

GPUs and the computational efficiency of Gaussian process based models

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April 15, 2015

- 1 Background
- 2 Migratory Bird Spatial Assignment Model
- 3 Speciated $PM_{2.5}$ Modeling
- 4 GPUs and Low Rank Approximations

The problem with GPs ...

Unless you are lucky (or clever), Gaussian process models are difficult to scale to large problems. For a Gaussian process $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$:

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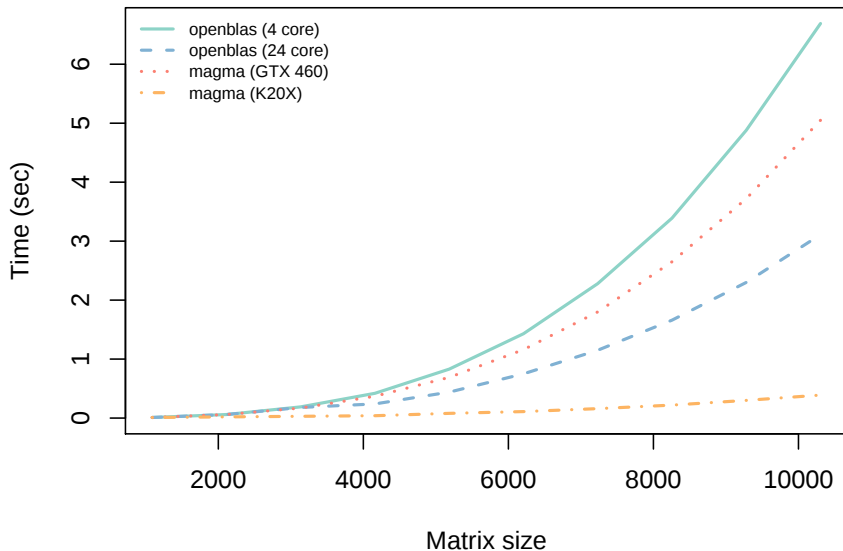
Cubic complexity?

Linear complexity? - Go for it

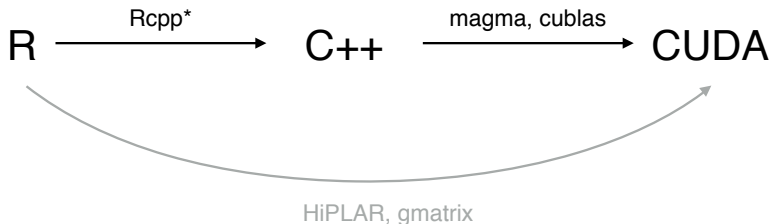
Quadratic complexity? - Pray

Cubic complexity? - Give up

Improving Cholesky



Tools and Optimization



Regardless of tools or workflow, measuring / profiling performance is critical.

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Background

Using intrinsic markers (genetic and isotopic signals) for the purpose of inferring migratory connectivity.

- Existing methods are too coarse for most applications
- Large amounts of data are available (>150,000 feather samples from >500 species)
- Genetic assignment methods are based on Wasser, et al. (2004)
- Isotopic assignment methods are based on Wunder, et al. (2005)

Data - DNA microsatellites and $\delta^2\text{H}$

Hermit Thrush (*Catharus guttatus*)

- 138 individuals
- 14 locations
- 6 loci
- 9-27 alleles / locus



Wilson's Warbler (*Wilsonia pusilla*)

- 163 individuals
- 8 locations
- 9 loci
- 15-31 alleles / locus



Allele Frequency Model

For the allele i , from locus l , at location k

$$\mathbf{y}_{\cdot lk} | \boldsymbol{\Theta} \sim \text{Mult}(\sum_i y_{ilk}, \mathbf{f}_{lk})$$

$$f_{ilk} = \frac{\exp(\Theta_{ilk})}{\sum_i \exp(\Theta_{ilk})}$$

$$\boldsymbol{\Theta}_{il} | \boldsymbol{\alpha}, \boldsymbol{\mu} \sim \mathcal{N}(\boldsymbol{\mu}_{il}, \boldsymbol{\Sigma})$$

$$\{\boldsymbol{\Sigma}\}_{ij} = \alpha_0 \exp\left(-(\{\mathbf{d}\}_{ij}/\alpha_1)^{\alpha_2}\right) + \alpha_3 \mathbb{1}_{i=j}$$

