Svante Pääbo, Wieland B. Huttner **Human-specific gene ARHGAP11B promotes basal progenitor amplification and neocortex expansion.** *Science* , 347(6229) 1465-1470 (2015)

Get published and forget.

Fast to write. Impossible to maintain or to evolve. Does not scale. Unteachable black art.

https://mbonnin.medium.com/may-2020-the-state-of-kotlin-scripting-99cb6cc57db1

Scripting with `kotlin`:
Fun, statically typed, with full IDE and library support



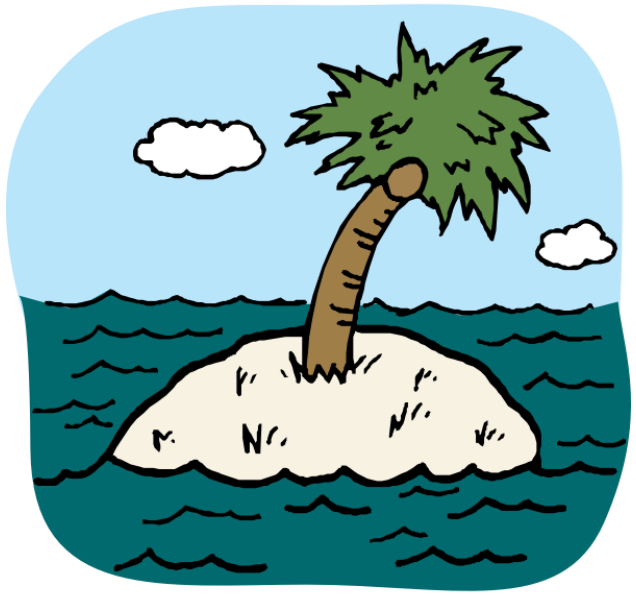
`kscript` Features Overview

- Installation
- Script Input Modes
- Script Configuration
- Text Processing Mode
- Treat yourself a REPL with `--interactive`
- Boostrap IDEA from a `kscript` let
- Deploy scripts as standalone binaries
- Embed kscript installer within your script
- FAQ
- Support
- How to contribute?
- Acknowledgements

Further Reading

- https://github.com/holgerbrandl/kscript
- KotlinConf2017 : kscript - Scripting Enhancements for Kotlin
- Talking Kotlin with Holger Brandl about kscript

What library would I take to a lonely island?



dplyr part of the tidyverse 1.0.7

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Overview

dplyr is a grammar of data manipulation, providing a consistent set of verbs that help you solve the most common data manipulation challenges:

- `mutate()` adds new variables that are functions of existing variables
- `select()` picks variables based on their names.
- `filter()` picks cases based on their values.
- `summarise()` reduces multiple values down to a single summary.
- `arrange()` changes the ordering of the rows.

These all combine naturally with `group_by()` which allows you to perform any operation "by group". You can learn more about them in `vignette("dplyr")`. As well as these single-table verbs, dplyr also provides a variety of two-table verbs, which you can learn about in `vignette("two-table")`.

If you are new to dplyr, the best place to start is the data transformation chapter in R for data science.

Links

Download from CRAN at
https://cloud.r-project.org/package=dplyr

Browse source code at
https://github.com/tidyverse/dplyr/

Report a bug at
htt

n more at
//r4ds.ha

Lice

Full license

Check what else is out there

- tablesaw which is (according to its authors) the *The simplest way to slice data in Java*
- kotliquery is a handy database access library
- Scala DataTable: a lightweight, in-memory table structure written in Scala
- joinery implements data frames for Java
- paleo which provides immutable Java 8 data frames with typed columns
- morpheus-core which is a data science framework implementing an R-like data-frame
- vectorz is a fast and flexible numerical library for Java featuring N-dimensional arrays
- koma is a scientific computing library written in Kotlin
- termsql converts text from a file or from stdin into SQL table using sqlite and query it instantly

> Great stuff, but not feature-complete enough, maintained or *kotlinesque* as needed for fluency and fun with data

holgerbrandl / krangl Public

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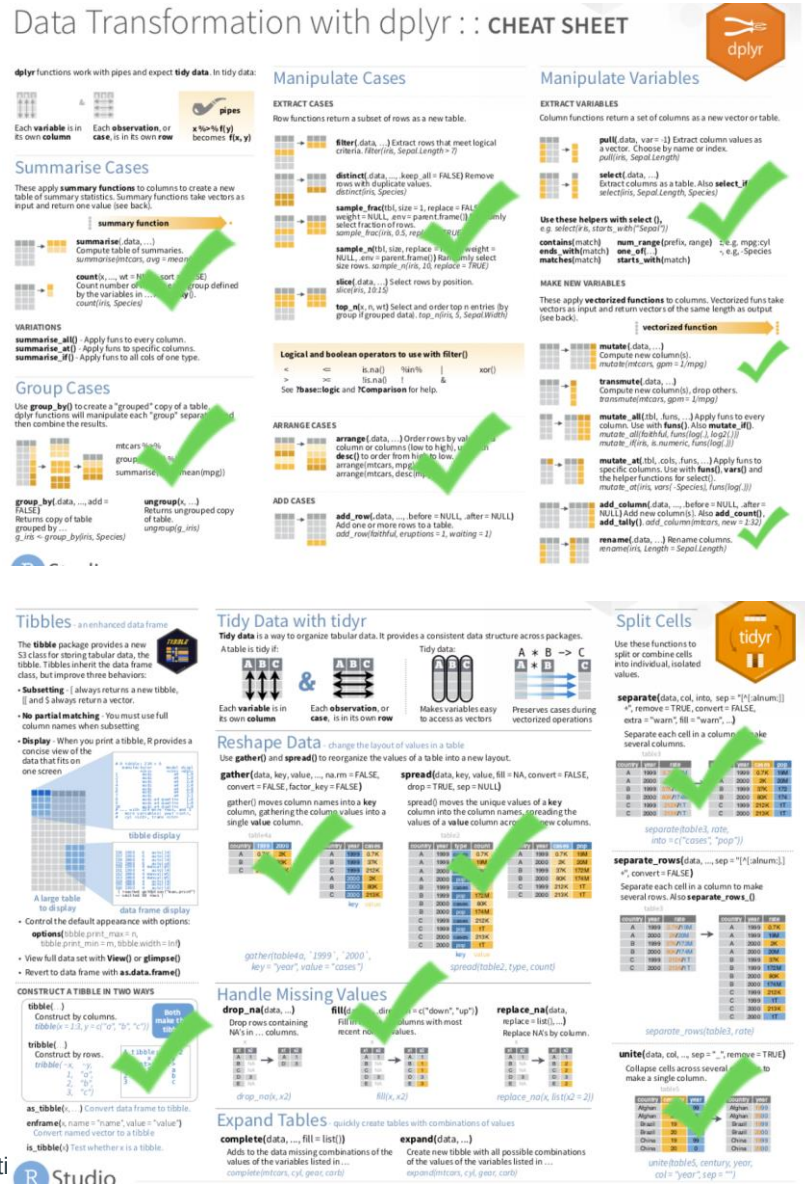
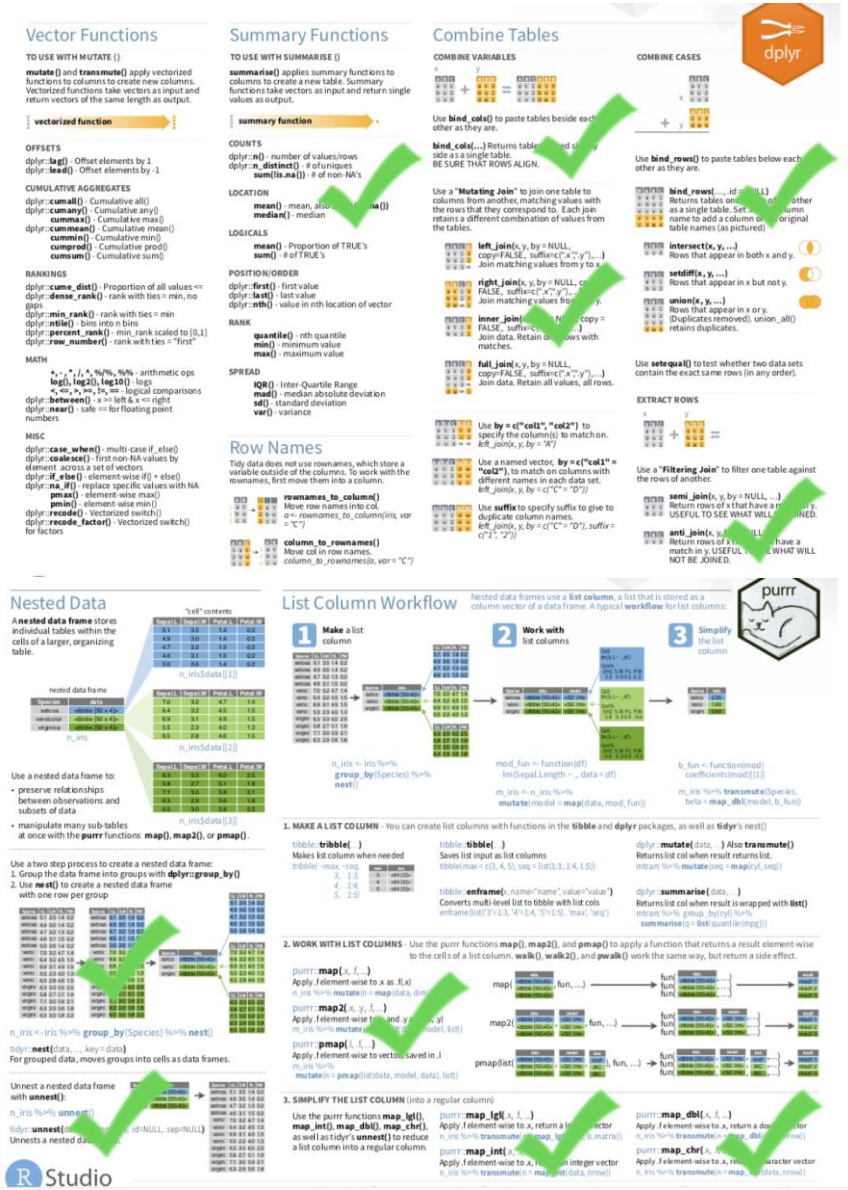
`krangl` is a {K}otlin library for data w{rangl}ing. By implementing a grammar of data manipulation using a modern functional-style API, it allows to filter, transform, aggregate and reshape tabular data.

