Modeling calculation kernels with Stan

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Context

With the current need for high performance computing, and the hardware complexity:

- How to predict the duration of calculations?
- How to check if the performance is normal?

For this talk:

1. Brief presentation of the context
2. Introduction to Bayesian sampling
3. Examples of application

Background on HPC and Polaris research

Modern context

- HPC systems use thousands of nodes, cache, hyperthreading, etc -> makes it difficult to predict performance
- Some functions are used everywhere, and called thousands of times

Polaris research

- Simulating HPL on smaller supercomputers to optimize it at a lesser cost
- Elaborated complex models but needed to evaluate and confirm the models

HPL simulation

Examples

- The blas library (especially matrix per matrix multiplication) is used by thousands of programs and constitutes most of HPL calculations.
- Performance variability is also caused by network communications
- Needs to check the models with bayesian sampling.

Bayes model

Model Let's say $y \sim \mathcal{N}(\mu, \sigma)$

- μ: Model parameters
- y: Dependent data (posterior)
- σ: Independent data (prior)

We observe some data and need to find model parameters

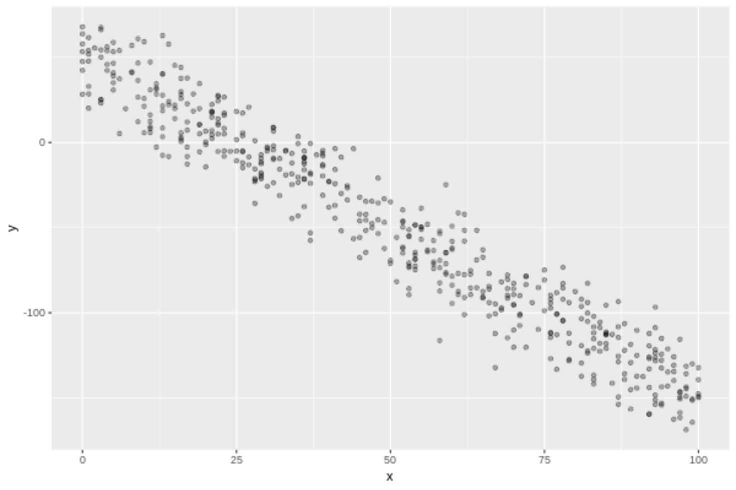
The vocabulary

- Posterior: The distribution of the parameters
- Likelihood: A function of the parameters, the model
- Prior: Existing knowledge of the system, guesses on the parameters values

$$\boxed{\underbrace{p(\mu|y,\sigma)}_{\text{Posterior}} \propto \underbrace{p(y|\mu,\sigma)}_{\text{Likelihood}}\underbrace{p(\mu,\sigma)}_{\text{Prior}}} \text{ assuming } y \sim \mathcal{M}(\mu, \sigma)$$

A Bayesian Sampler, Stan

With a simple example



Using this data, we'll try to find the parameters that were used to generate it.

The Stan model

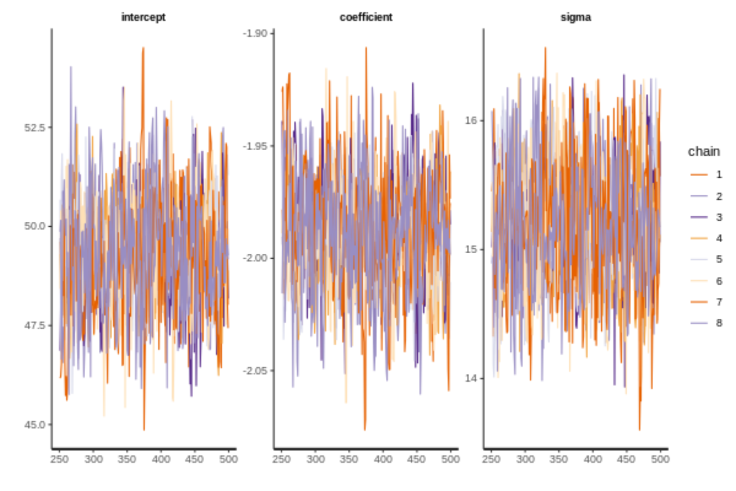
```
library(rstan)

modelString = "data { // the observations
    int<lower=1> N; // number of points
    vector[N] x;
    vector[N] y;
}
parameters { // what we want to find
    real intercept;
    real coefficient;
    real<lower=0> sigma; // indication: sigma cannot be negative
}
model {
    // We define our priors
    intercept   ~ normal(0, 10); // We know that all the parameters follow a nor
    coefficient ~ normal(0, 10);
    sigma       ~ normal(0, 10);

    // Then, our likelihood function
    y ~ normal(coefficient*x + intercept, sigma);
}
"
sm = stan_model(model_code = modelString)
```