Genetic Assignment Model

Assignment model using Hardy-Weinberg equilibrium allowing for genotyping (δ) and single amplification (γ) errors.

$$P(S_G|\mathbf{f}, k) = \prod_l P(i_l, j_l|\mathbf{f}, k)$$

$$P(i_l, j_l|\mathbf{f}, k) = \begin{cases} \gamma P(i_l|\mathbf{f}, k) + (1 - \gamma)P(i_l|\tilde{\mathbf{f}}, k)^2 & \text{if } i = j \\ (1 - \gamma)P(i_l|\mathbf{f}, k)P(j_l|\mathbf{f}, k) & \text{if } i \neq j \end{cases}$$

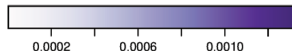
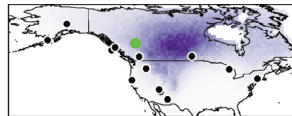
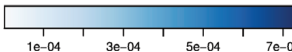
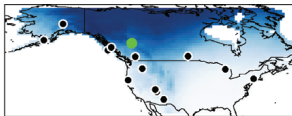
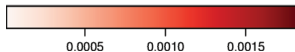
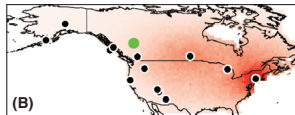
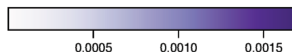
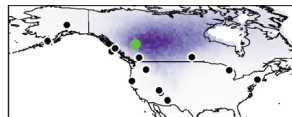
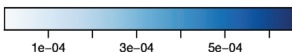
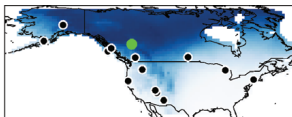
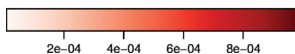
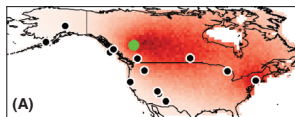
$$P(i_l|\mathbf{f}, k) = (1 - \delta)f_{lik} + \delta/m_l$$

Combined Model

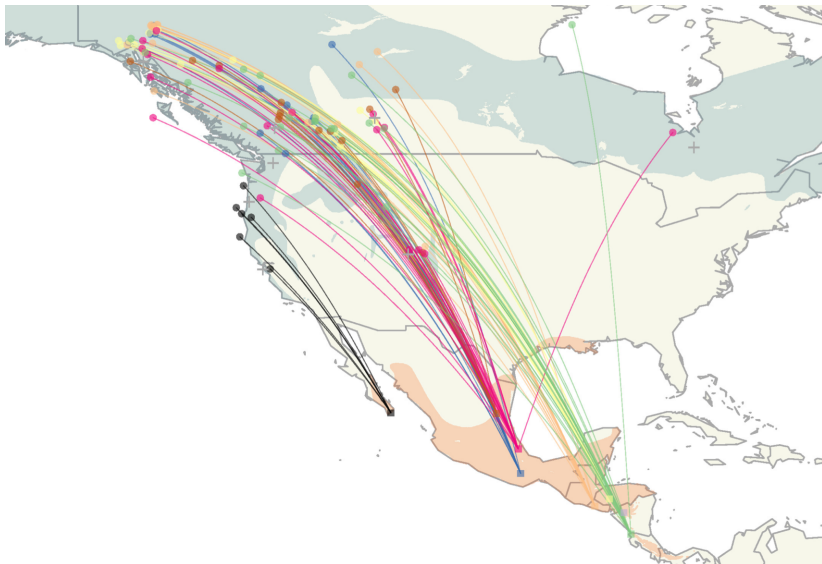
Genetic

Isotopic

Combined



Migratory Connectivity



Implementation

Model fitting is done via MCMC (MH within Gibbs)

- Original implementation in pure C++ with minimal dependencies (Wasser, et al. (2004))
- Rewritten using R / C++ via Rcpp(Armadillo)
 - Code closer to matrix notation (and R)
 - Transparent use of high performance LAPACK implementations
 - R Package - isoscatR - <https://github.com/rundel/isoscatR>
- Model fitting performance is quite good
 - 300,000 iterations in ~ 5.5 minutes
- Bottleneck in drawing posterior predictive samples
 - 1,000 iterations in ~ 30 minutes

