From flop to success in academic software development

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Inria

"Most lines of code written by programmers in academia never reach an audience"

G. Varoquaux, March 19th 2015

"Most lines of code written by programmers in academia never reach an audience"

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- Technical problems: making software
- Marketing problems: unknown users

This talk [TL;DR]*

- Choose your battles

  projects that solve a problem

- Win them

  software production

⋆ Too Long, Didn't Read

Please allow me to introduce myself

I'm a man of wealth and taste
I've been around for a long, long year

- Physicist gone bad
  - Neuroscience, Machine learning
- Worked in a software startup
  - Enthought: scientific computing consulting in Python
- Coder (done my share of mistake)
  - Mayavi, scikit-learn, joblib...
- Scipy community
  - Chair of scipy and EuroScipy conferences
- Researcher (PI) at INRIA

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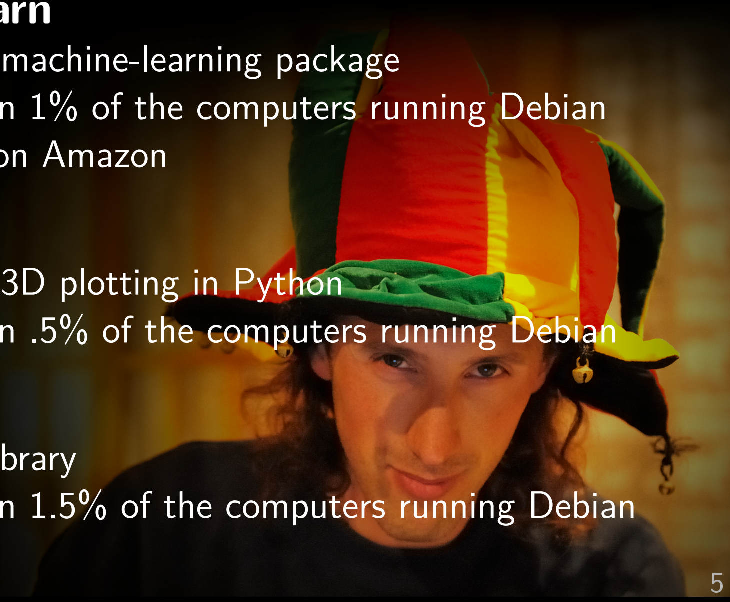


- **Scikit-learn**

  Reference machine-learning package

  Installed on 1% of the computers running Debian

  16 books on Amazon

- **Mayavi**

  Reference 3D plotting in Python

  Installed on .5% of the computers running Debian

- **joblib**

  Backend library

  Installed on 1.5% of the computers running Debian

Software for scientific research

Reproducible science: enabling falsification

Replicating

A 3rd party redoing the work

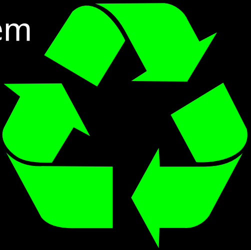
Code and data made available

Reproducing

New analysis on different data / code coming to the same conclusion

Reusing

Applying the approach to a new problem



Let us enable reusable research

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Code and data made available

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New analysis on different data / code coming to the same conclusion

Arguments for BSD license

No strings attached

Can tinker with it

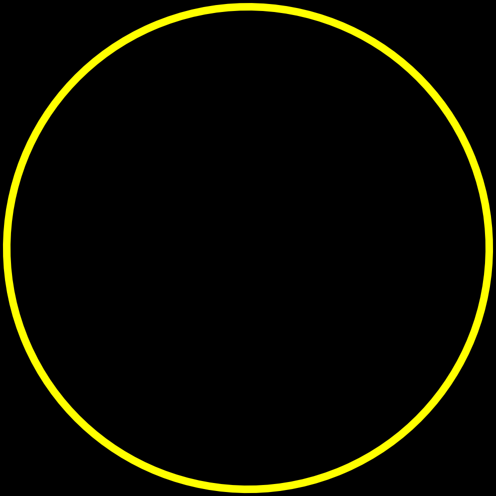
Reusing

Applying th

Let us enable reusable research

The advancement of knowledge

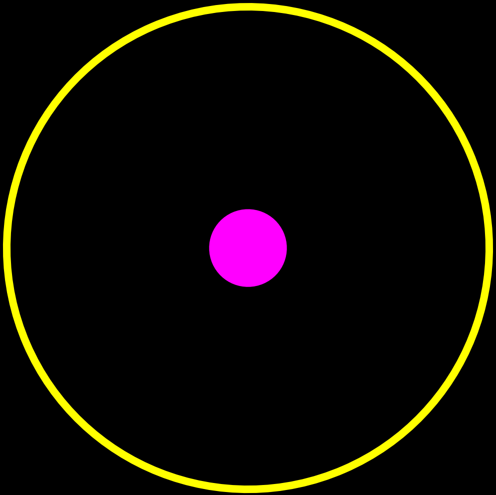
Imagine a circle that contains human knowledge