Making the fit and checking the results

```
data = list(N=nrow(df),x=df$x,y=df$y)
fit = sampling(sm,data=data, iter=500, chains=8)

print(fit)

Inference for Stan model: ea4b5a288cf5f1d87215860103a9026e.
8 chains, each with iter=500; warmup=250; thin=1;
post-warmup draws per chain=250, total post-warmup draws=2000.

                mean se_mean   sd     2.5%      25%      50%      75%    97.5%
intercept      49.86    0.04 1.36    47.14    48.94    49.87    50.82    52.40
coefficient    -2.00    0.00 0.02    -2.04    -2.01    -2.00    -1.98    -
1.95
sigma          15.03    0.01 0.47    14.18    14.70    15.02    15.35    15.99
lp__        -1615.90    0.04 1.12 -1618.80 -1616.45 -1615.62 -1615.05 -1614.58
            n_eff Rhat
intercept    1070 1.00
coefficient  1042 1.00
sigma        1042 1.01
lp__          871 1.00

Samples were drawn using NUTS(diag_e) at Wed Jun 19 17:07:18 2019.
For each parameter, n_eff is a crude measure of effective sample size,
and Rhat is the potential scale reduction factor on split chains (at
convergence, Rhat=1).
```

Checking the convergence

```
stan_trace(fit)
```



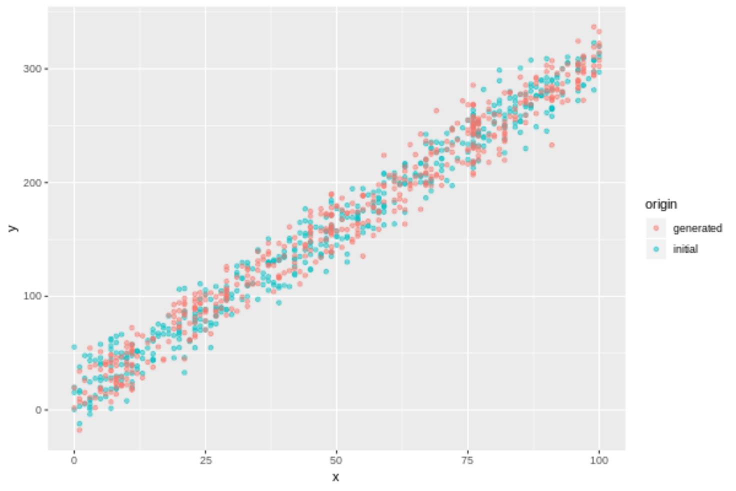
Generating new data

- Generating new data to check the results and model's accuracy.

```
modelString = "data {
    int<lower=1> N;
    vector[N] x;
    vector[N] y;
}
parameters { // what we want to find
    real intercept;
    real coefficient;
    real<lower=0> sigma;
}
model {
    intercept   ~ normal(0, 10);
    coefficient ~ normal(0, 10);
    sigma       ~ normal(0, 10);
    y ~ normal(coefficient*x + intercept, sigma);
}
generated quantities {
   real x_pos = x[categorical_rng(rep_vector(1,N) / N)];
   real y_pos; // posterior predictions
   y_pos = normal_rng(coefficient*x_pos+intercept, sigma);
}
"
sm = stan_model(model_code = modelString)
```

Plotting the new data

```
extracted=rstan::extract(fit)
df_generated = data.frame(x=extracted$x_pos, y=extracted$y_pos, origin='generate
ggplot(tmp, aes(x=x, y=y, color=origin)) + geom_point(alpha=0.5)
```



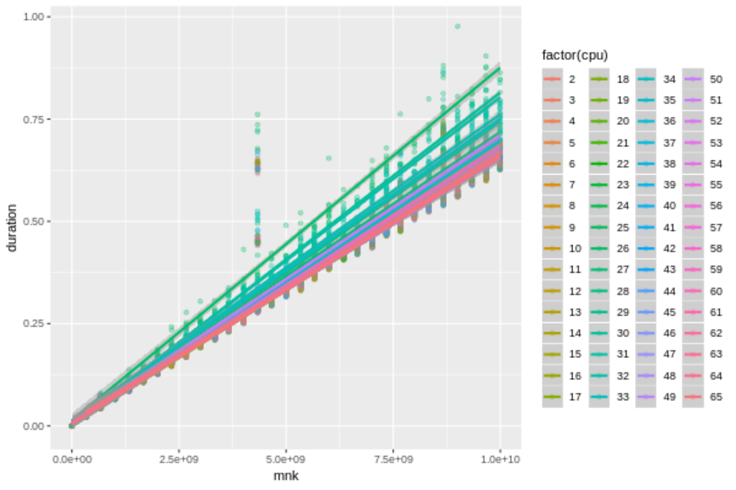
The importance of the priors

- The priors are necessary to have convergence in the fit
- Non-informative prior vs informative (careful not to have a falsely informative one and introduce bias)
- A little bit of precision is better, but initialisation values can make the trick