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To do so we sample from:

$$\Theta_p | \Theta_m \sim \mathcal{N}(\mu_p + \Sigma_{pm} \Sigma_m^{-1} (\Theta_m - \mu_m), \Sigma_p - \Sigma_{pm} \Sigma_m^{-1} \Sigma_{mp})$$

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Algorithm steps

- 1 Calculate Σ_{pm} , Σ_p , and $\Sigma_p - \Sigma_{pm} \Sigma_m^{-1} \Sigma_{mp}$
- 2 Calculate $\text{Chol}(\Sigma_p - \Sigma_{pm} \Sigma_m^{-1} \Sigma_{mp})$
- 3 Sample from MVN
- 4 Calculate allele frequencies

Posterior predictive sampling timings

Step	CPU (secs)	CPU+GPU (secs)	Rel. Performance
1. Covariances	1.080	0.046	23.0
2. Cholesky	0.467	0.208	2.3
3. Sample	0.049	0.052	0.9
4. Allele Freq	0.129	0.127	1.0
Total	1.732	0.465	3.7

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- × CV runs $\begin{bmatrix} 166 \text{ for Hermit Thrush} \\ 179 \text{ for Wilson's Warbler} \end{bmatrix}$

- Relatively small changes in one function resulted in 3 - 4x improvement
 - Cross validation results in two days instead of a week
 - 1-2 weeks of implementation, 1 week of tweaking / testing
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- Issues
 - External library dependency makes package development (much) more complicated
 - Additional code verbosity and complexity

Improving Covariance Calculations

Covariance is assumed to be stationary and isotropic

- Elements of the covariance matrix can be calculated independently
- Small scale “embarrassingly parallel”
- Implementation is straight forward
(if we don't worry about things like symmetry)

```
__global__ void powered_exponential_cov_kernel(double* dist, double* cov,
                                              const int nm, const double sigma2,
                                              const double phi, const double kappa)
{
    int n_threads = blockDim.x * blockDim.x;
    int pos = blockDim.x * blockIdx.x + threadIdx.x;

    for (int i = pos; i < nm; i += n_threads)
    {
        cov[i] += sigma2 * exp( -pow(dist[i] * phi, kappa) );
    }
}
```

Building core tools

Common set of (expensive) tasks for GP models

- Covariance calculation
- Cholesky of Cov.
- Inverse of Cov.

Goal is to make performing these tasks on a GPU as painless as possible and allow interoperability with GPU (magma, CUBLAS) and CPU (Armadillo) libraries.

- GPU matrix class
- Modern resource management (RAII, move semantics)
- Simple translation between GPU and CPU memory

R Package - RcppGP - <https://github.com/rundel/RcppGP>

CPU vs GPU code

```
arma::mat prop_Sigma = arma::exp(-prop_phi * d_CIF);  
arma::mat prop_Sigma_U = arma::chol(prop_Sigma);  
  
double prop_Sigma_log_det = 2*arma::accu(arma::log(prop_Sigma_U.diag()));  
  
arma::mat prop_Sigma_U_inv = arma::inv(arma::trimatu(prop_Sigma_U));  
arma::mat prop_Sigma_inv = prop_Sigma_U_inv * prop_Sigma_U_inv.t();
```

```
exponential_cov_gpu(d_CIF_gpu.mat, cov_gpu.mat, nr_CIF, nr_CIF, 1.0, prop_phi, 64);  
cov_gpu.chol('L', false);  
  
double prop_Sigma_log_det = 2*arma::accu(arma::log(cov_gpu.get_mat().diag()));  
  
cov_gpu.inv_chol('L', true);  
arma::mat prop_Sigma_inv = cov_gpu.get_mat();
```

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Fine particulate matter ($\text{PM}_{2.5}$) is an EPA regulated air pollutant linked to a variety of adverse health effects

- Classified based on particle size ($< 2.5 \mu\text{m}$ diameter)
- Major species: Sulfate, Nitrate, Ammonium, Soil, Carbon.
- Minor species: trace elements (K, Mg, Ca), heavy metals (Cu, Fe), etc.
- Complex spatio-temporal dependence between species

Speciated PM_{2.5} Sources

- Chemical Speciation Network (CSN) - 221 stations
- Interagency Monitoring of Protected Visual Environments (IMPROVE) - 172 stations

