

Speeding up Python with Rust

Summer school on modelling and complex systems 2021

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Motivating Example

Crash Course in Rust

Motivating Example Revisited

Next Steps

Motivating Example

A model

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Scaled Student T Distribution

Throughout this we will use a known model, with likelihood function based around the Scaled Student T Distribution, with priors as straightforward as they can be - the idea is to show work flow and ideas, not a specific model.

$$x \sim t_{\nu}(\mu, \sigma^2)$$

$$\mu \propto \text{const.}$$

$$\sigma^2 \propto \text{const.}$$

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$$\mu \propto \text{const.}$$

$$\sigma^2 \propto \text{const.}$$

Subordinate Representation

$$x \sim \mu + N\sqrt{\frac{\nu\sigma^2}{\chi_{\nu}^2}}$$

Another Representation

$$x \sim N(\mu, V)$$

$$V \sim \text{Inv-}\chi^2(\nu, \sigma^2)$$

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We will cheat a bit (i.e. make the model better in terms of learning it) and extend the above to allow better mixing:

$$x \sim N(\mu, \alpha^2 U)$$
$$U \sim \text{Inv-}\chi^2(\nu, \tau^2)$$

A model

Here, $\alpha^2 U$ plays the role of V , and $\alpha\tau = \sigma - \alpha$ is a 'mixing' parameter, helps with MCMC. The full conditional for Gibbs are as follows:

Source: *Bayesian Data Analysis 3rd ed.* Gelman et al. pp. 295

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.

$$U_i | \alpha, \mu, \tau^2, \nu, \sim \text{Inv-}\chi^2 \left(\nu + 1, \frac{\nu\tau^2 + ((x_i - \mu)/\alpha)^2}{\nu + 1} \right)$$

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- $$\mu | \alpha, \tau^2, U, \nu, x \sim N \left(\frac{\sum \frac{1}{\alpha^2 U_i} x_i}{\sum \frac{1}{\alpha^2 U_i}}, \frac{1}{\sum \frac{1}{\alpha^2 U_i}} \right)$$

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- $$\tau^2 | \alpha, \mu, U, \nu, x \sim \text{Gamma} \left(\frac{\nu n}{2}, \frac{\nu}{2} \sum \frac{1}{U_i} \right)$$

A model

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- $$\tau^2 | \alpha, \mu, U, \nu, x \sim \text{Gamma} \left(\frac{\nu n}{2}, \frac{\nu}{2} \sum \frac{1}{U_i} \right)$$

- $$\alpha^2 | \mu, \tau^2, U, \nu, x \sim \text{Inv-}\chi^2 \left(n, \frac{1}{n} \sum \frac{(x_i - \mu)^2}{U_i} \right)$$

Python implementation

```
class ScaledTModel(object):

    __slots__ = ['_data', '_data_size', '_nu',...]

    def __init__(self, data, nu):
        pass

    def run(self, burnin, sample_size):
        pass

    def get_mu(self):
        pass

    def get_sigma2(self):
        pass

    def _update_mu(self):
        pass

    def _update_tau2(self):
        pass

    def _update_alpha2(self):
        pass

    def _update_extended_vars(self):
        pass

    def _sampleScaledInvChiSquare(self, ni, scale):
        pass
```


Pure Python implementation

```
def __init__(self, data, nu):  
    print("making a model")  
    self._data = data  
    self._data_size = len(data)  
    self._nu = nu  
  
    self._extended_vars = [0.0] * self._data_size  
    self._tau2 = 1  
    self._mu = sum(data) / self._data_size  
    self._alpha2 = 1  
  
    self._update_extended_vars()
```

Pure Python implementation

```
def _update_mu(self):
    variance = 0.0
    expected_value = 0.0
    for i in range(self._data_size):
        tmp = 1.0/self._extended_vars[i]
        variance += tmp
        expected_value += tmp * self._data[i]

    variance /= self._alpha2
    expected_value /= self._alpha2
    variance = 1.0 / variance
    expected_value = expected_value * variance
    self._mu = random.gauss(expected_value, math.sqrt(variance))
```