`krangl` is heavily inspired by the amazing `dplyr` for R. `krangl` is written in Kotlin, excels in Kotlin, but emphasizes as well on good java-interop. It is mimicking the API of `dplyr`, while carefully adding more typed constructs where possible.

https://github.com/holgerbrandl/krangl

~~Copy~~ Learn from the best, learn from `dplyr`





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How to get your data into `krangl`

Define tables inline

```
val users = dataFrameOf(
    "firstName", "lastName", "age", "hasSudo")(
    "max", "smith" , 53, false,
    "eva", "miller", 23, true,
    null , "meyer" , 23, null)
```

Read & write from tsv, csv, json, jdbc, etc.

```
val tornados = DataFrame.readCSV(pathAsStringFileOrUrl)
// do stuff
tornados.writeCSV(File("tornados.txt.gz"))
```

- Guess column types & default parameters
- Built-in missing value support

Example: Summarize Flights by Date

```
flightsData
    .groupBy("year", "month", "day")
    .select({ range("year", "day") }, { listOf("arr_delay", "dep_delay") })
    .summarize(
        "mean_arr_delay" `=` { it["arr_delay"].mean(removeNA = true) },
        "mean_dep_delay" to  { it["dep_delay"].mean(removeNA = true) }
    )
    .filter { (it["mean_arr_delay"] gt  30)  OR  (it["mean_dep_delay"] gt  30) }
    .sortedBy("mean_arr_delay")
```

year	month	day	mean_arr_delay	mean_dep_delay
2013	10	11	18.9229	31.2318
2013	5	24	24.2574	30.3407
2013	6	2	26.075	34.0133
2013	6	26	27.3174	30.61175
2013	6	10	28.0222	30.61945
2013	7	8	29.6488	37.2966
2013	8	22	29.9767	33.6004
2013	2	27	31.252	37.7632

To type or not to type?

- *Static types* are cool, but most data has no type
- It's more robust/fun to use types and they allow for better design
- Many data attributes are very fluent

```
data class Employee(val id:Int, val name:String)
val staffStats = listOf(Employee(1, "John"), Employee(2, "Anna"))
    .predictNumSickDays()      // new type!
    .addPerformanceMetrics()   // new type!
    .addSalaries()             // new type!
    .correlationAnalysis()     // odd generic signature :-|
```

- R/python lack static typing, which make such workflows more fluent/fun to write

```
staff %>%
    mutate(sick_days=predictSickDays(name)) %>%   # table with another column
    left_join(userPerf) %>%                       # and some more columns
    left_join(salaries) %>%                       # and even more columns
    select_if(is.numeric) %>%
    correlate(type="spearman")                    # correlate numeric attributes
```

Mix typed and untyped data

```
val dataFrame : DataFrame =
```

employee:Employee	sales:List<Sale>	age:Int	address:String	salary:Double
Employee(23, "Max")	listOf(Sale(...), Sale())	23	"Frankfurt"	50.3E3
...	...	...	...	...

```
// aggregations like
dataFrame.groupBy("age").count()
dataFrame.summarize("mean_salary"){ mean(it["salaray"])}

// integration like
val df: DataFrame = dataFrame.leftJoin(otherDF)

// transformations like
dataFrame.addColumn("intial"){ it["employee"].map<Employee>{ it.name.first() }}
```

- `krangl` includes methods to go back and forth between untyped and typed data
- Best method ever `asDataFrame()` for every Iterable
- Flattening of complex types with `df.unfold<Car>("vehicle")`

Bumpy API corners in `krangl`

Lists in table formulas cause operator confusion

```
users.addColumn("age_plus_3") { it["user"].map<User> { it.age } + 3 } // extend list with 3
users.addColumn("age_plus_3") { it["user"].map<User> { it.age + 3 } } // correct
users.addColumn("age_plus_3") { it["age"] + 3 }   // works because `DataCol.plus` can be defined
```

Incomplete vectorization for operators

Some (`+`, `-`, `*`, `!`) can be overridden for collections, but others cannot (e.g. all arithmetic and boolean comparison ops)

No vectorization for `>`, `&& ==`, etc. in table forumlas → Use function calls or not so pretty `gt`, `AND`, `eq`, etc.