Total PM_{2.5} Sources

- Federal Reference Method (FRM) - 949 stations

Model Output

- Community Multi-scale Air Quality (CMAQ) - 12 km grid

Data Issues

- Monitoring frequency
- Total vs Sum of Species

Species Model Details

For the 5 major species (Sulfate, Nitrate, Ammonium, Soil, Carbon) and the two networks (CSN, IMPROVE):

$$C_t^i(\mathbf{s}) = Z_t^i(\mathbf{s}) + \epsilon_{C,t}^i(\mathbf{s})$$

$$I_t^i(\mathbf{s}) = Z_t^i(\mathbf{s}) + \epsilon_{I,t}^i(\mathbf{s})$$

where $Z_t^i(\mathbf{s})$ are the latent “true” concentrations of species i at time t and locations $\mathbf{s}$, and is given by

$$Z_t^i(\mathbf{s}) = \max \left(0, \tilde{Z}_t^i(\mathbf{s}) \right)$$

$$\tilde{Z}_t^i(\mathbf{s}) = \beta_{0,t}^i + \beta_{0,t}^i(\mathbf{s}) + \beta_{1,t}^i Q_t^i(B_s)$$

Total PM_{2.5} Model Details

For total PM_{2.5} from the three networks (CSN, IMPROVE, FRM):

$$C_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{C,t}^{tot}(\mathbf{s})$$

$$I_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{I,t}^{tot}(\mathbf{s})$$

$$F_t^{tot}(\mathbf{s}) = Z_t^{tot}(\mathbf{s}) + \epsilon_{F,t}^{tot}(\mathbf{s})$$

where $Z_t^{tot}(\mathbf{s})$ are the latent “true” concentration of total PM_{2.5} at time t and locations $\mathbf{s}$, which is given by the sum of the major species and the “other” species concentrations.

$$Z_t^{tot}(\mathbf{s}) = \sum_{i=1}^5 Z_t^i(\mathbf{s}) + Z_t^o(\mathbf{s})$$

$$Z_t^o(\mathbf{s}) = \max \left(0, \tilde{Z}_t^o(\mathbf{s}) \right) \quad \tilde{Z}_t^o(\mathbf{s}) = \beta_{0,t}^o + \beta_{0,t}^o(\mathbf{s}) + \beta_{1,t}^o Q_t^o(B_s)$$

Spatial Dependence

Spatial dependence enters the model through the $\beta_{0,t}^i(\mathbf{s})$ parameters for $i \in \{0, 1, 2, 3, 4, 5\}$.

$$\beta_{0,t}^i(\mathbf{s}) = \sigma_t^i w_t^i(\mathbf{s})$$

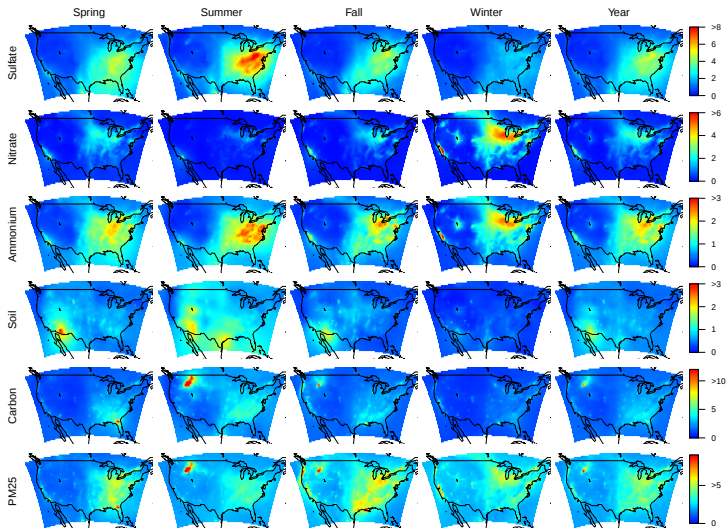
where $w_t^i(\mathbf{s})$ are zero mean, variance 1, Gaussian processes with exponential correlation given by

$$\text{corr}(w_t^i(\mathbf{s}), w_t^i(\mathbf{s}')) = \exp(-\phi_t^i |\mathbf{s} - \mathbf{s}'|)$$

