Faster Computation for Hierarchical Bayesian Models with Rcpp Packages

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The findings and conclusions in this presentation are those of the authors and should not be construed to represent any official USDA or US Government determination or policy.

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Outline

Motivation

Introduction of Rcpp Packages

Examples

Conclusion

Motivation

> "Sometimes R code just isn't fast enough."
>
> – Hadley Wickham

- Problem: How to combine survey and auxiliary data to improve the county-level estimates for crops?
- Application: Bayesian small area models
- Potential bottlenecks of R code: subsequent iterations, repeatedly calling functions, loops in Markov chain Monte Carlo (MCMC) algorithms
- One solution: rewriting key functions in C++ through **Rcpp packages**

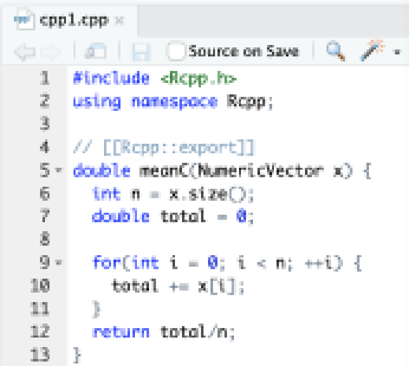
Rcpp Packages

- **Rcpp** is a R package to extend R with C++ codes developed by Dirk Eddelbuettel and Romain Francois (2013) .
  - Speed
  - New Things
- **RcppArmadillo** is a Rcpp extension package that provides all the functionality of Armadillo, focusing on **matrix math**.
  - Easy-to-use
  - Further speedup

Using sourceCpp() in R

- The Rcpp::sourceCpp function parses the C++ file (.cpp) and makes C++ functions available as R functions.