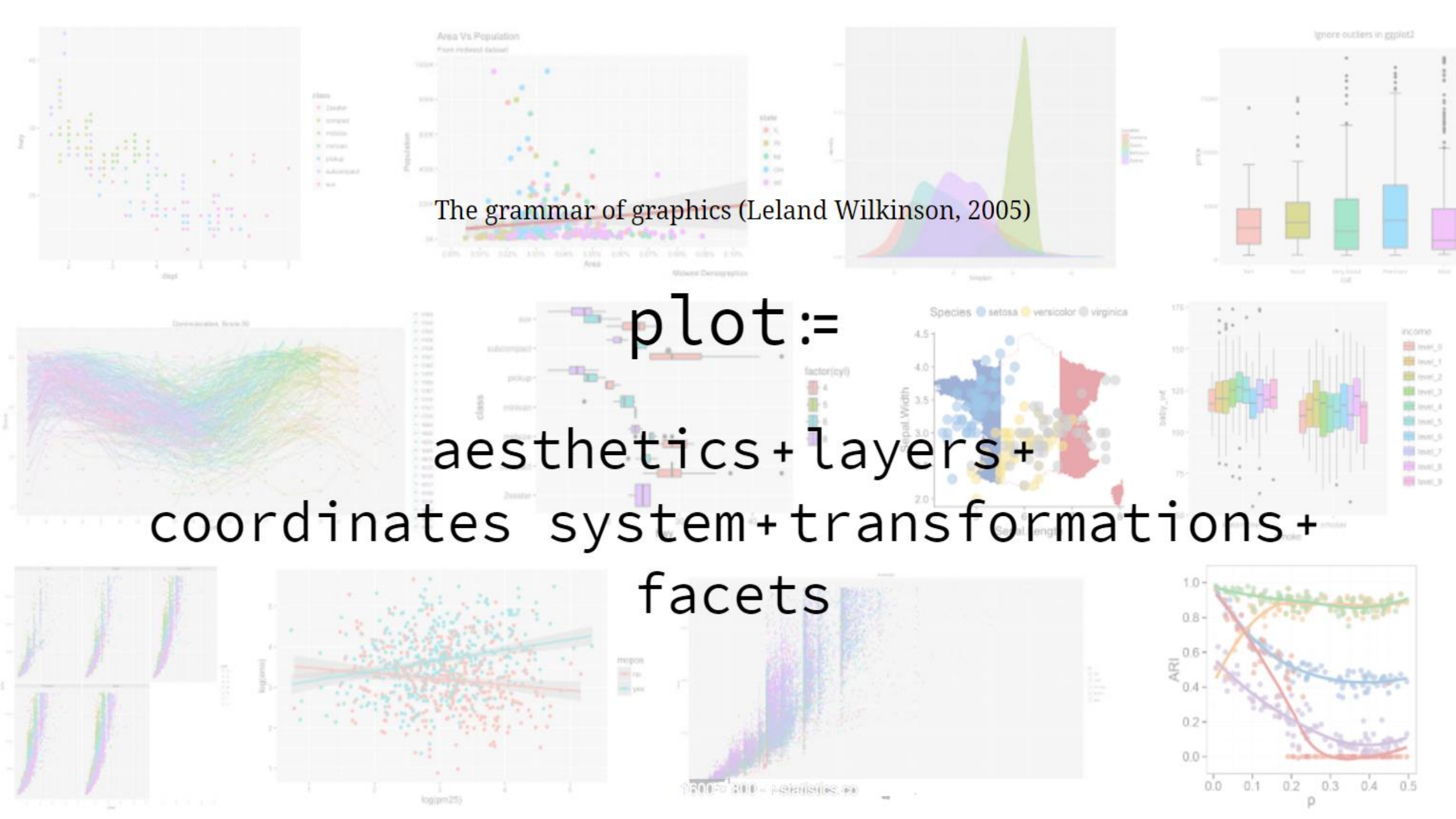
Next steps

Promising API, great learning experience.

Project still in flux towards a convenient and consistent API design

Next steps

- Date column support
- Better lambda receiver contexts
- Performance (indices, avoid list and array copies, compressed columns)
- Use dedicated return type for table formula helpers (like `mean`, `rank`) to reduce runtime errors
- More bindings to other jvm data-science libraries
- Better documentation & cheatsheets
- `Sequence` vs `Iterable`?
- Pluggable backends like native or SQL



The grammar of graphics (Leland Wilkinson, 2005)

```
plot :=
  aesthetics + layers +
  coordinates system + transformations +
  facets
```

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kravis - A {k}otlin {gra}mmar for data {vis}ualization

Maven Central 0.8.1 build failing

Visualizing tabular and relational data is the core of data-science. `kravis` implements a grammar to create a wide range of plots using a standardized set of verbs.

The grammar implemented by `kravis` is inspired from `ggplot2`. In fact, all it provides is a more typesafe wrapper around it. Internally, `ggplot2` is used as rendering engine. The API of `kravis` is highly similar to allow even reusing their excellent cheatsheet.

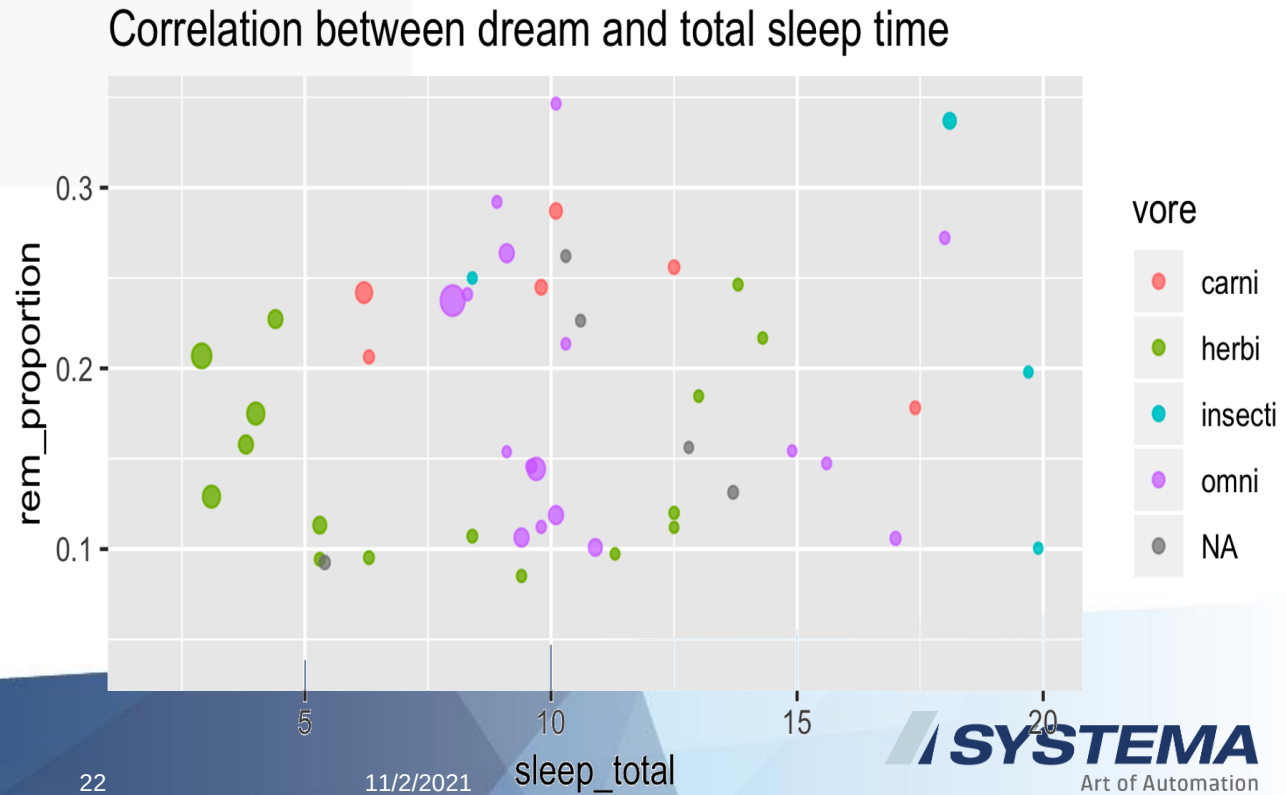
R is required to use `ggplot`. However, `kravis` works with various integration backend ranging such as docker or remote webservices.