Pure Python implementation

```
def _update_tau2(self):
    x = 0.0
    for i in range(self._data_size):
        x += 1.0 / self._extended_vars[i]
    self._tau2 = random.gammavariate(
        self._data_size * self._nu / 2.0,
        2.0 / (self._nu * x),
    )

def _update_alpha2(self):
    x = 0.0
    for i in range(self._data_size):
        x += (self._data[i] - self._mu) *
            (self._data[i] - self._mu) / self._extended_vars[i]
    x /= self._data_size
    self._alpha2 = self._sampleScaledInvChiSquare(self._data_size, x)
```

Pure Python implementation

```
def _update_extended_vars(self):
    for i in range(self._data_size):
        x = (self._data[i] - self._mu) *
            (self._data[i] - self._mu) / self._alpha2
        self._extended_vars[i] = self._sampleScaledInvChiSquare(
            self._nu + 1, (self._nu * self._tau2 + x) / (self._nu + 1))

@property
def get_mu(self):
    return self._results_mu

@property
def get_sigma2(self):
    return self._results_sigma2
```

Pure Python implementation

```
def run(self, burn_in = 1000, sample_size = 2000):
    self._results_mu = [0.0] * sample_size
    self._results_sigma2 = [0.0] * sample_size
    for _ in range(burn_in):
        self._update_extended_vars()
        self._update_alpha2()
        self._update_mu()
        self._update_tau2

    for i in range(sample_size):
        self._update_extended_vars()
        self._update_alpha2()
        self._update_mu()
        self._update_tau2
        self._results_mu[i] = self._mu
        self._results_sigma2[i] = self._alpha2 * self._tau2
```

Pure Python implementation

```
from great_model.python_great_model import ScaledTModel as PythonModel
import numpy as np
from timeit import timeit

nu = 6
mu = -3.14
sigma2 = 30
data_size = 500
z = np.random.randn(data_size)
x = np.random.chisquare(nu, data_size)

t_data = mu + z * np.sqrt(sigma2 * nu / x)

p_model = PythonModel(t_data, nu)

exec_time = timeit('p_model.run(2000, 2000)',
globals=globals(), number = 10)
print(f"Average run time of Pure Python model: {exec_time * 1000 / 10:3.5f} ms")
Average run time of Pure Python model: 10404.53057 ms
```

That's a bit more than 10 seconds.

Numpy implementation

```
def __init__(self, data, nu):
    print("making a model")
    self._data = np.asarray(data)
    self._data_size = len(data)
    self._nu = nu

    self._rng = default_rng()
    # Some starting values
    self._extended_vars = np.zeros(self._data_size)
    self._tau2 = 1
    self._mu = sum(data) / self._data_size
    self._alpha2 = 1

    self._update_extended_vars()

    # temporary data holders, so that we reuse memory
    self._tmp_with_data_size = np.zeros(self._data_size)
    self._tmp_with_data_size2 = np.zeros(self._data_size)
```

Numpy implementation

```
def _update_mu(self):
    np.reciprocal(self._extended_vars, out=self._tmp_with_data_size)
    self._tmp_with_data_size2 = self._data * self._tmp_with_data_size

    variance = self._tmp_with_data_size.sum()
    expected_value = self._tmp_with_data_size2.sum()

    variance /= self._alpha2
    expected_value /= self._alpha2
    variance = 1.0 / variance
    expected_value = expected_value * variance
    self._mu = self._rng.normal(expected_value, math.sqrt(variance))
```


Numpy implementation

```
def _update_tau2(self):
    np.reciprocal(self._extended_vars, out=self._tmp_with_data_size)
    x = self._tmp_with_data_size.sum()
    self._tau2 = self._rng.gamma(self._data_size * self._nu / 2.0, 2.0 / (self._nu * x))

def _update_alpha2(self):
    x = 0.0
    self._tmp_with_data_size = self._data - self._mu
    self._tmp_with_data_size = (self._tmp_with_data_size *
                                self._tmp_with_data_size) / self._extended_vars
    x = self._tmp_with_data_size.sum()
    x /= self._data_size
    self._alpha2 = self._sampleScaledInvChiSquare(self._data_size, x)
```

Numpy implementation

```
def _update_extended_vars(self):
    x = (self._data - self._mu) * (self._data - self._mu) / self._alpha2
    self._extended_vars = self._sampleScaledInvChiSquareN(
        self._nu + 1,
        (self._nu * self._tau2 + x) / (self._nu + 1),
    )

def _sampleScaledInvChiSquareN(self, ni, scale):
    x = self._rng.chisquare(ni, size=len(scale))
    return ni * scale / x
```