Courtesy of Matt Might, via Stefan van der Waalt

The advancement of knowledge

By the time you finish elementary school, you know a little



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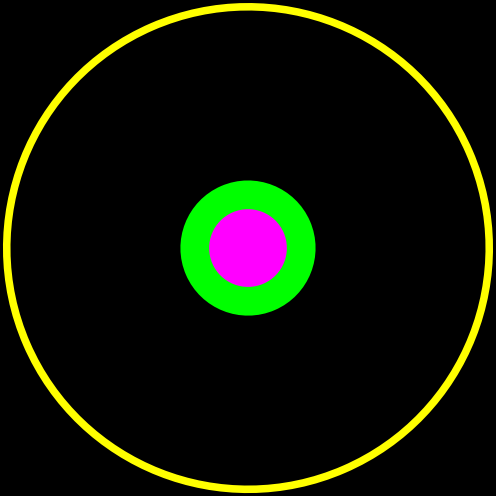
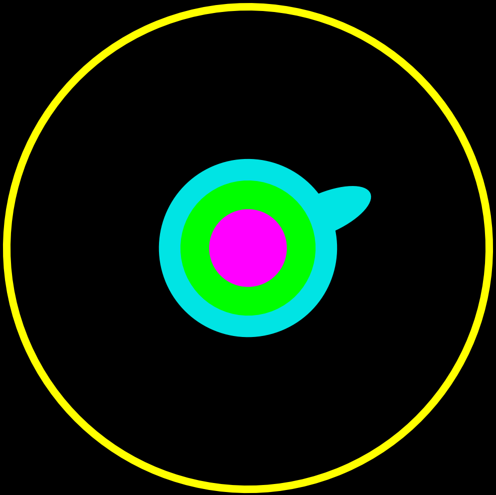
High school takes you a little bit further



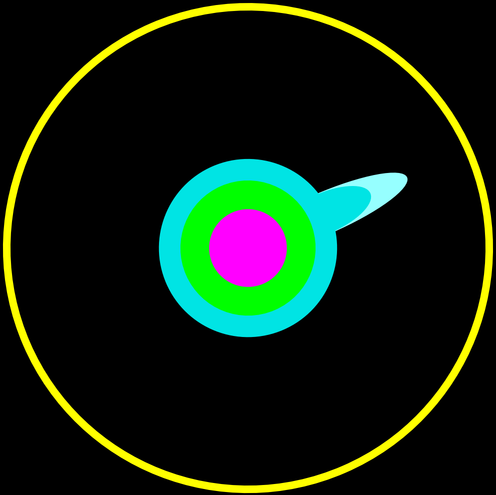
Courtesy of Matt Might, via Stefan van der Waalt

With a bachelors degree, you gain a speciality



Courtesy of Matt Might, via Stefan van der Waalt

A master's degree deepens this speciality



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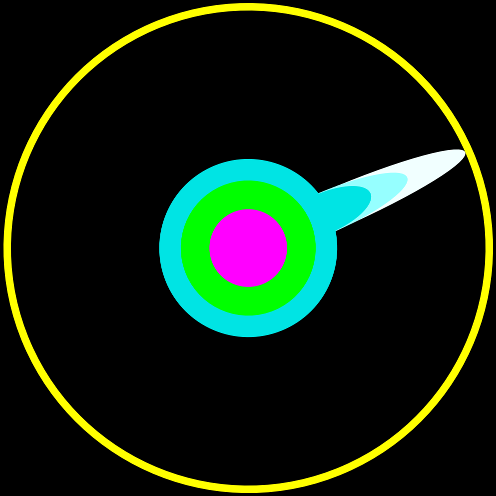
The advancement of knowledge