Example: Calculate mean of $x_i, i = 1, \ldots, 10^5$, where $x_i \sim U(0,1)$.



```cpp
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
double meanC(NumericVector x) {
  int n = x.size();
  double total = 0;

  for(int i = 0; i < n; ++i) {
    total += x[i];
  }
  return total/n;
}
```

```r
Rcpp::sourceCpp('cpp1.cpp')
x <- runif(1e5)
microbenchmark(
        mean(x), #build-in R mean() function
        meanC(x) #C++ function
)
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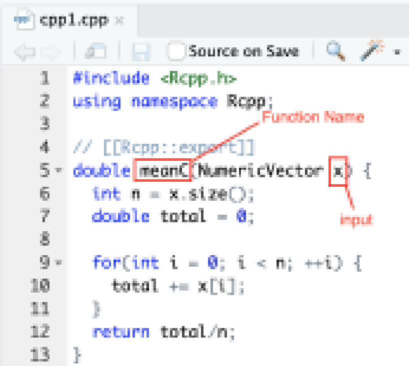

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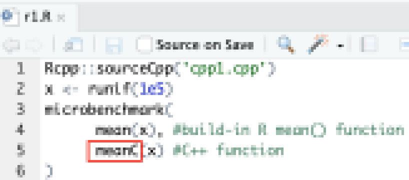

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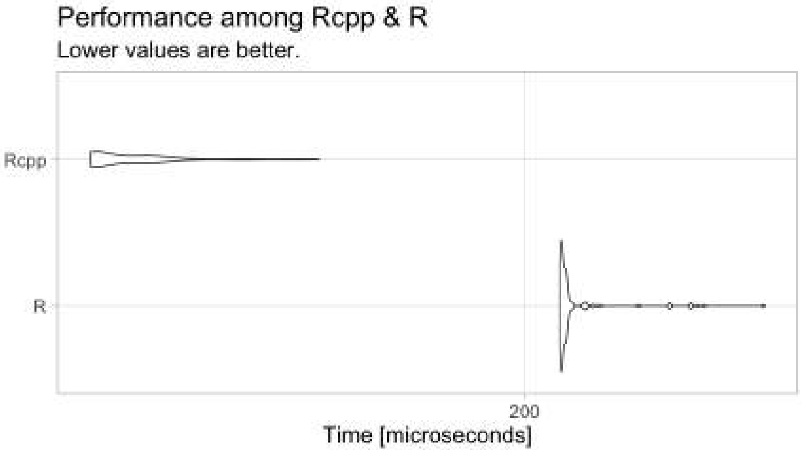
Comparison



name	min	mean	median	max	times
Rcpp	105.432	151.448	109.209	228.249	100
R	210.845	237.125	235.366	396.785	100

MCMC in Bayesian Computation

- MCMC is a sampling method to draw random samples from distributions.
- Each random sample is used as a stepping stone to generate the next one (chains).
- Gibbs sampler, Metropolis-Hastings sampler and many others are widely used in Bayesian inference.
- Involve **loops** and **calling functions repeatedly** within loops.

Rcpp (C++) and RcppArmadillo are useful tools for efficient MCMC computation.

Simulated Data

Data: simulated planted acres data in Illinois (Nandram et al., 2019 and Battese et al., 1988)

- Survey estimates $\hat{\theta}_i, \ i = 1, \ldots, 102$
- Survey standard errors $\hat{\sigma}_i, \ i = 1, \ldots, 102$
- Covariates: corn and soybean planted acres from land observatory satellites (LANDSAT)

Fay-Herriot Model

Fay-Herriot Model (1979) in small area estimation:

$$\hat{\theta}_i | \theta_i \overset{ind}{\sim} N(\theta_i, \hat{\sigma}_i^2),$$

$$\theta_i | \boldsymbol{\beta}, \delta^2 \overset{ind}{\sim} N(\mathbf{x}_i' \boldsymbol{\beta}, \delta^2),\ \ i = 1, \ldots, n,$$

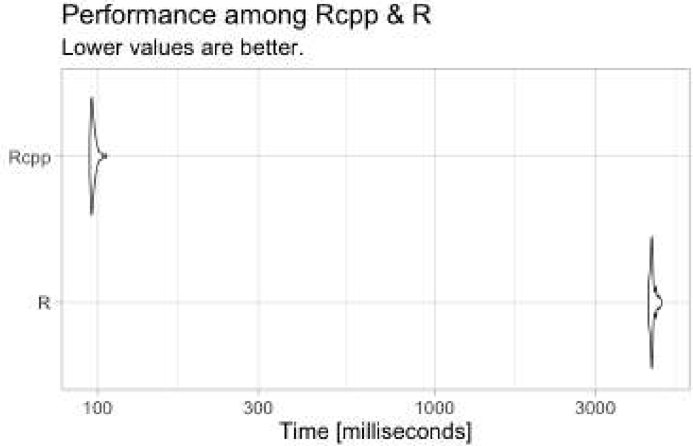
Priors for the parameters: $\pi(\boldsymbol{\beta}) \propto 1; \pi(\delta^2) \propto \frac{1}{\delta^2}$.