https://github.com/holgerbrandl/kravis

Can we map a scripting API into a statically typed language?

```
import krangl.*
import kravis.*

sleepData
    .addColumn("rem_proportion") { it["sleep_rem"] / it["sleep_total"] }
        // Analyze correlation
    .plot(x = "sleep_total", y = "rem_proportion", color = "vore", size = "brainwt")
        .geomPoint(alpha = 0.7)
        .guides(size = LegendType.none)
        .title("Correlation between dream and total sleep time")
```



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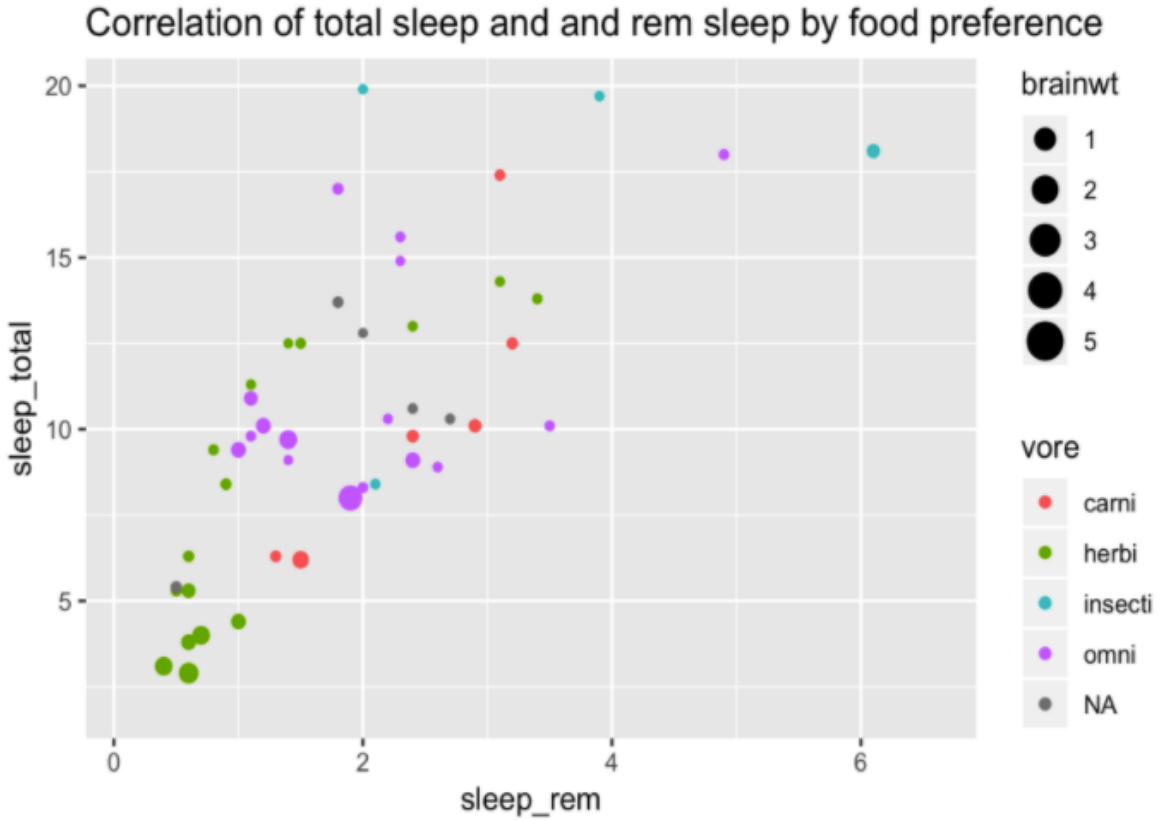
Example: Typed API

Use any `Iterable<T>` to build a plot. :-)

```
val sleepPatterns : List<SleepPattern> = ...

//  deparse records using property references
sleepPatterns
    .plot(
        x = SleepPattern::sleep_rem,
        y = SleepPattern::sleep_total,
        color = SleepPattern::vore,
        size = SleepPattern::brainwt
    )
    .geomPoint()
    .title("Correlation of total sleep " +
     "and and rem sleep by food preference")
```



System Architecture

```
irisData.plot(x="Species" , y="Petal.Length" )
    .geomBoxplot()
    .geomPoint(position = PositionJitter(width = 0.1), alpha = 0.3)
    .title("Petal Length by Species")
```

Dockerized R

Local R Installation

Remote R
(via Rserve)

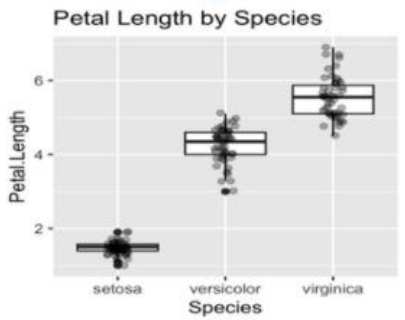
Later: JRI

```
ggplot(mapping = aes(x = `Species`, y = `Petal.Length`), data = data01) +
    geom_boxplot(stat = 'boxplot') +
    geom_point(stat = 'identity', position = position_jitter(width = 0.1), alpha = 0.3) +
    ggtitle("Petal Length by Species")
```

SVG, PNG, JPG, PDF, EPS

JavaFx Device

Swing Device



Jupyter

File IO

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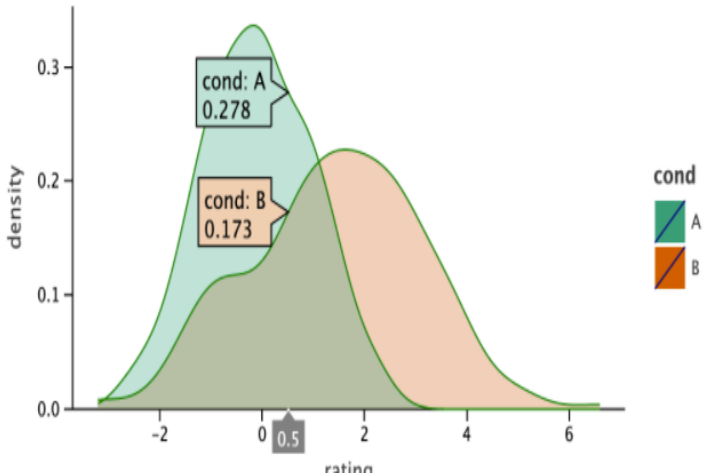
`lets-plot` as modern alternative

- Removes annoying dependency on R (which is great!!)
- `lets-plot` provides a kotlin-native rendering backend, more interactivity
- Currently, still limited method support and customizability compared to `kravis`

```
val rand = java.util.Random()
val data = mapOf<String, Any>(
    "rating" to List(200) { rand.nextGaussian() } + List(200) { rand.nextGaussian() * 1.5 + 1.5 },
    "cond" to List(200) { "A" } + List(200) { "B" }
)

var p = lets_plot(data)
p += geom_density(color="dark_green", alpha=.3) {x="rating"; fill="cond"}
p + ggsize(500, 250)
```

- Execute the added code to evaluate the plotting capabilities of Lets-Plot.