Numpy implementation

```
def run(self, burn_in = 1000, sample_size = 2000):
    self._results_mu = np.zeros(sample_size)
    self._results_sigma2 = np.zeros(sample_size)
    for _ in range(burn_in):
        self._update_extended_vars()
        self._update_alpha2()
        self._update_mu()
        self._update_tau2

    for i in range(sample_size):
        self._update_extended_vars()
        self._update_alpha2()
        self._update_mu()
        self._update_tau2
        self._results_mu[i] = self._mu
        self._results_sigma2[i] = self._alpha2 * self._tau2
```

Numpy implementation

```
from great_model.numpy_great_model import ScaledTModel as NumpyModel
import numpy as np
from timeit import timeit

nu = 6
mu = -3.14
sigma2 = 30
data_size = 500
z = np.random.randn(data_size)
x = np.random.chisquare(nu, data_size)

t_data = mu + z * np.sqrt(sigma2 * nu / x)

n_model = NumpyModel(t_data, nu)

exec_time = timeit('n_model.run(2000, 2000)',
                    globals=globals(), number = 10)
print(f"Average run time of Numpy model: {exec_time * 1000 / 10:3.5f} ms")
Average run time of Numpy model: 356.86459 ms
```

That's more like it... Can we do better? And how much better?

Crash Course in Rust

Good because

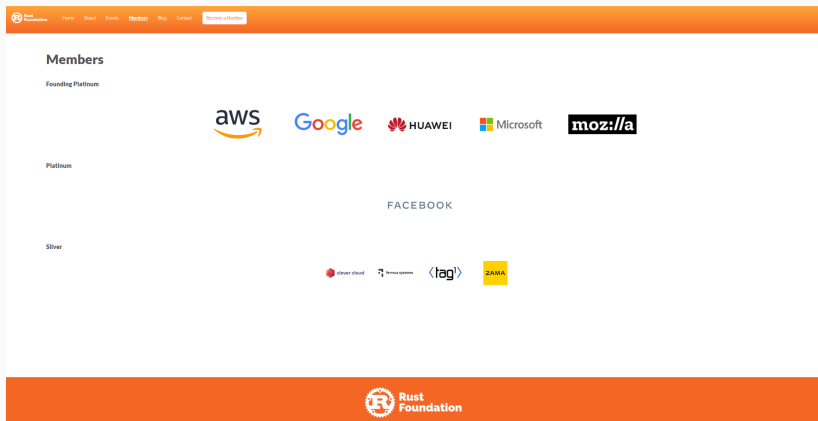
- A compiled, strongly typed, systems programming language (thing C/C++)
- Fast - about the same performance as C/C++
- Memory safe
- With great interoperability
- Outstanding tooling

Good because

- A compiled, strongly typed, systems programming language (thing C/C++)
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Bad because

- Steep learning curve
- Long compile times
- A somewhat young language



Hello World for scientists

```
fn main() {  
    // the type is not necessary in this case  
    let x: f64 = 1_000_000.0;  
  
    // no type cast - it is inferred by the compiler  
    let y = {  
        let z = x / 100.0;  
        // notice the missing colon  
        // this is the return value of the block  
        z  
    };  
  
    println!("The value of y is {}", y);  
}
```

One more Hello World

```
fn main() {  
    // this variable we will want to change  
    let mut x: f64 = 0.0;  
  
    for i in 1..=10 {  
        // we perform a cast, as i is not f64  
        x += i as f64;  
    }  
    // we recreate the value x to remove mutability  
    let x = x;  
    // we take the address of the variable x  
    let y = &x;  
  
    // we pass a reference, but still get what we want  
    println!("The sum of the first 10 natural numbers is {}", y);  
}
```

One more Hello World 2

```
struct MyStruct {
    has_value: bool,
    large_vector: Vec<f64>,
}

fn freeFlowFunction(x: &[f64]) -> f64 {
    unimplemented!();
}

impl MyStruct {
    // method functions for the struct
    fn increate_x(&mut self) {
        self.x += 1;
    }
}

impl fmt::Debug for MyStruct {
    // implement a trait for MyStruct - in this case,
    // how to present the struct in debug messages
    fn fmt(&self, f: &mut fmt::Formatter<'_>) -> fmt::Result {
        todo!()
        // almost never need to do this:
        // annotate the struct definition with
        // #[derive(Debug)] and the compiler will handle it
    }
}
```