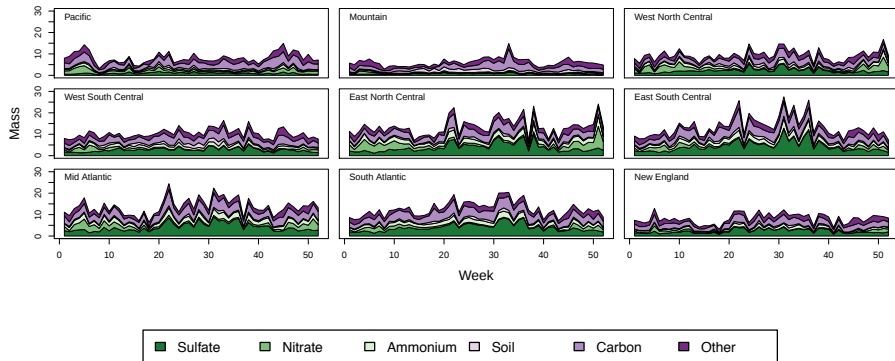
Additional dependence between species is introduced via coregionalization,

$$\begin{pmatrix} \beta_{0,t}^i(\mathbf{s}) \\ \beta_{0,t}^j(\mathbf{s}) \end{pmatrix} = \mathbf{A}_t \begin{pmatrix} w_t^i(\mathbf{s}) \\ w_t^j(\mathbf{s}) \end{pmatrix}.$$

Model results



Model results



MCMC performance

Parameter	CPU (secs)	CPU+GPU (secs)	Rel. Performance
β_0, β_1	0.00029	0.00030	0.97
$\beta_0(s)$	0.09205	0.09132	1.00
σ^2	0.00383	0.00385	0.99
ϕ	0.46084	0.25174	1.83
τ_i^2, τ_{tot}^2	0.00003	0.00003	1.00
Total	0.55708	0.34729	1.60

Run times

Total run time for model fitting (50,000 iterations):

- CPU - 7.7 hours
 - CPU+GPU - 4.8 hours
- × 52 weeks

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$\times 3$ model variants
 $\times 10$ for cross validation

- Established infrastructure makes a huge difference in development time
 - 1 hour to go from CPU implementation to CPU+GPU implementation
 - Code shown previously is 2/3 of the changes necessary [Code](#)
- In practice, was easier to run CPU only code across more servers (configuration time / effort)
 - Not possible (or at least easy) for models variants that are not independent in time.
 - There will be ~ 20 desktops with GPUs available in the department (available via Condor)
- Rcpp Attributes offer huge advantages in development and deployment
 - Simplifies external dependencies (locally)
 - Full compatibility is the goal for RcppGP

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Low rank approximations

For a Gaussian process

$$Y(\mathbf{s}) = \mathbf{x}(\mathbf{s})' \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon, \quad \epsilon \sim N(0, \tau^2 I)$$

$$w(\mathbf{s}) \sim N(0, \mathbf{C}(\mathbf{s})), \quad \mathbf{C}(\mathbf{s}, \mathbf{s}') = \sigma \rho(\mathbf{s}, \mathbf{s}' | \theta)$$

we can approximate $\mathbf{C}(\mathbf{s})$ with a low rank approximation with the form $\mathbf{U} \mathbf{S} \mathbf{V}'$ where $\mathbf{U}$ and $\mathbf{V}$ are $n \times k$ and $\mathbf{S}$ is $k \times k$.

Low rank approximations

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This allows for the use of the Sherman-Morrison-Woodbury formula for the inverse (and determinant),

$$\mathbf{C}(\mathbf{s})^{-1} \approx (\mathbf{A} + \mathbf{U} \mathbf{S} \mathbf{V}')^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1} \mathbf{U} (\mathbf{S}^{-1} + \mathbf{V}' \mathbf{A}^{-1} \mathbf{U})^{-1} \mathbf{V}' \mathbf{A}^{-1}.$$

Gaussian Predictive Processes

For a rank k approximation,

- Pick k knot locations $\mathbf{s}^*$
- Calculate knot covariance ($\mathbf{C}(\mathbf{s}^*)$) and knot cross-covariance ($\mathbf{C}(\mathbf{s}^*)^{-1}$)
- Approximate full covariance

$$\mathbf{C}(\mathbf{s}) \approx \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s}).$$

- Systematically underestimates variance, inflates τ^2 .
- Modified predictive process corrects this using

$$\mathbf{C}(\mathbf{s}) \approx \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s}) + \text{diag}\left(\mathbf{C}(\mathbf{s}) - \mathbf{C}(\mathbf{s}, \mathbf{s}^*) \mathbf{C}(\mathbf{s}^*)^{-1} \mathbf{C}(\mathbf{s}^*, \mathbf{s})\right).$$