The full conditional distributions for Gibbs sampling are:

1. $\boldsymbol{\beta} | \delta^2 \sim MVN\Big((\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i')^{-1} (\sum_{i=1}^n \mathbf{x}_i' \boldsymbol{\beta}), \delta^2 (\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i')^{-1} \Big)$,
2. $\theta_i | \boldsymbol{\beta}, \delta^2 \overset{ind}{\sim} N(\lambda_i \hat{\theta}_i + (1 - \lambda_i) \mathbf{x}_i' \boldsymbol{\beta}, (1 - \lambda_i) \delta^2),\ \ \lambda_i = \frac{\delta^2}{\delta^2 + \hat{\sigma}_i^2}$,
3. $\delta^2 | \boldsymbol{\theta}, \boldsymbol{\beta} \sim IG\Big(\frac{n-1}{2}, \frac{1}{2} \sum_{i=1}^n (\theta_i - \mathbf{x}_i' \boldsymbol{\beta})^2 \Big)$.

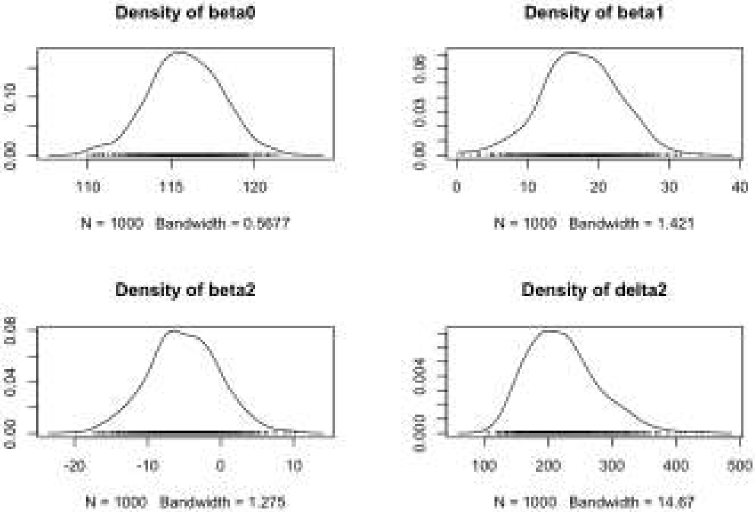
Comparison

12,000 iterations with 2,000 burn-in and pick every 10^{th} sample

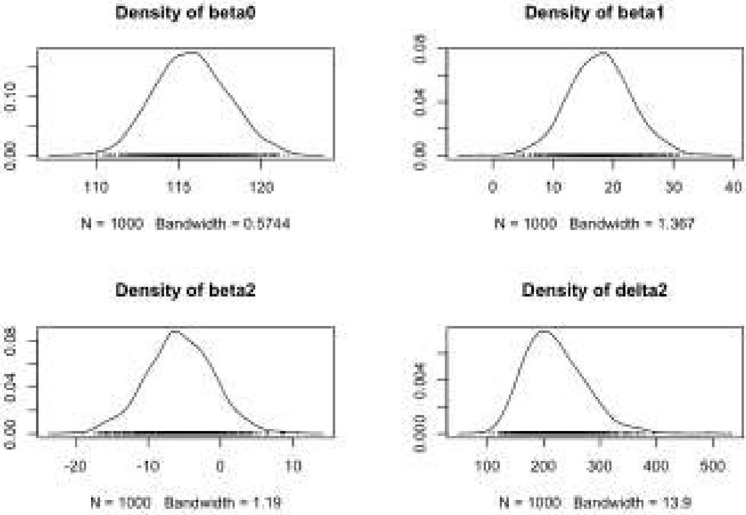


name	min	mean	median	max	times
Rcpp	94.863	97.285	96.621	106.362	100
R	4707.729	4856.196	4829.291	4912.025	100

Comparison - R density plots



Comparison - Rcpp density plots



Fay-Herriot Model with Benchmarking Constraints

In some applications, we need to incorporate benchmarking constraints into the model. For example, the county-level estimates should be summed to state target and they need to cover certain values. The model with inequality constraints:

$$\hat{\theta}_i|\theta_i \overset{ind}{\sim} N(\theta_i,\ \hat{\sigma}_i^2),\ i = 1, \ldots, n,$$

$$\theta_i|\boldsymbol{\beta}, \delta^2 \overset{ind}{\sim} N(\mathbf{x}_i'\boldsymbol{\beta}, \delta^2),\ \theta_i \geq c_i, \sum_{i=1}^{n} \theta_i \leq a,$$

where $\mathbf{C} = (c_1, \ldots, c_n)'$ are known and fixed and a is state target. The priors are $\pi(\boldsymbol{\beta}) \propto 1; \delta^2 \propto \frac{1}{(1+\delta^2)^2}$.

Joint Posterior Distribution

The posterior density is

$$\pi(\boldsymbol{\theta}, \boldsymbol{\beta}, \delta^2 | \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\sigma}}^2) = \frac{\prod_{i=1}^{n} \phi((\theta_i - \mathbf{X}'\boldsymbol{\beta})/\delta)\phi((\theta_i - \hat{\theta}_i)/\hat{\sigma}_i)}{\int_{\theta \in V} \prod_{i=1}^{n} \phi((\theta_i - \mathbf{X}'\boldsymbol{\beta})/\delta) d\theta}, \; \boldsymbol{\theta} \in V,$$