One more Hello World 2f2f aka Family

```
fn a_fun(x: String) {  
    if x.len() % 2 == 0 {  
        println!("Even");  
        return;  
    }  
    println!("Odd");  
}  
  
fn main() {  
    let x = "Summer School 2021".to_string();  
    a_fun(x);  
    println!("x was: '{} ' ", x);  
}
```

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        return;  
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}  
  
fn main() {  
    let x = "Summer School 2021".to_string();  
    a_fun(x);  
    println!("x was: '{}'", x);  
}
```

```
error[E0382]: borrow of moved value: `x`  
--> src\main.rs:701:26  
699 |     let x = "Summer School 2021".to_string();  
    |         - move occurs because `x` has type `String`, which does not implement the `Copy` trait  
700 |     a_fun(x);  
    |         - value moved here  
701 |     println!("x was: '{}'", x);  
    |                             ^ value borrowed here after move  
  
error: aborting due to previous error; 1 warning emitted
```

Figure 1: "Not a bad way to explain the error in the code"

Rules of ownership

1. Each object can be used only once - it is "moved" every time
2. Out of scope objects are destroyed and cannot be used
3. Each block produces a value that goes one scope up
4. All objects have a lifetime that constrains which scopes they may be moved out of

Source: <https://chrismorgan.info/blog/rust-ownership-the-hard-way/>

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There are always exceptions to any rule...

1. Object that implement the special trait *Copy* (think as if on every "=" we do a copy)
2. Reference borrowing - you can have as many as you like immutable references to an object or one mutable

Source: <https://chrismorgan.info/blog/rust-ownership-the-hard-way/>

1. Functional tools (could possibly be faster than loops)

```
let sum_squares = a_vec.iter().map(|v| v * v).sum();
```

2. Algebraic types

```
enum IpAddr {  
    V4(u8, u8, u8, u8),  
    V6(String),  
}
```

3. Destructuring and matching

```
let as_string = match ip {  
    IpAddr::V4(a, b, c, d) => format!("{}", a, b, c, d),  
    IpAddr::V6(s) => s.clone()  
};
```

4. Anyone can implement a Trait for their Struct

Two important Enums

- `enum Result<T, E> {
 Ok(T),
 Err(E),
}`

You either get the value or get an error - Rust doesn't have exceptions that can get swept under the rug.

- `enum Option<T> {
 None,
 Some(T),
}`

None is only part of this enum, again forcing you to handle missing values.

- The ownership, type system and the borrow checker are some of what guarantees the memory safety in Rust. The compiler proves that no Segmentation Faults, memory leaks etc. cannot happen - otherwise, you get compile time error.
- "Fearless concurrency" - the same checks are done when multiple threads are involved, so two threads accessing the same memory location with read and write is not possible (mostly).
- If that was all, Rust would be too rigid and unusable, hence

unsafe

code word. This signals to the compiler: "I, the human, checked this piece of code and it is fine." You are free to do whatever in these sections (e.g. pointer arithmetic).

Some example tools for development (non exhaustive)

- **rustc** - the compiler (already saw the error messages)
- **rustup** - updater of the above
- **cargo** - package manager (crate in rust parlance)
- **cargofmt** - formatter (so the code looks nice)
- **clippy** - linter (helps find potential issues)
- **rust-analyzer** - IDE support (i.e. code completion) can integrate into your favorite text editor

Motivating Example Revisited

- Python C Package - write directly C code (i.e. extend CPython)
- Cython - mixture of Python and C (C++) syntax - this is parsed to C and then compiled as above
- With enough dedication any language that can build a dynamic library (and some C files to be link the two) can be used for Python modules (e.g. GoLang)

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Enter PyO3:

- A Rust bindings for Python
- Most of the 'magic' happens with the help of annotations
- Several different ways to actually build the package.

Definition

```
#[pyclass]
struct ScaledTModel {
    data_size: usize,
    nu: f64,
    tau2: f64,
    mu: f64,
    alpha2: f64,

    extended_vars: Vec<f64>,
    data: Vec<f64>,
    result_mu: Vec<f64>,
    result_sigma2: Vec<f64>,
}
#[pymodule]
fn rust_great_model(_py: Python, m: &PyModule) -> PyResult<()> {
    m.add_class::<ScaledTModel>()?;