Banerjee, Gelfand, Finley, Sang (2008) Finley, Sang, Banerjee, Gelfand (2008)

Low Rank Approximations via Random Projections

- 1 Starting with an $m \times n$ matrix $\mathbf{A}$.
- 2 Draw an $n \times k + p$ Gaussian random matrix $\mathbf{\Omega}$.
- 3 Form $\mathbf{Y} = \mathbf{A}\mathbf{\Omega}$ and compute its QR factorization $\mathbf{Y} = \mathbf{Q}\mathbf{R}$.
- 4 Form the $k + p \times n$ matrix $\mathbf{B} = \mathbf{Q}'\mathbf{A}$.
- 5 Compute the SVD of the small matrix $\mathbf{B}$, $\mathbf{B} = \hat{\mathbf{U}}\mathbf{S}\mathbf{V}'$.
- 6 Form the matrix $\mathbf{U} = \mathbf{Q}\hat{\mathbf{U}}$.

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Resulting approximation has nicely bounded expected error,

$$\mathbb{E} \|\mathbf{A} - \mathbf{USV}'\| \leq \left[1 + \frac{4\sqrt{k+p}}{p-1} \sqrt{\min(m, n)} \right] \sigma_{k+1}.$$

Halko, Martinsson, Tropp (2011)

Random Matrix Low Rank Decompositions and GPs

Preceding algorithm can be modified slightly to take advantage of the positive definite structure of a covariance matrix.

- 1 Starting with an $n \times n$ covariance matrix $\mathbf{A}$.
- 2 Draw an $n \times k + p$ Gaussian random matrix $\mathbf{\Omega}$.
- 3 Form $\mathbf{Y} = \mathbf{A}\mathbf{\Omega}$ and compute its QR factorization $\mathbf{Y} = \mathbf{Q}\mathbf{R}$
- 4 Form the $k + p \times k + p$ matrix $\mathbf{B} = \mathbf{Q}'\mathbf{A}\mathbf{Q}$.
- 5 Compute the eigen decomposition of the small matrix $\mathbf{B}$,
 $\mathbf{B} = \hat{\mathbf{U}}\mathbf{S}\hat{\mathbf{U}}'$.
- 6 Form the matrix $\mathbf{U} = \mathbf{Q}\hat{\mathbf{U}}$.

Once again we have a bound on the error,

$$\mathbb{E} \|\mathbf{A} - \mathbf{Q}(\mathbf{Q}'\mathbf{A}\mathbf{Q})\mathbf{Q}'\| = \mathbb{E} \|\mathbf{A} - \mathbf{U}\mathbf{S}\mathbf{U}'\| \lesssim c \cdot \sigma_{k+1}.$$

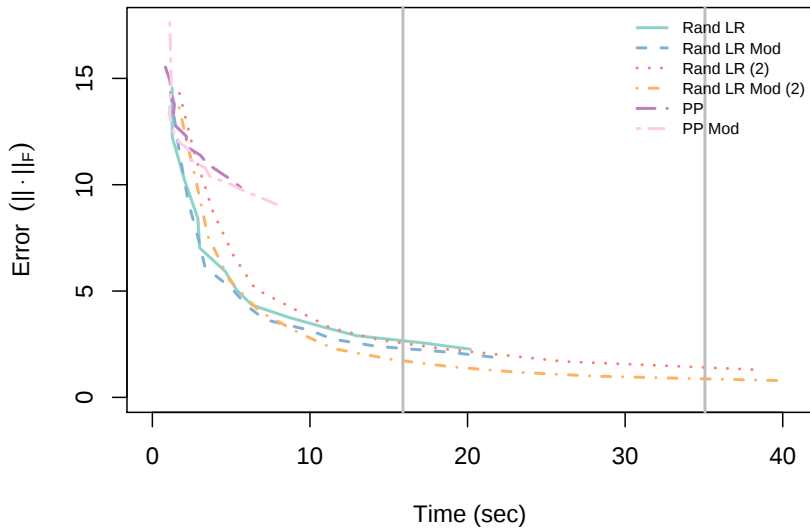
Halko, Martinsson, Tropp (2011), Banerjee, Dunson, Tokdar (2012)

Low Rank Approximations and GPUs

Both predictive process and random matrix low rank approximations are good candidates for acceleration using GPUs.