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Data Science with Kotlin Tutorial

→ Mammalian Sleep Patterns

Further reading: Data science with `kotlin`

Tutorials

- https://kotlinlang.org/docs/data-science-overview.html
- http://holgerbrandl.github.io/krangl/10_minutes/
- http://holgerbrandl.github.io/krangl/data_manip/

Talks

- KotlinConf2017 - A wild ride through New York City with Holger Brandl
- KotlinNight2018 - Kotlin's emerging data-science ecosystem with Holger Brandl
- KotlinConf 2019 Making Kotlin Ready for Data Science by Roman Belov

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- Kotlin Slack channels science and data-science & github

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Smart Manufacturing

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SAP Portfolio

Resources

Integration

Automation

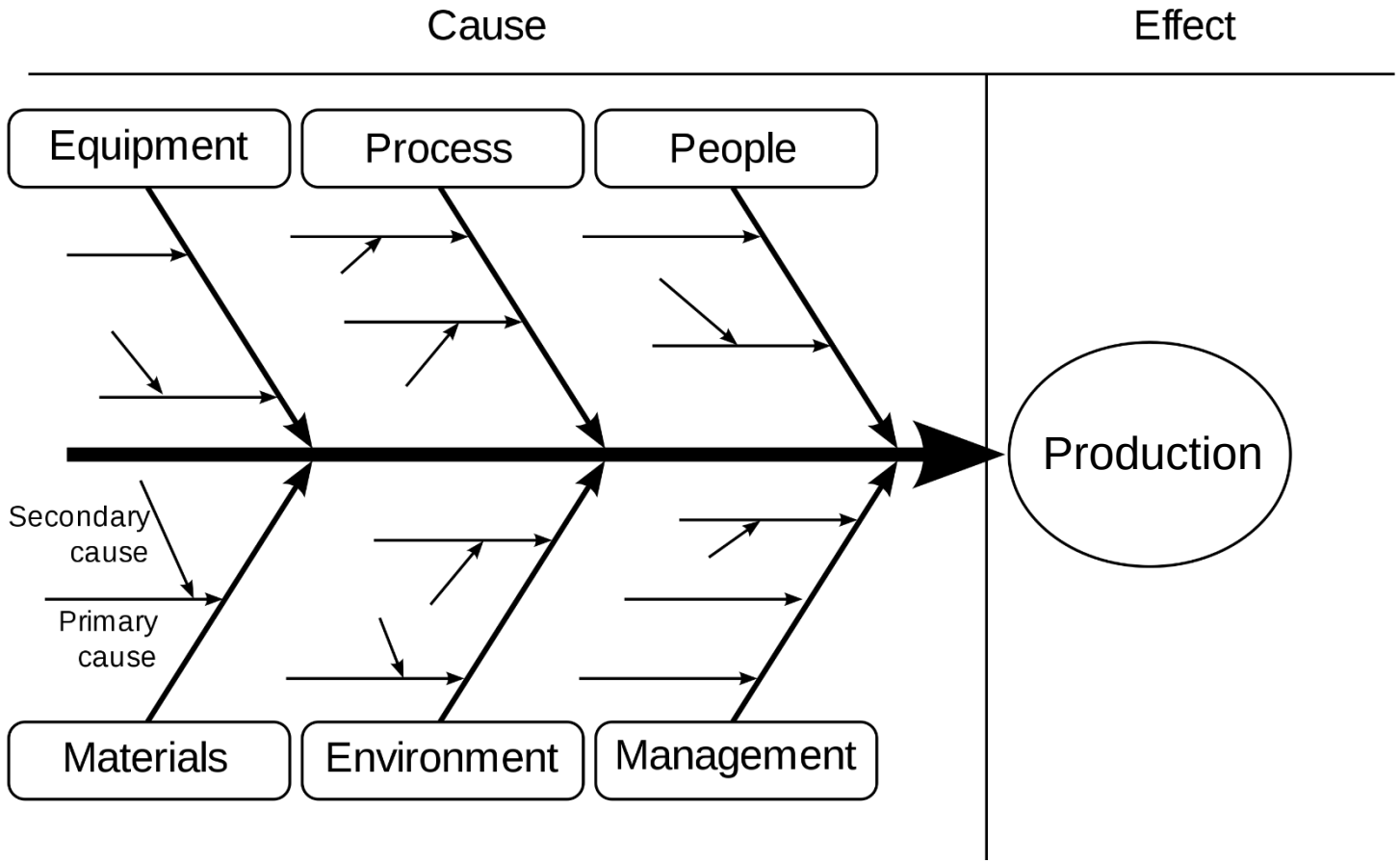
Optimization

Visualization

Migration

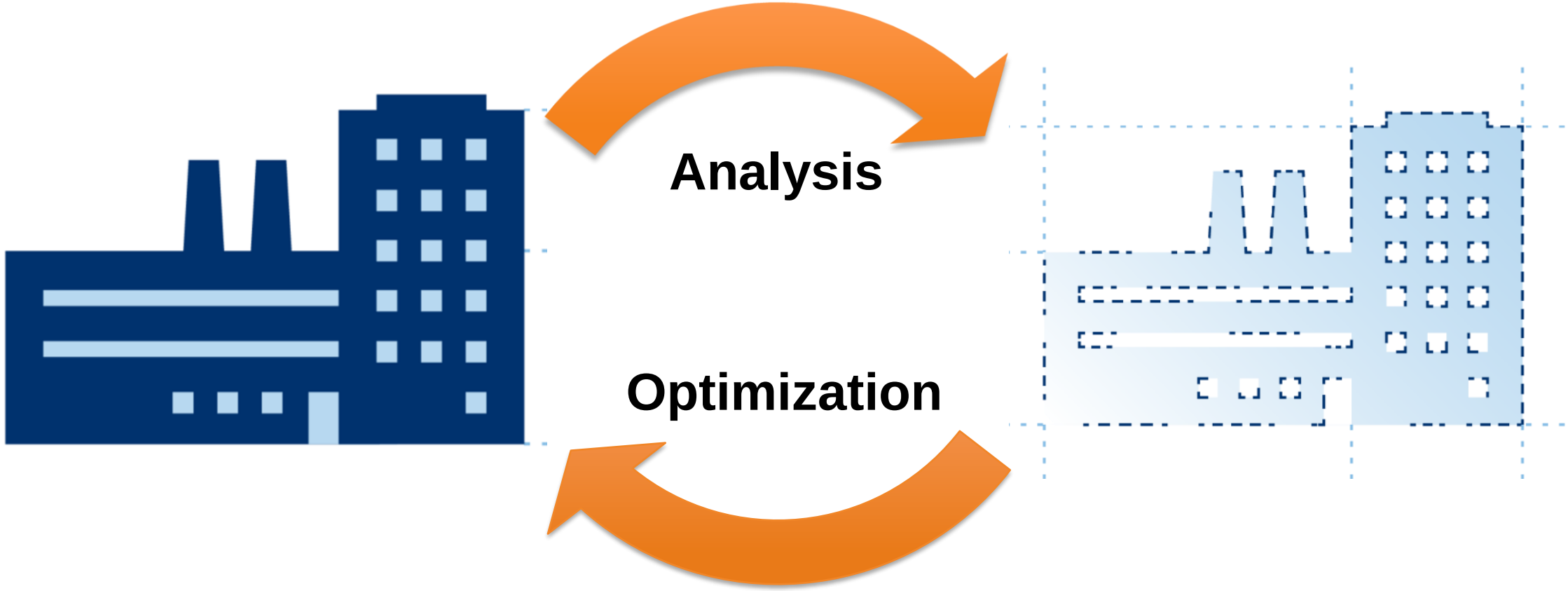
Optimization is the art of maximizing manufacturing efficiency, throughput, OEE, yield, and quality by monitoring, analyzing, and iteratively tuning manufacturing processes.