    Ok(())
}
```


Exposed methods

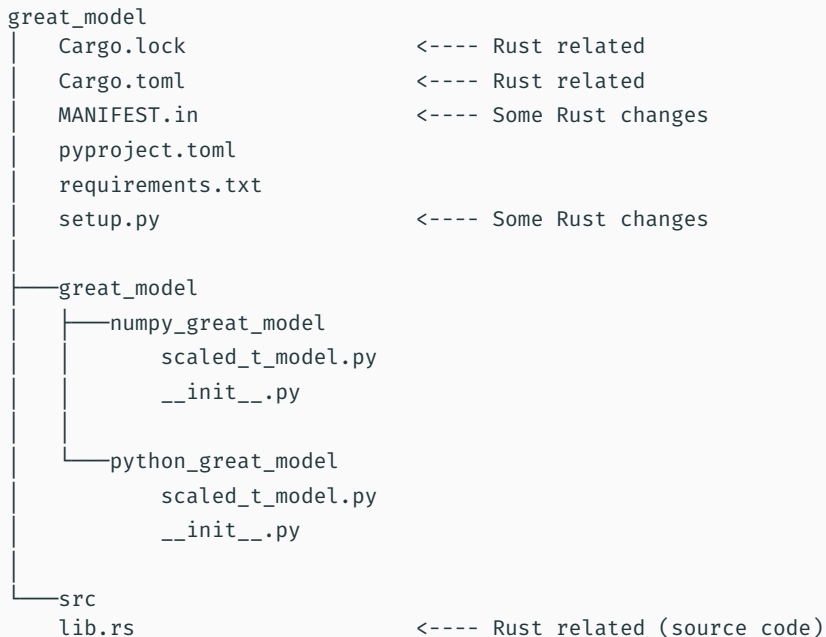
```
#[pymethods]
impl ScaledTModel {
    #[new]
    fn new(data: Vec<f64>, nu: f64) -> Self {
        println!("making a rust model");
        ScaledTModel {
            // skipped in slides!
        }
    }

    #[getter]
    fn get_mu(&self) -> PyResult<Vec<f64>> {
        Ok(self.result_mu.clone())
    }

    #[getter]
    fn get_sigma2(&self) -> PyResult<Vec<f64>> {
        Ok(self.result_sigma2.clone())
    }

    fn run(&mut self, burn_in: usize,
          sample_size: usize) -> PyResult<()> {
        todo!()
    }
}
```

Folder Structure



Cargo.toml

```
[package]
name = "great_model"
version = "1.0.0"
edition = "2018"

# See more keys and their definitions at
# https://doc.rust-lang.org/cargo/reference/manifest.html

[lib]
name = "great_model"
# "cdylib" is necessary to produce a shared
# library for Python to import from.
#
# Downstream Rust code (including code in `bin/`, `examples/`,
# and `tests/`) will not be able to use the code unless the "rlib" or
# "lib" crate type is also included, e.g.:
# crate-type = ["cdylib", "rlib"]
crate-type = ["cdylib"]

[dependencies]
rand = "0.8.4"
rand_distr = "0.4.1"
rand_xoshiro = "0.6.0"

[dependencies.pyo3]
version = "0.14.1"
features = ["extension-module"]
```

A MANIFEST.in file consists of commands, one per line, instructing setuptools to add or remove some set of files from the distribute package .

```
include pyproject.toml Cargo.toml
recursive-include src *
```

pyproject.toml specifies the minimum build system for python (basically - make setup.py work)

```
[build-system]
requires = [
    "setuptools>=42",
    "wheel",
    "setuptools-rust"
]
build-backend = "setuptools.build_meta"
```

```
1  import setuptools
2  from setuptools_rust import Binding, RustExtension
3
4  setuptools.setup(
5      name="great-model",
6      version="1.0.0",
7      author="Metodi Nikolov",
8      author_email="metodi.nikolov@gmail.com",
9      classifiers=[
10         "Programming Language :: Python :: 3",
11         "License :: OSI Approved :: MIT License",
12         "Operating System :: OS Independent",
13     ],
14     rust_extensions=[RustExtension("great_model.rust_great_model",
15                                   binding=Binding.PyO3)],
16     zip_safe=False,
17     packages=setuptools.find_packages(),
18     python_requires=">=3.8",
19 )
```

Lines 2, 14-16 are need for the rust bindings, the rest are standard python package.

Implementing the model