The different models for dgemm

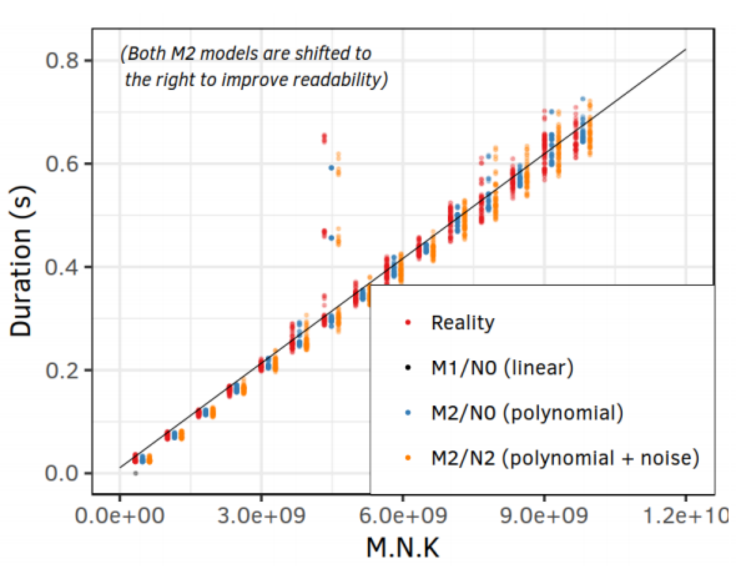
The theory behind it

- Dgemm's duration depends on the matrix size, but also on the CPU used to run it



The possible models

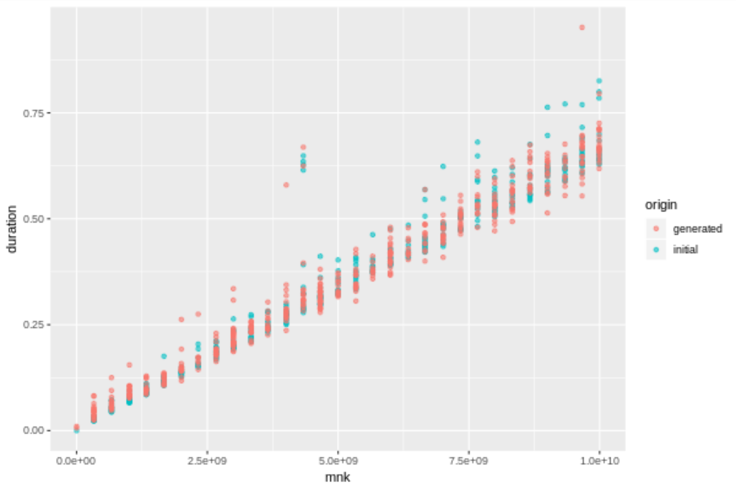
Different possible models, some more accurate than others:



A M-2 N-2 MODEL (POLYNOMIAL WITH NOISE DEPENDING ON X)

```
modelString = "data {
    int<lower=0> N;
    vector[N] mnk;
    vector[N] duration;
    vector[5] mu_mean; //the priors for mu and sigma
    vector[5] mu_sd;
    vector[5] sigma_mean;
    vector[5] sigma_sd;
}
parameters {
    vector[5] mu_raw; vector[5] sigma_raw;
}
transformed parameters {
    vector[5] mu; vector[5] sigma;
    for(j in 1:5){
      mu[j] = mu_mean[j] + mu_raw[j] * mu_sd[j];
      sigma[j] = sigma_mean[j] + sigma_raw[j] * sigma_sd[j];}
}
model {
    mu_raw ~ normal(0,1); sigma_raw ~ normal(0,1);
    duration ~ normal(mu[1]*mnk + mu[2]*mn + mu[3]*mk + mu[4]*nk + mu[5],
    sigma[1]*mnk + sigma[2]*mn + sigma[3]*mk + sigma[4]*nk + sigma[5]);
}
"
```