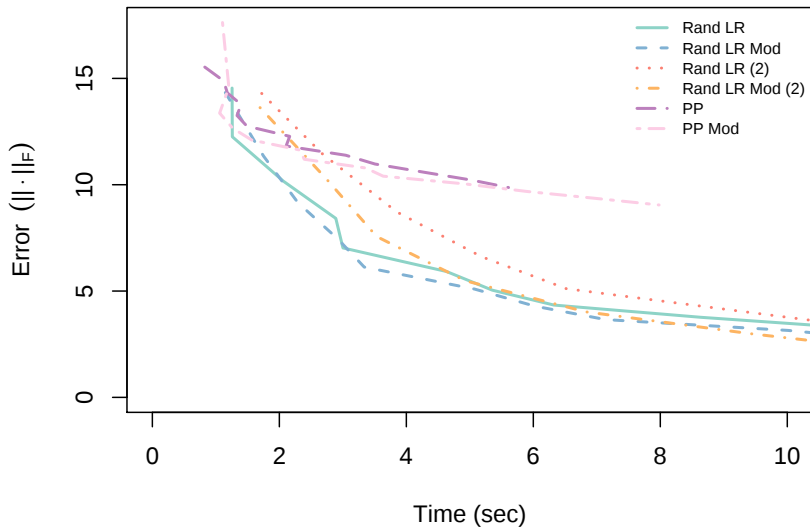
- Both use Sherman-Woodbury-Morrison to calculate the inverse (involves matrix multiplication, addition, and a small matrix inverse).
- Predictive processes involves several covariance matrix calculations (knots and cross-covariance) and a small matrix inverse.
- Random matrix low rank involves a large matrix multiplication ($\mathbf{A}\mathbf{\Omega}$) and several small matrix decompositions (QR, eigen).
- Functionality for both approaches included in current version of RcppGP (inv_lr and inv_pp).

Matrix inverse (fixed rank, strong dependence)



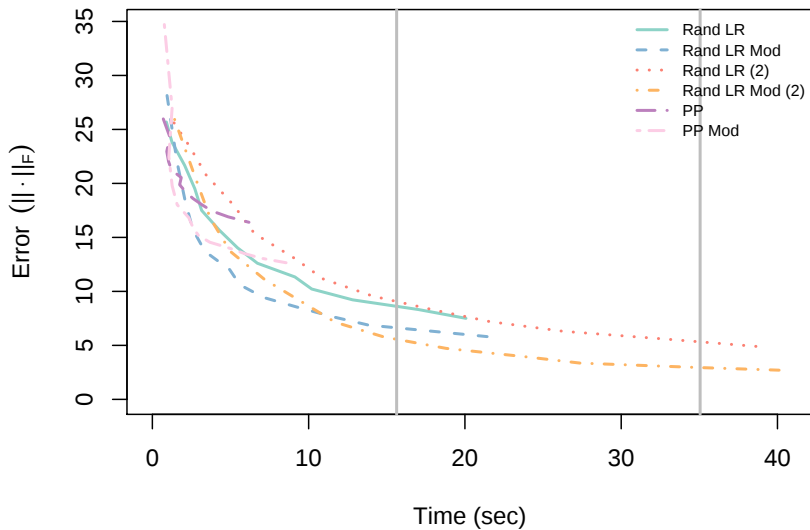
$n = 15000, \quad k = \{100, \dots, 4900\}$

Matrix inverse (fixed rank, strong dependence)



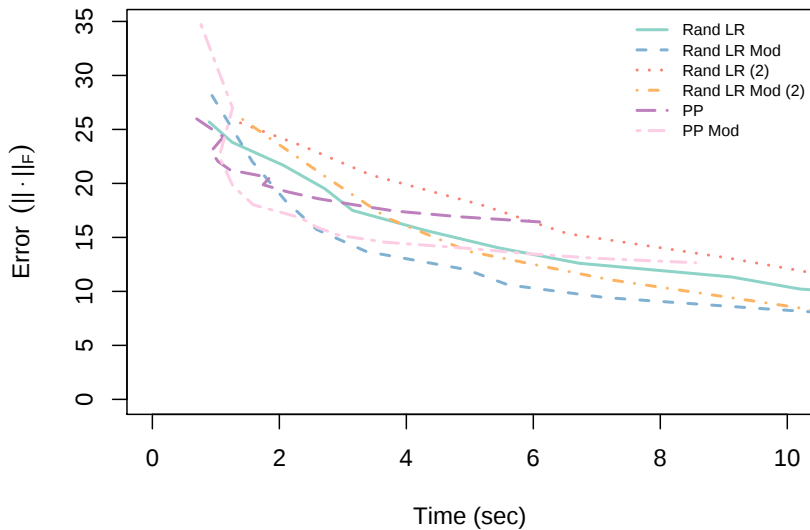
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Matrix inverse (fixed rank, weak dependence)