```
fn run(&mut self, burn_in: usize, sample_size: usize) -> PyResult<()> {  
    let mut rng = Xoshiro256Plus::seed_from_u64(0);  
    for _ in 0..burn_in {  
        self.update_extended_vars(&mut rng);  
        self.update_alpha2(&mut rng);  
        self.update_mu(&mut rng);  
        self.update_tau2(&mut rng);  
    }  
  
    self.result_mu.resize(sample_size, 0.0);  
    self.result_sigma2.resize(sample_size, 0.0);  
  
    for i in 0..sample_size {  
        self.update_extended_vars(&mut rng);  
        self.update_alpha2(&mut rng);  
        self.update_mu(&mut rng);  
        self.update_tau2(&mut rng);  
        self.result_mu[i] = self.mu;  
        self.result_sigma2[i] = self.alpha2 * self.tau2;  
    }  
    Ok(())  
}
```

Implementing the model

```
fn update_mu<R>(&mut self, rng: &mut R)
    where
        R: Rng,
{
    let mut tmp: f64;
    let mut variance = 0.0;
    let mut expected_value = 0.0;
    for (datum, ext_var) in self.data.iter().
        zip(self.extended_vars.iter()) {
        tmp = 1.0 / ext_var;
        variance += tmp;
        expected_value += datum * tmp;
    }
    variance /= self.alpha2;
    expected_value /= self.alpha2;
    variance = 1.0 / variance;
    expected_value = expected_value * variance;

    self.mu = expected_value + variance.sqrt() *
        rng.sample::<f64, _>(StandardNormal);
}
```

Implementing the model

```
fn update_tau2<R>(&mut self, rng: &mut R)
  where
    R: Rng,
{
  let x: f64 = self.extended_vars.iter().map(|x| 1.0 / x).sum();
  let scale = 2.0 / (self.nu * x);
  let gamma = Gamma::new(
    (self.data_size as f64) * self.nu / 2.0,
    scale,
  ).expect(&format!(
    "Failed at creation of Gamma, shape:{:}, scale: {:?}",
    (self.data_size as f64) * self.nu / 2.0,
    2.0 / (self.nu * x)
  )),
  );
  self.tau2 = gamma.sample(rng);
}
```


Implementing the model

```
fn update_alpha2<R>(&mut self, rng: &mut R)
    where
        R: Rng,
{
    let mu = self.mu;
    let mut x = self
        .data
        .iter()
        .zip(self.extended_vars.iter())
        .map(|(datum, ext_var)| (datum - mu) * (datum - mu) / ext_var)
        .sum();
    x /= self.data_size as f64;
    self.alpha2 = sample_scaled_inv_chi_square(rng, self.data_size as _, x);
}
```

Implementing the model

```
fn update_extended_vars<R>(&mut self, rng: &mut R)
    where
        R: Rng,
{
    let mut x: f64;
    let mu = self.mu;
    let alpha2 = self.alpha2;
    let tau2 = self.tau2;
    let nu = self.nu + 1.0;

    let nutau2 = self.nu * tau2;
    let chi = ChiSquared::new(nu).expect(
        "Failed at creation of ChiSquared");
    for i in 0..self.data_size {
        let datum = self.data[i];
        x = (datum - mu) * (datum - mu) * alpha2;
        self.extended_vars[i] = (nutau2 + x) / chi.sample(rng);
    }
}
```

Rust implementation

```
from great_model.rust_great_model import ScaledTModel as RustModel
import numpy as np
from timeit import timeit

nu = 6
mu = -3.14
sigma2 = 30
data_size = 500
z = np.random.randn(data_size)
x = np.random.chisquare(nu, data_size)

t_data = mu + z * np.sqrt(sigma2 * nu / x)

r_model = RustModel(t_data, nu)

exec_time = timeit('r_model.run(2000, 2000)',
                    globals=globals(), number = 10)
print(f"Average run time of Rust model: {exec_time * 1000 / 10:3.5f} ms")
Average run time of Rust model: 113.34160 ms
```

Next Steps

- Language <https://www.rust-lang.org/>
- The Book <https://doc.rust-lang.org/stable/book/>
- Good introduction <https://tourofrust.com/>
- Reference (work in progress)
<https://doc.rust-lang.org/stable/reference/>
- Reddit <https://www.reddit.com/r/rust/>
- <https://github.com/MetodiNikolov/SummerSchool2021>

Thank you!

Thank you for the attention!