# Speeding up Python with Rust

Summer school on modelling and complex systems 2021

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Motivating Example Model Crash Course in Rust PyO3 Motivating Example Model Revisited Next Steps

Motivating Example Model

Say that you have come up with a very interesting Bayesian model for the data you have. The model is not supported by the standard packages for inference (e.g. PyMCMC, Stan), so you will have to code it yourself.

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:

$$x \sim t_{\nu}(\mu, \sigma^2)$$
  
 $\mu \propto \text{const.}$   
 $\sigma^2 \propto \text{const.}$ 

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## Subordinate Representation

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

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#### **Another Representation**

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#### **Another Representation**

$$\mathbf{X} \sim \mathit{N}(\mu, \mathbf{V})$$
 
$$\mathbf{V} \sim \mathit{Inv-}\chi^2(\nu, \sigma^2)$$

NB: There is a V for each data point!

$$\begin{aligned} \mathbf{X} &\sim \mathit{N}(\mu, \alpha^2 \mathit{U}) \\ \mathit{U} &\sim \mathit{Inv-}\chi^2(\nu, \tau^2) \end{aligned}$$

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 $\mathbf{U} \sim \text{Inv-}\chi^2(\nu, \tau^2)$ 

$$\mathsf{U}_i|\alpha,\mu,\tau^2,\nu,\sim \mathsf{Inv-}\chi^2\left(\nu+1,\frac{\nu\tau^2+((\mathsf{X}_i-\mu)/\alpha)^2}{\nu+1}\right)$$

$$\mathbf{X} \sim N(\mu, \alpha^2 \mathbf{U})$$
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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:

•

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

•

$$\mu | \alpha, \tau^2, U, \nu, \mathsf{X} \sim \mathsf{N}\left(\frac{\sum \frac{1}{\alpha^2 U_i} \mathsf{X}_i}{\sum \frac{1}{\alpha^2 U_i}}, \frac{1}{\sum \frac{1}{\alpha^2 U_i}}\right)$$

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

$$\begin{split} &U_i|\alpha,\mu,\tau^2,\nu,\sim \text{Inv-}\chi^2\left(\nu+1,\frac{\nu\tau^2+((\textbf{X}_i-\mu)/\alpha)^2}{\nu+1}\right) \\ &\mu|\alpha,\tau^2,U,\nu,\textbf{X}\sim \textit{N}\left(\frac{\sum\frac{1}{\alpha^2U_i}\textbf{X}_i}{\sum\frac{1}{\alpha^2U_i}},\frac{1}{\sum\frac{1}{\alpha^2U_i}}\right) \\ &\tau^2|\alpha,\mu,U,\nu,\textbf{X}\sim \text{Gamma}(\frac{\nu\textbf{n}}{2},\frac{\nu}{2}\sum\frac{1}{U}) \end{split}$$

$$\mathbf{X} \sim N(\mu, \alpha^2 \mathbf{U})$$

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$$\begin{split} & \textit{$U_i|\alpha,\mu,\tau^2,\nu,\sim \text{Inv-}\chi^2\left(\nu+1,\frac{\nu\tau^2+((\textit{$\chi_i-\mu$})/\alpha)^2}{\nu+1}\right)$} \\ & \mu|\alpha,\tau^2,\textit{$U,\nu$},\textit{$\chi\sim \textit{$N}\left(\frac{\sum\frac{1}{\alpha^2\textit{$U_i$}}\textit{$\chi_i$}}{\sum\frac{1}{\alpha^2\textit{$U_i$}}},\frac{1}{\sum\frac{1}{\alpha^2\textit{$U_i$}}}\right)$} \\ & \tau^2|\alpha,\mu,\textit{$U,\nu$},\textit{$\chi\sim \text{Gamma}(\frac{\nu n}{2},\frac{\nu}{2}\sum\frac{1}{\textit{$U_i$}})$} \\ & \alpha^2|\mu,\tau^2,\textit{$U,\nu$},\textit{$\chi\sim \text{Inv-}\chi^2\left(n,\frac{1}{n}\sum\frac{(\textit{$\chi_i-\mu$})^2}{\textit{$U_i$}}\right)$} \end{split}$$

```
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
```

```
def __init__(self, data, nu):
    print("making a model")
    self._data = np.asarray(data)
    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)
    self._tmp_with_data_size2 = np.zeros(self._data_size)
    self._tmp_with_data_size2 = np.zeros(self._data_size)
```

```
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._rmg.normal(expected_value, math.sqrt(variance))
```

```
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._data_size
```

```
def run(self. burn in = 1000. sample size = 2000):
        self. results mu = np.zeros(sample size)
        self. results sigma2 = np.zeros(sample size)
        print("Starting Burn-in")
        for _ in range(burn_in):
               self._update_extended_vars()
                self._update_alpha2()
                self. update mu()
                self. update tau2
        print("Starting Data run")
        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
```

```
from great_model.python_great_model import ScaledTModel as Model
import numpy as np

nu = 6
mu = -3.14
ssigma2 = 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)
g_model = Model(t_data, nu)
%timeit g_model.run(2000, 2000)
```

On my local machine %timeit reports 8 seconds of execution.

Crash Course in Rust

PyO3

Motivating Example Model
Revisited

# Next Steps

► Gelman, A.; Carlin, J. B.; Stern, H. S. & Rubin, D. B. (2014), *Bayesian Data Analysis*, Chapman and Hall/CRC