The generated data



A M_H-2 N_H-2 MODEL (DEPENDING ON THE HOST)

- Much like the previous model, but with different observations for each host
- Added a variable for the number of hosts, and used matrixes instead of vectors for all the parameters.

```
modelString = "data {
    int hosts;
}
parameters {
    matrix[hosts,5] mu_raw;
    matrix[hosts,5] sigma_raw;
}
transformed parameters {
    matrix[hosts,5] mu;
    matrix[hosts,5] sigma;
}
model {
    for(i in 1:hosts){
      duration[i] ~ normal(mu[i,1]*mnk[i]+mu[i,2]*mn[i]+mu[i,3]*mk[i]+
      mu[i,4]*nk[i]+mu[i,5], sigma[i,1]*mnk[i]+sigma[i,2]*mn[i]+
      sigma[i,3]*mk[i]+sigma[i,4]*nk[i]+sigma[i,5]);}
}
"
```

A hierarchical M_H-1 N_H-2 model

- Useful to find the value of hyperparameters from which we get the parameters
- From this we could calculate new parameters for new CPUs
- Here μ-alpha and σ-alpha are the hyperparameters for alpha, and the same goes for the other parameters

$\mu - alpha \sim \mathcal{N}(alpha_{\mu}, alpha_{\sigma})$ with alpha_μ and alpha_σ the priors

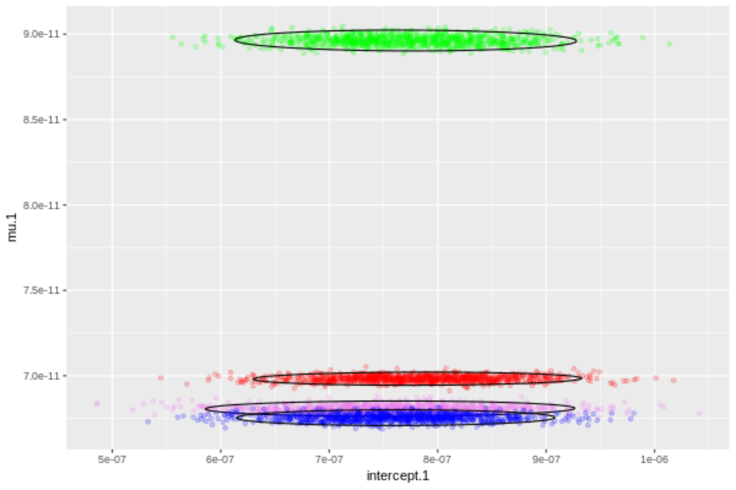
$\sigma - alpha \sim \mathcal{N}(0, 1)$

$alpha[i] \sim \mathcal{N}(\mu - alpha, \sigma - alpha)$

$duration[i] \sim \mathcal{N}(alpha[i] * mnk + beta[i], teta[i] * mnk + gamma[i])$

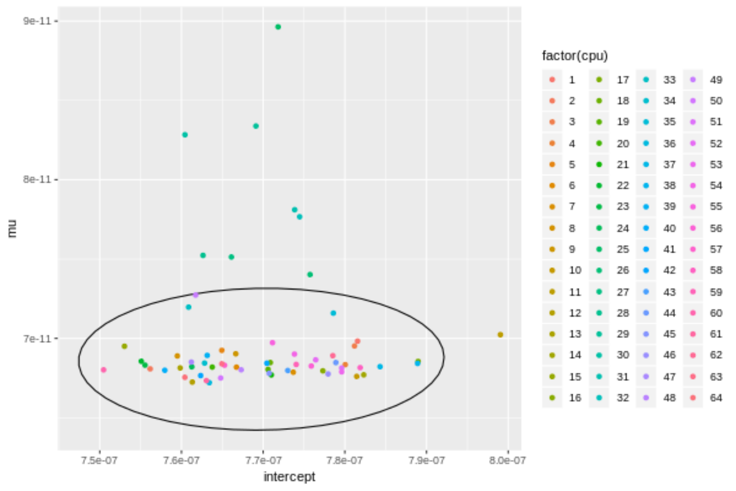
Posterior visualisation

The posterior with models depending on the host shows a lot of difference between hosts (here we have 3 ”average” CPU and a slow one):



Posterior visualisation

If we look at the means of the parameters' values for each host, we get a range of values in which most hosts are.



The follow up

- Modeling other calculation kernels
- Modeling the network communications
- Parsing and converting Stan code to C, to generate new data more efficiently
- Anomaly detection