Research papers take you to the edge of human knowledge



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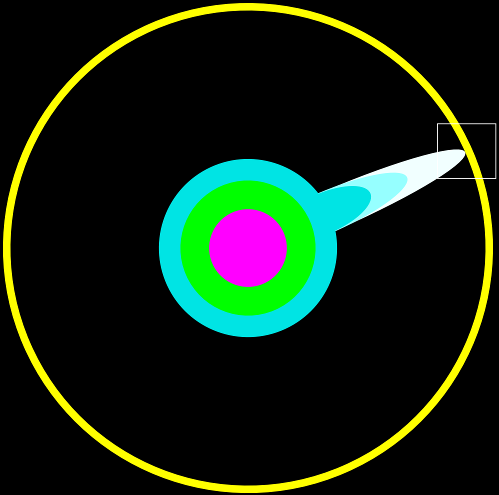
Once you are at the boundary, you focus



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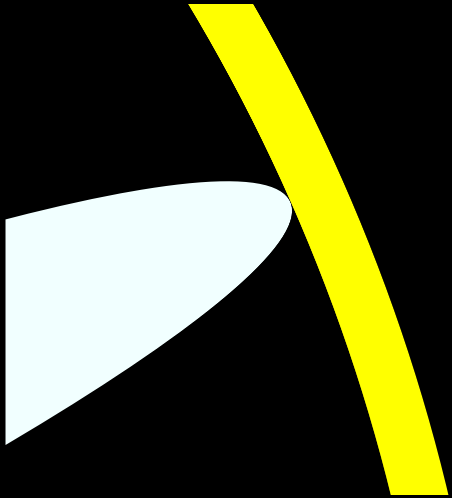
You push at the boundary for a few years



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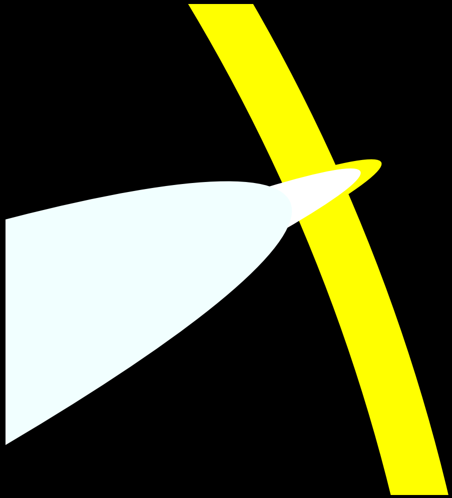
And one day it yields



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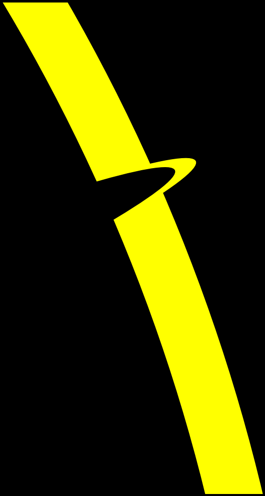
The advancement of knowledge

That dent you've made, is called a PhD



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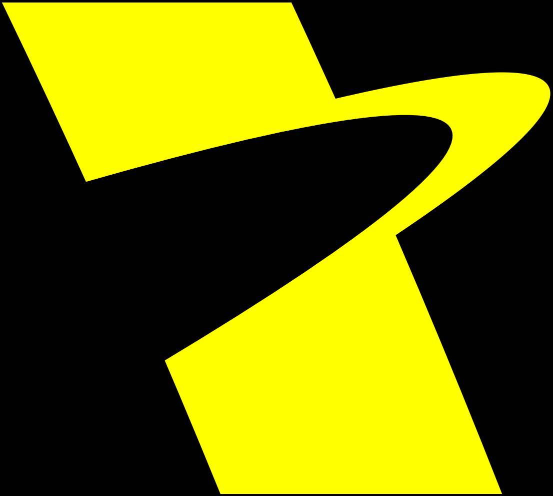
Of course, the world looks different to you now