where $\phi(\cdot)$ is the standard normal density and the support of $\boldsymbol{\theta}$ is

$$V = \left\{ c_i \leq \theta_i, \sum_{i=1}^{n} \theta_i \leq a, \; i = 1, \ldots, n \right\}.$$

Awkward joint posterior distribution and intractable.

Computation

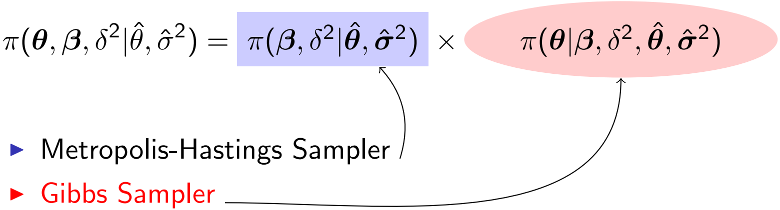
Our strategy:

$$\pi(\boldsymbol{\theta}, \boldsymbol{\beta}, \delta^2 | \hat{\theta}, \hat{\sigma}^2) = \pi(\boldsymbol{\beta}, \delta^2 | \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\sigma}}^2) \times \pi(\boldsymbol{\theta} | \boldsymbol{\beta}, \delta^2, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\sigma}}^2)$$

- Metropolis-Hastings Sampler

Computation

Our strategy:



$$\pi(\boldsymbol{\theta},\boldsymbol{\beta},\delta^2|\hat{\theta},\hat{\sigma}^2) = \pi(\boldsymbol{\beta},\delta^2|\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\sigma}}^2) \times \pi(\boldsymbol{\theta}|\boldsymbol{\beta},\delta^2,\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\sigma}}^2)$$

- Metropolis-Hastings Sampler
- Gibbs Sampler

Metropolis-Hastings Sampler

We will draw $(\boldsymbol{\beta}, \delta^2)$ samples from $\pi(\boldsymbol{\beta}, \delta^2 | \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\sigma}}^2)$. The proposal density is

$$(\boldsymbol{\beta}, \log(\delta^2)) \sim MVN(\hat{\boldsymbol{\beta}}_p, \sigma^2 \hat{\Sigma}_p)$$
$$\nu/\sigma^2 \sim \Gamma(\nu/2, 1/2)$$

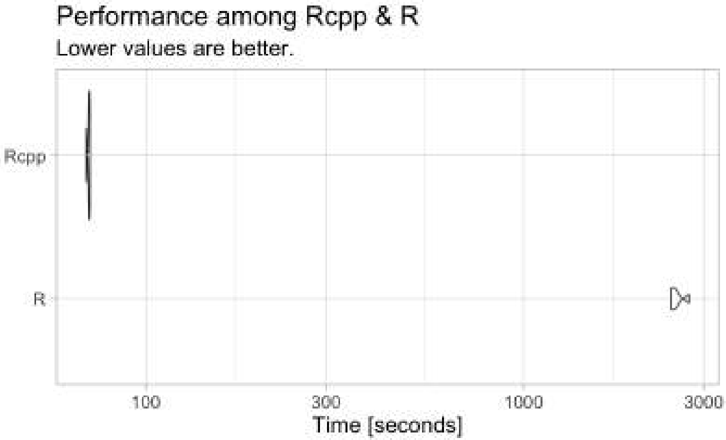
Bottleneck:

For each iteration h:

- **Generate**: Generate a candidate $(\boldsymbol{\beta}^c, \log(\delta^2)^c)$ from proposal density;
- **Calculate**: Calculate the acceptance ratio $\alpha = \pi(\boldsymbol{\beta}^c, \log(\delta^2)^c)/\pi(\boldsymbol{\beta}^{(h)}, \log(\delta^2)^{(h)})$;
- **Accept or Reject** candidate based on the comparison between α and $u \sim U(0, 1)$.

Comparison

10,000 iterations with 2,000 burn-in and pick every 8^{th} sample