Cause and consequence in production planning

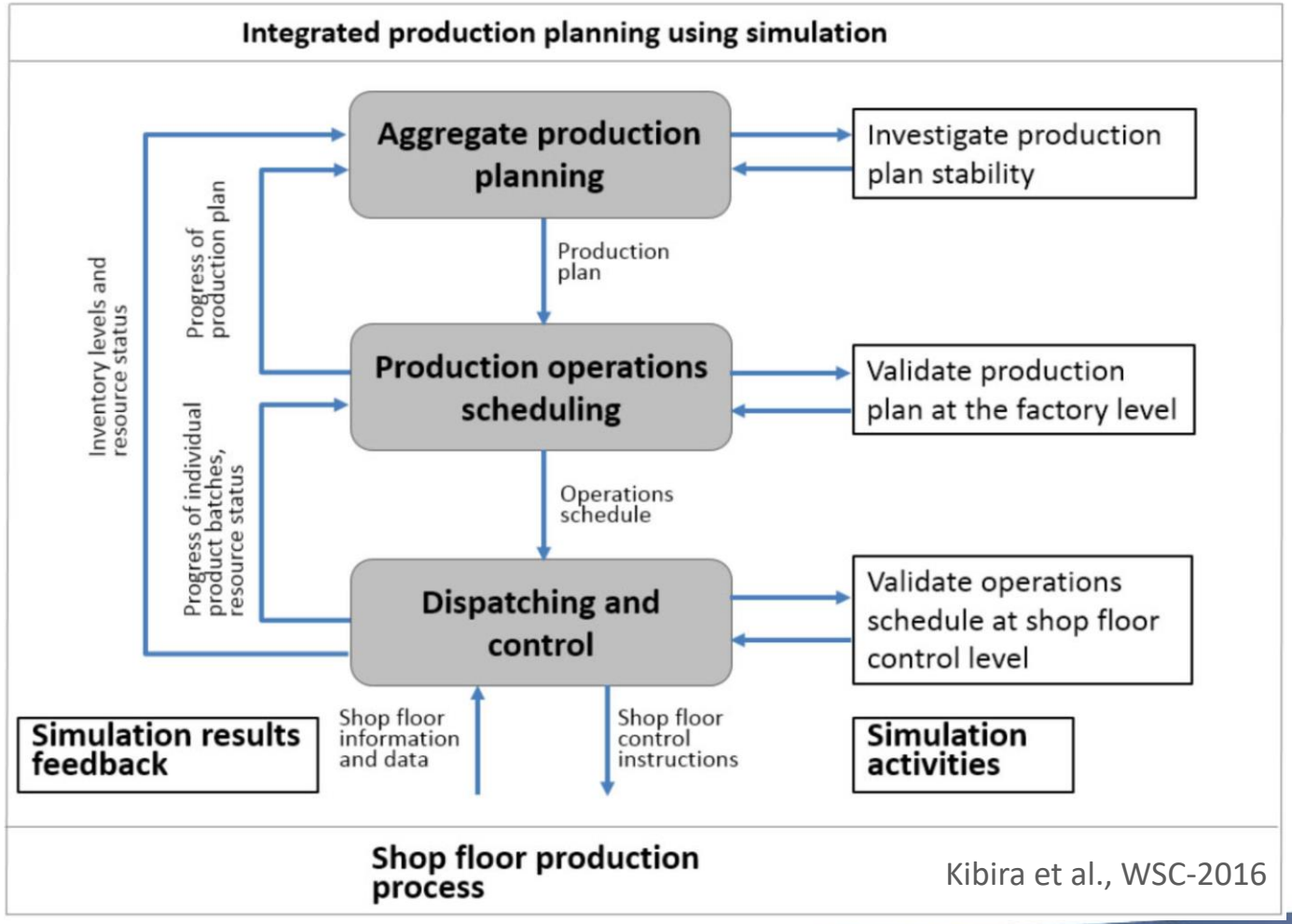


- Complex interplay of human, machine, material and methods
- Not always following intuition

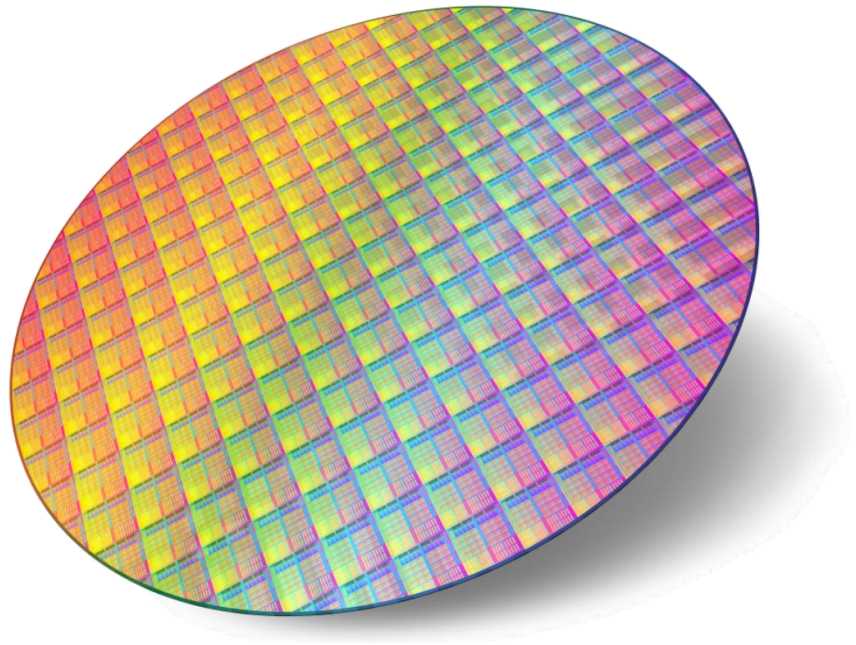
How to optimize a complex system?



How to produce more in complex industries?



Kibira et al., WSC-2016



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Welcome to `kalasim`

`kalasim` is a discrete event simulator that enables complex, dynamic process models. It provides a statically typed API, dependency injection, modern persistence, structured logging and automation capabilities.

`kalasim` is written in Kotlin, is designed around suspendable coroutines for process definitions, runs on the JVM for performance and scale, is built with koin as dependency wiring framework, and is using common-math for stats and distributions. See acknowledgements for further references.

Table of contents

Core Features

`kalasim` is a generic process-oriented discrete event simulation (DES) engine.

- Simulation entities have a generative process description that defines the interplay with other entities
- There is a well-defined rich process interaction vocabulary, including hold, request, wait or passivate
- An event trigger queue maintains future action triggers and acts as sole driver to progress simulation state
- Built-in monitoring and statistics gathering across the entire API

First Example

Key Types

- `Component`
- `Resource`
- `State`

Key methods

- `request`
- `hold`

```
////Cars.kts
import org.kalasim.*

class Driver : Resource()
class TrafficLight : State<String>("red")

class Car : Component() {

    val trafficLight = get<TrafficLight>()
    val driver = get<Driver>()

    override fun process() = sequence {
        request(driver) {
            hold(1.0, description = "driving")

            wait(trafficLight, "green")
        }
    }
}

createSimulation(enableConsoleLogger = true) {
    dependency { TrafficLight() }
    dependency { Driver() }

    Car()
}.run(5.0)
```