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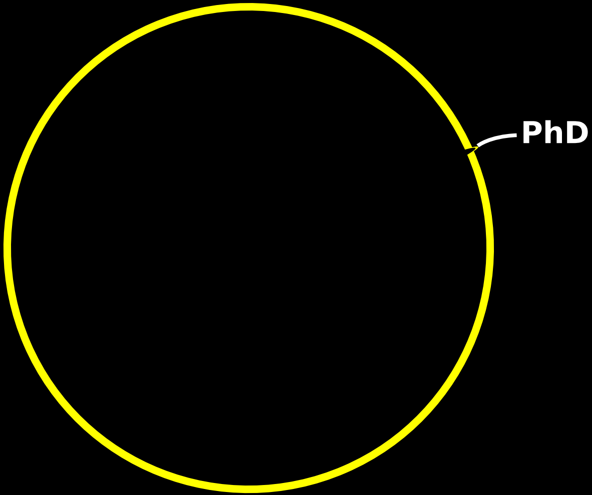
But don't forget the big picture



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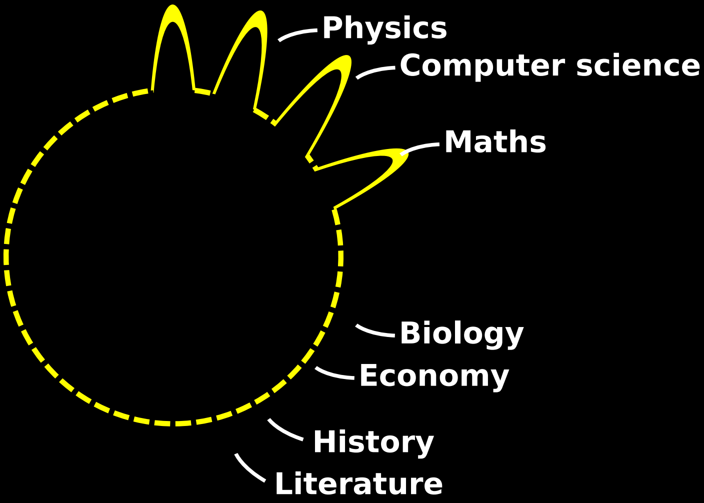
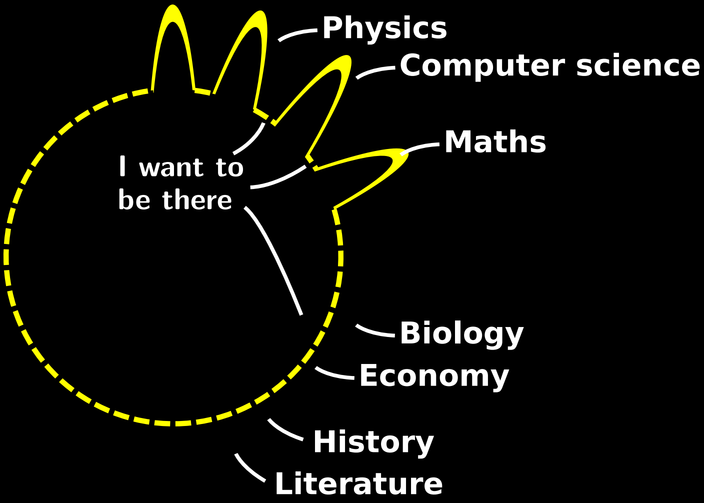
The advancement of knowledge

This is an optimistic view



This is an optimistic view



Translationnal computational science

Computational science

The use of computers and mathematical models to address scientific research

Translationnal computational science

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In medecine: bring bench science to medical practice

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Computational science

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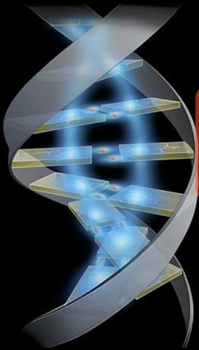
In medecine: bring bench science to medical practice



Translational computational science?

Pick a problem to work on

Take the "easy" route

There needs to be a market screeming for the software (in academia and in industry)

Refine your *vision*

Pull, not push

Design driven be need

Having an impact

Having an impact

Pick the right battles: viable projects

Project idea

A software implementing:

i) machine learning

and ***ii)*** neuroimaging

and ***iii)*** a graphical user interface

and ***iv)*** 3D plotting

Pick the right battles: viable projects

Project idea

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Pick the right battles: viable projects

Define project scope and vision

- Break down projects by expertise
- Don't solve hard problems
- Know the software landscape
- Don't target markets that will not yield contributors