name	min	mean	median	max	times
Rcpp	69.527	70.554	70.711	71.073	10
R	2451.688	2540.393	2519.215	2741.561	10

Gibbs Sampler for $\boldsymbol{\theta}$

The conditional posterior density of θ_i is

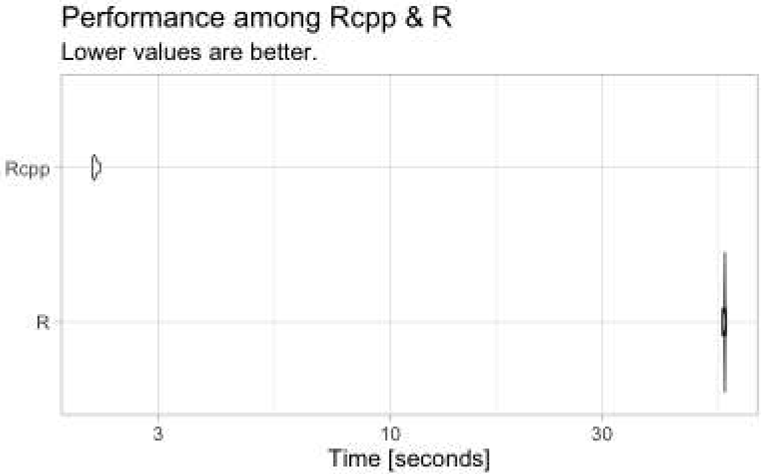
$$\theta_i | \boldsymbol{\theta}_{(i)}, \boldsymbol{\beta}, \delta^2, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\sigma}}^2 \sim N\Big(\mu_i, \phi_i\Big), \ \theta_i \in V_i,$$

where μ_i and ϕ_i related to $\boldsymbol{\beta}$ and δ^2 and

$$V_i = \Big\{ c_i \leq \theta_i \leq a - \sum_{j=1, j \neq i}^{n-1} \theta_j \Big\}, \ i = 1, \ldots, n.$$

Bottleneck:
Each θ_i related to other $\boldsymbol{\theta}$s based on the V_i.
For one iteration, we need to loop n times.

Comparison



name	min	mean	median	max	times
Rcpp	2.130	2.162	2.153	2.213	10
R	55.934	56.615	56.696	57.134	10

Convergence Diagnostics

- M-H: 1,000 samples of $(\boldsymbol{\beta}^{(h)}, \delta^{2(h)}), h = 1, \ldots, 1000$.
- Gibbs: for each $(\boldsymbol{\beta}^{(h)}, \delta^{2(h)})$, we run 100 times Gibbs sampler and pick the last set of $\boldsymbol{\theta}$.

	pm	psd	lb	ub	gewe.pval	ess
β_0	116.22	2.01	112.43	120.06	0.45	909
β_1	16.74	4.58	7.75	25.29	0.40	870
β_2	-4.81	4.23	-13.14	3.35	0.24	968
δ^2	325.96	60.78	206.98	469.46	0.64	827

- Rcpp vs R code: **72s** vs **2576s** for 102 samples size in the constraint Bayesian model.

Conclusion

- Rcpp functions can reduce the running time by a significant factor and reasonable in further production for county-level estimates in NASS.
- Large data set or complicated hierarchical Bayesian models: Rcpp packages
  - Pros: incorporating C++ code into R workflow easily; substantially speed up MCMC computation in R
  - Cons: learning curve and long coding time
- Small data set or simple, classic Bayesian models: such as RJags and RStan
  - Pros: Easy-to-use; less coding time
  - Cons: Black-box sampler; not for non-standard problems

Reference

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Thank You!

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