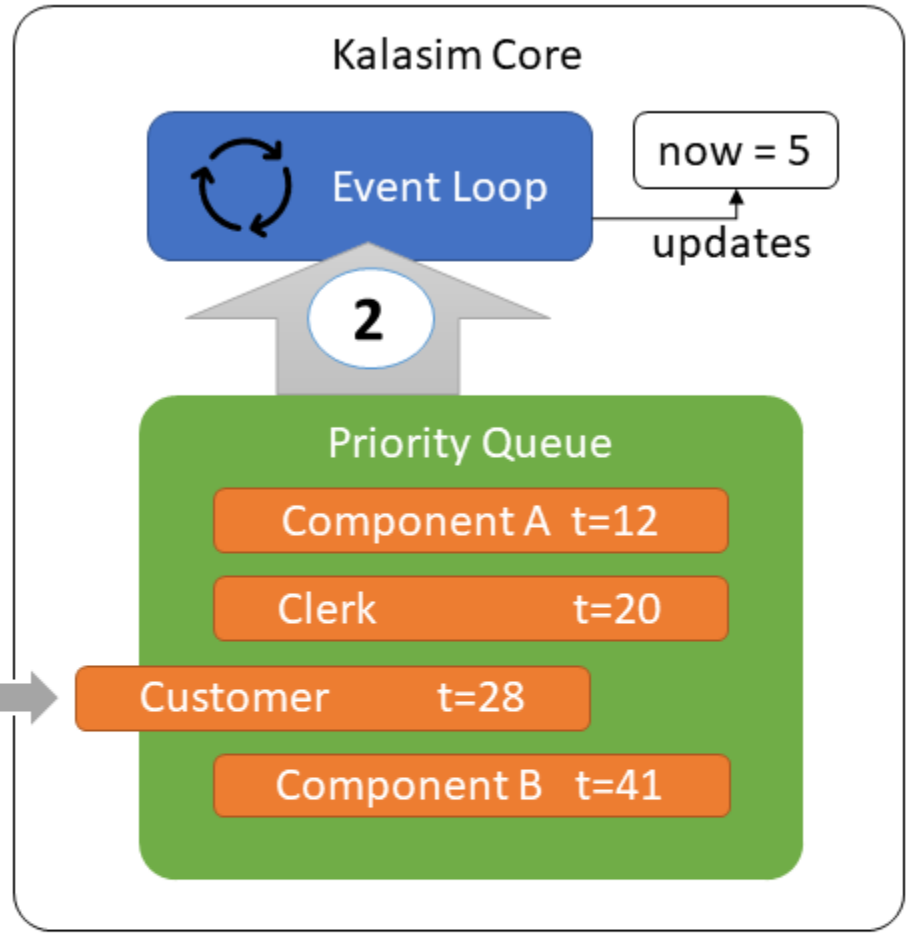
Event Loop Architecture

```
class Customer(val clerk: Resource) : Component() {

    override fun process() :Sequence<Component> = sequence {
        // do shopping
        hold(ticks = 23.0)

        // wait for an empty counter
        request(clerk)

        // billing process
        hold(ticks = 2.0, priority = HIGH)
    }
}
```



1. Stall customer's `process` execution and insert it into event queue by time (and optional priority to resolve ambiguities)
2. Poll, while queue is not empty and resume (or start) `process`
3. Event loop will continue execution here. Components are terminated once `process` end has been reached

Source https://github.com/thomasnield/kotlinconf-datascience-talk

Why another DES engine?

- Simmer, Salabim, SimJulia, SimPy, DSOL, …
- UI-driven commercial vendors: AnyLogic, SIMIO

Kotlin vs Python

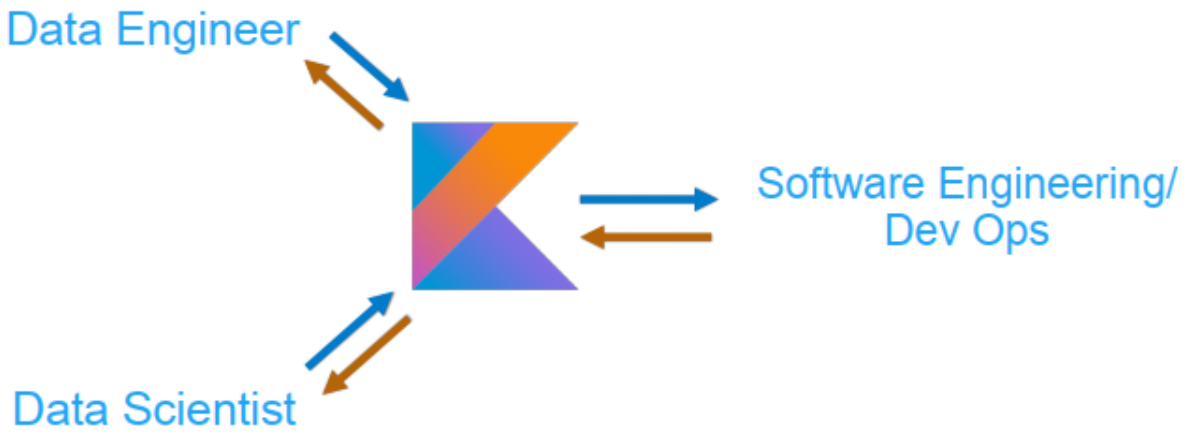
Static vs Dynamic

Python is a powerful, flexible platform with a simple syntax and rich ecosystem of libraries.

Dynamic typing makes Python flexible for ad hoc analysis, but it is challenging to use in production.

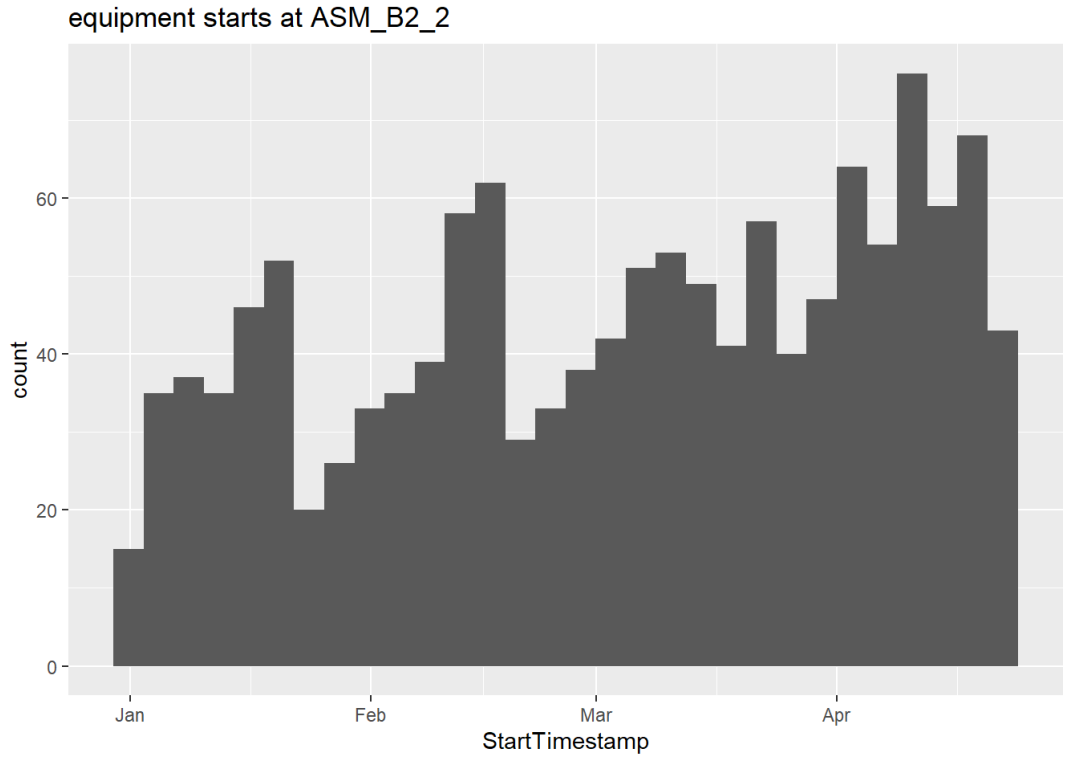
- Dynamic types allow improvised data structures to be defined at runtime.
- Dynamic typing can quickly create difficulties in maintaining, testing, and debugging codebases, especially as the codebase grows large.