Need a vision = elevator pitch

Pick the right battles: viable projects

Define project scope and vision

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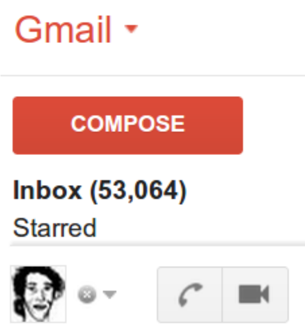
Need a vision = elevator pitch

Your research (PhD) probably does not qualify
⇒ need to cherry-pick contributions

Open source and community development

Code maintenance too expensive to be alone

scikit-learn ∼ 300 email/month   nipy ∼ 45 email/month
joblib ∼ 45 email/month   mayavi ∼ 30 email/month



"Hey Gael, I take it you're too busy. That's okay, I spent a day trying to install XXX and I think I'll succeed myself. Next time though please don't ignore my emails, I really don't like it. You can say, 'sorry, I have no time to help you.' Just don't ignore."

Open source and community development

Code maintenance too expensive to be alone

scikit-learn ~ 300 email/month   nipy ~ 45 email/month
joblib ~ 45 email/month   mayavi ~ 30 email/month

Your "benefits" come from a fraction of the code

- Data loading?   Maybe?
- Standard algorithms?   Nah

Share the common code...

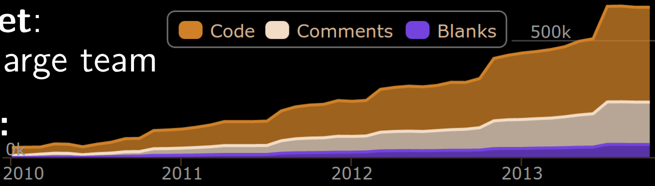
...to avoid dying under code

Code becomes less precious with time

And somebody might contribute features

Huge feature set:
benefits of a large team

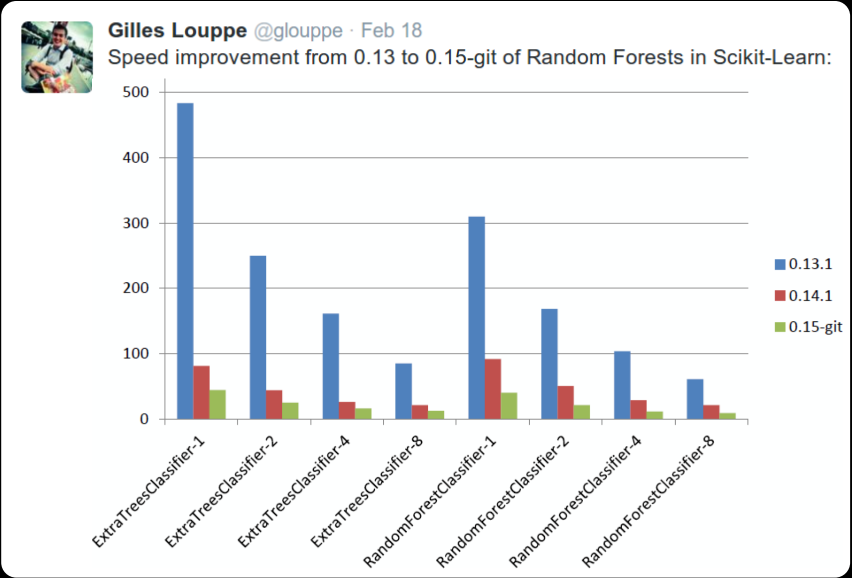
Project growth:



- More than 200 contributors
- $\sim$ 12 core contributors
- 1 full-time INRIA programmer from the start

Estimated cost of development: **$ 6 millions**
COCOMO model,
`http://www.ohloh.net/p/scikit-learn`

Communities: many eyes makes code fast



L. Buitinck, O. Grisel, A. Joly, G. Louppe, J. Nothman, P. Prettenhofer

You need a community

6 steps to a community-driven project

1. Focus on **quality**
2. Build great **docs and examples**
3. Use **github**
4. Limit the technicality of your codebase
5. Releasing and packaging matter
6. Focus on your contributors,
   give them credit, decision power

http://www.slideshare.net/GaelVaroquaux/scikit-learn-dveloppement-communautaire

What's in a scientific-computing environment

- Interaction...
  - $\longrightarrow$ script...
    - $\longrightarrow$ module...
      - ↺ interaction again...
- **Consolidation**, progressively
- Low tech and short turn-around times

Choose your weapons

Python, what else?