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Matrix inverse (fixed rank, weak dependence)



$n = 15000, \quad k = \{100, \dots, 4900\}$

Rand. Matrix Low Rank Decompositions for Prediction

This approach can also be used for prediction, if we want to sample

$$\mathcal{N}(0, \Sigma) \text{ with } \Sigma \approx \mathbf{U}\mathbf{S}\mathbf{U}' = (\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}')(\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}')'$$

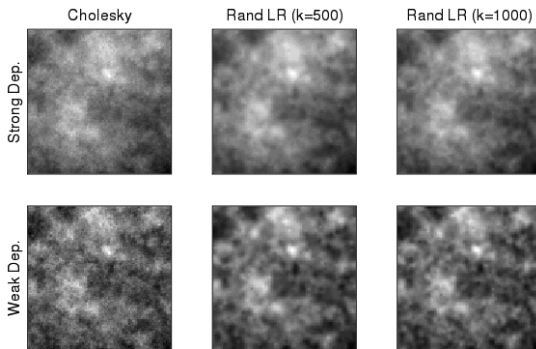
then $X_{pred} = (\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}') \times \mathbf{Z}$ where $Z_i \sim \mathcal{N}(0, 1)$.

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$$n = 1000, \quad p = 10000$$

Dehdari, Deutsch (2012)

- Refinement of RcppGP
 - Transition to header only implementation
 - Transparent GPU to CPU failover
 - Support for fixed error (instead of rank) random matrix low rank decomposition
 - Thinking about out-of-memory based approaches
- Future of GPUs, CUDA, and Magma
 - Single vs. Multi-GPU algorithms
 - Mixed precision algorithms
 - NVBLAS
 - Unified memory
 - cuSolver

Acknowledgments

Migratory Connectivity

- John Novembre - UChicago
- Thomas Smith - UCLA
- Kristen Ruegg - UCLA, UCSC
- Center for Tropical Research,
UCLA IoES

Speciated PM_{2.5}

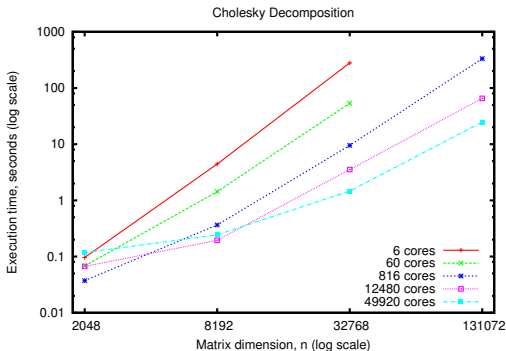
- Alan Gelfand - Duke
- Dave Holland - EPA
- Erin Schliep - Duke

RcppGP <https://github.com/rundel/RcppGP>
Talk <https://github.com/rundel/Presentations>

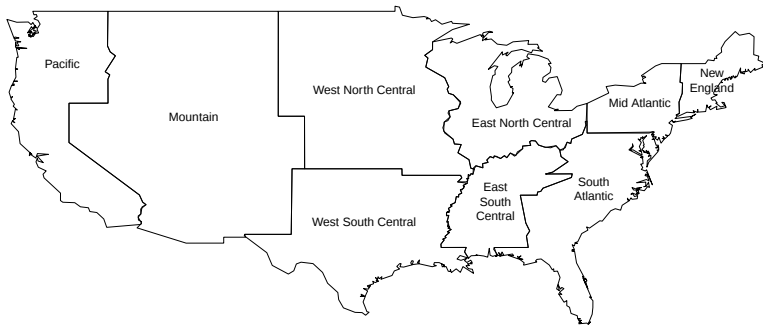
Another Approach

bigGP is an R package written by Chris Paciorek, et al.

- Specialized implementation of LA operation for GPs
- Designed to run on large super computer clusters
- Uses both shared and distributed memory
- Able to fit models on the order of $n = 65k$ (32 GB Cov. matrix)



Regions



[Back](#)