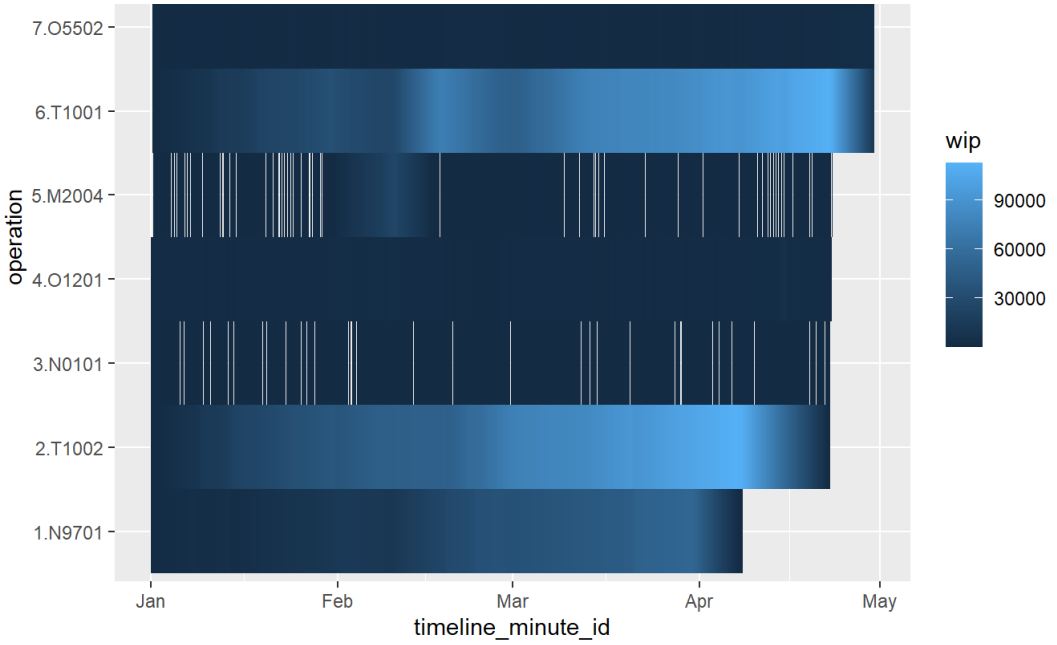
One language, One Codebase, One Platform



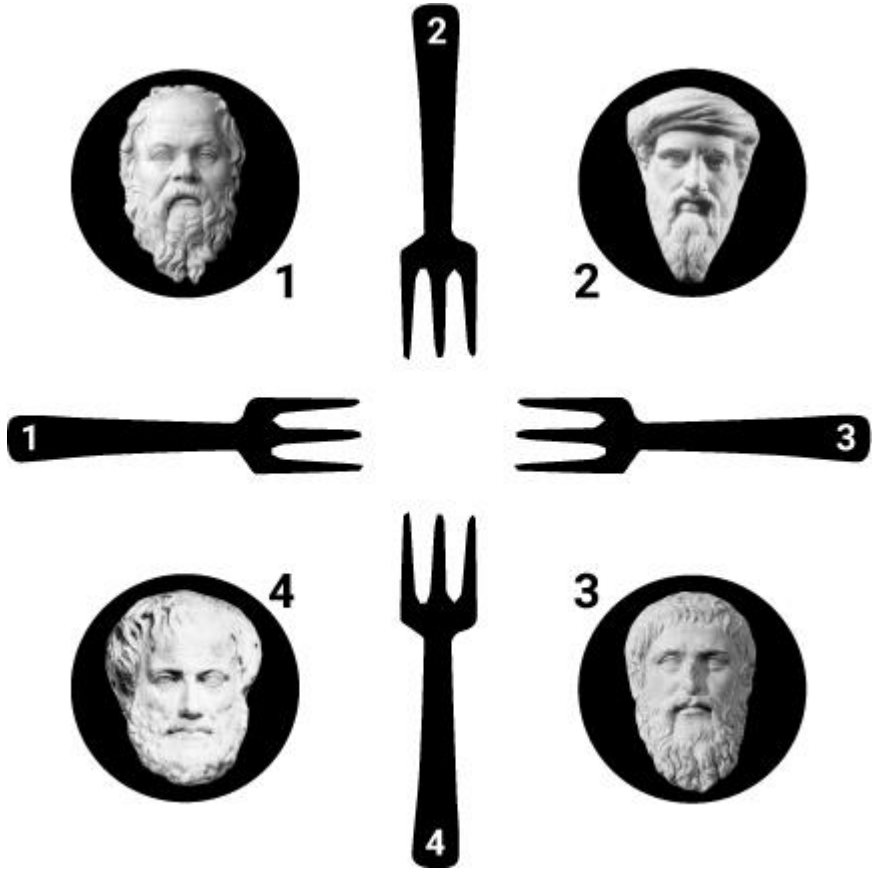
Can we model a semiconductor fab with `kalasim`?

- Yes, we can!





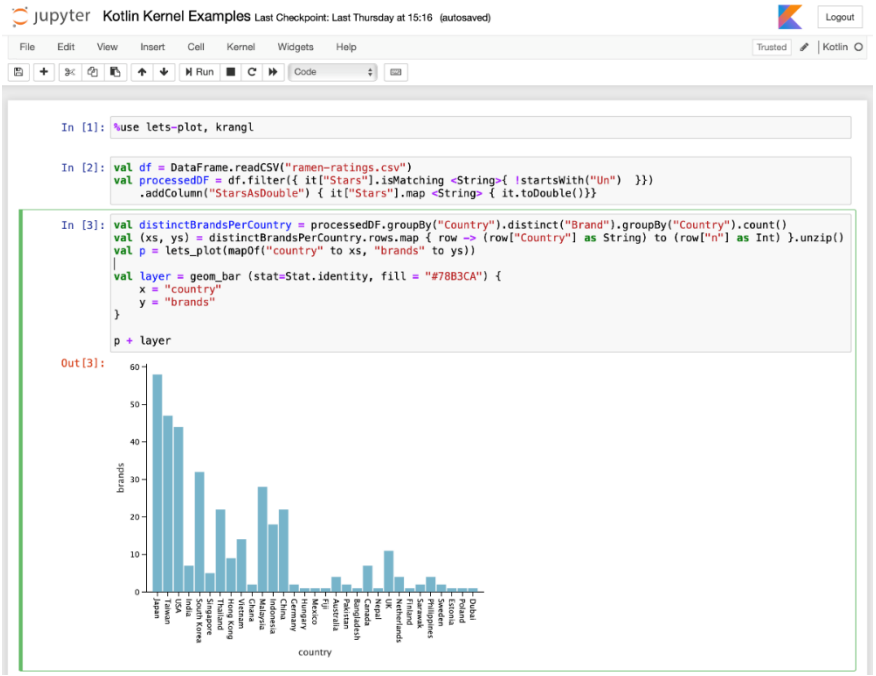
Example: Let’s have some food with Dining Philosophers



https://www.kalasim.org/examples/dining_philosophers/

Quo vadis, `kotlin` for science?

- Amazing language for modelling & prototyping
- Great projects KotlinDL or multik
- Awesome jupyter kernel
- Tooling barrier easy to climb for developers but harder for data scientists
- Slow data-science community adoption
- Multiplatform & Huge JVM ecosystem



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Thank you! Stay in touch!

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