- Interactive language
- Easy to read / write
- General purpose

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- Interactive language
- Easy to read / write
- General purpose

Old virtual machine / compiler

Younger languages promissing (Julia)

but will they get adoption beyond science?

Python, what else?

Use numpy arrays

- scikit-learn
- scikit-image

...

It's about plugin things together

Software architecture for science

- "Scriptability" is paramount
- In an application: MVC (model, view, controller)

Model
Numerical or data-processing core

View
Ouput: graphs, or files
Must enable headless use

Controller
Input: dialogs, or **an API**
Avoid input as files: not expressive

- Dialogs should never be far from the code
  Dialog generation: traits, IPython widgets
- Reactive programming:
  dialogs modify object, and the model updates

Don't own the `main`

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  Dialog **In Mayavi**: script generation for free
- Reactive programming:
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Quality is free*

* This is a book, by Philip Crosby

You need quality

- Quality will give you users

  Bugs give you bad rap

- Quality will give you developers

  Contribute to learn and improve

- Quality will make your developers happy

  People need to be proud of their work

Do less, do better

Goes against the grant-system incentive

Quality: what & how

Great documentation

- Simplify, but don't dumb down
- Focus on what the user is trying to solve

Great APIs

- Example-based development
- If something is hard to explain, rethink the concepts
- Limit the number of different concepts and objects
- Consistency, consistency, consistency

Good numerics

- Write tests based on mathematical properties
- When a user finds an instability, write a new test

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Quality enables reuse

Beyond mere reproducibility

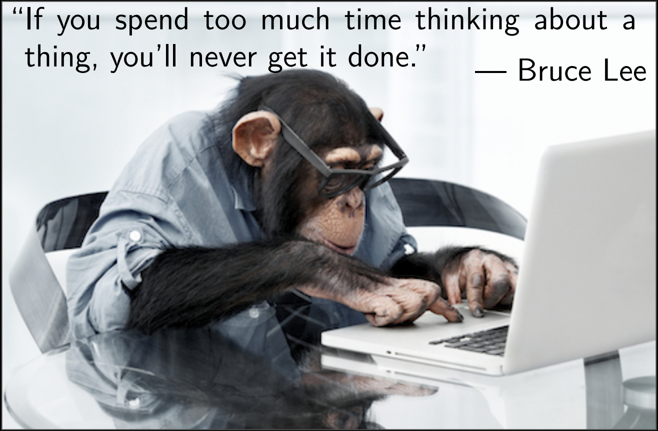
Good numerics

- Write tests based on mathematical properties
- When a user finds an instability, write a new test

Be productive

Be productive

"If you spend too much time thinking about a thing, you'll never get it done." — Bruce Lee



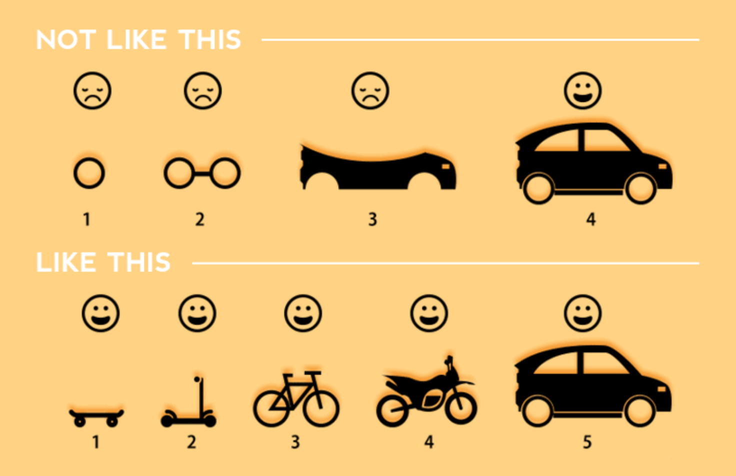
Limited resources are good

- Need success in the short term, not the long term

- The startup culture: fail fast
  Quickly identify non-viable projects

- The simpest solution that works is the best

Short cycles, limited ambitions



- Keep coming back to your users
- Release early, release often

Complexity increase superlinearly

[An Experiment on Unit Increase in Problem Complexity, Woodfield 1979]

25% increase in problem complexity

$\Rightarrow$ 100% increase in code complexity

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The 80/20 rule

80% of the usecases can be solved
with 20% of the lines of code

Avoid feature creep

Simplicity

Complexity increase superlinearly

[An Experiment on Unit Increase in Problem Complexity, Woodfield 1979]

25% increase in problem complexity

$\Rightarrow$ 100% increase in code complexity

The 80/20 rule

80% of the usecases can be solved with 20% of the lines of code

Avoid feature creep

Use objects sparingly

Don't use classes for the sake of it

Software engineering

Software development is an industrial process

It's time to adopt engineering practices

Amateur practices that work for small projects
do not scale

Software engineering good practices

- Coding convention, good naming
- Version control

  Use git + github

- Unit testing

  If it's not tested, it's broken or soon will be.

- Make a package,

  with controlled dependencies and compilation

...

Things we did right (maybe)

Mayavi: 3D visualization in Python

Success factors

- Building upon VTK — Great power
- Component model (UI)
- Internals open to the world

$\Rightarrow$ from interaction to scripting

Limiting factors

- Building upon VTK — A lot of complexity
- Codebase too complex and object-oriented (bound to VTK)
- Users of GUIs do not turn into developers
- Composition is an API killer

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Parallel for loop

```
>>> from joblib import Parallel, delayed
>>> Parallel(n_jobs=2)(delayed(sqrt)(i**2)
...                         for i in range(8))
 [0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
```

- On-demand dispatch to ease memory consumption
- Threading and processes backends

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...                     for i in range(8))
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```

Memoize pattern

```
mem = joblib.Memory(cachedir='.')
g = mem.cache(f)
b = g(a)        # computes a using f
c = g(a)        # retrieves results from store
```

Success factors

- Simplicity of use
- Patterns we really, really need (pull not push)

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- Simplicity of use
- Patterns we really, really need (pull not push)

Limiting factor

- Vision of the project unclear
- Positioning with regards to landscape unclear (parallel computing world fuzzy)
- Tricky code inside

Success factors

- **Right project vision**

  Machine learning without learning the machinery

  Black box that can be opened

  Right trade-off between ”just works” and versatility
  (think Apple vs Linux)

  We’re not going to solve all the problems for you
  I don’t solve hard problems

  Feature-engineering, domain-specific cases...
  Python is a programming language. Use it.

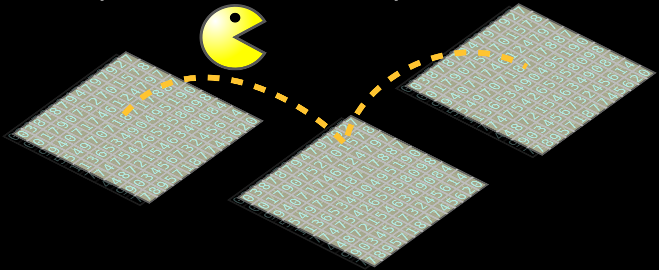
Cover all the 80% usecases in one package

Success factors

- **Right project vision**
- **High-level programming**
  - Optimize algorithmes, not for loops
  - Know perfectly Numpy and scipy
  - Use Cython, quad not C/C++

Success factors

- **Right project vision**
- **High-level programming**
- **Good API design**
  - separate data from operations



Success factors

- **Right project vision**
- **High-level programming**
- **Good API design**
  - separate data from operations
  - Object API exposes a data-processing language

fit, predict, transform, score, partial_fit

  - Instantiated without data but with all parameters

Success factors

- **Right project vision**
- **High-level programming**
- **Good API design**
- **Great community**
  - Github + code review

Success factors

- **Right project vision**
- **High-level programming**
- **Good API design**
- **Great community**
- **Great documentation**

Success factors

- Right project vision
- High-level programming
- Good API design
- Great community
- Great documentation

Limiting factors

- Tricky numerical code
- Our own success $\Rightarrow$ huge volume

From flop to success in academic software

1. Choose the project well

Not all battles can be fought

Make sure that there is a market

Don't solve (too many) hard problems

From flop to success in academic software

1. Choose the project well
2. Reach a community

Users: market your project

Developers: community-driven development

@GaelVaroquaux

From flop to success in academic software

1. Choose the project well
2. Reach a community
3. Make good software

With quality, software engineering
Usability matters

@GaelVaroquaux

From flop to success in academic software

1. Choose the project well
2. Reach a community
3. Make good software