Leveraging GPU Libraries for Efficient Computation of Bayesian Spatial Assignment Models in R

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August 1, 2012

Project Background

Developing methods to make use of 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)

Preliminary Data (microsats and $\delta^2\mathrm{H}$):

- Hermit Thrush (*Catharus guttatus*) - 138 Individuals, 14 Locations, 6 Loci, 9-27 Alleles
- Wilson's Warbler (*Wilsonia pusilla*) - 163 Individuals, 8 Locations, 9 Loci, 15-31 Alleles

Allele Frequency Model

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

$$\boldsymbol{y_{l\cdot k}} \sim \mathsf{MN}\left(n_{lk} = \textstyle\sum_i y_{lik}, \boldsymbol{f_{l\cdot k}}\right)$$

$$f_{lik} = \frac{\exp(X_{lik})}{\sum_i \exp(X_{lik})} \qquad \boldsymbol{X}_{li} \sim \mathcal{N}(\boldsymbol{M}_{li}, \boldsymbol{\Sigma})$$

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Likelihood:

$$\begin{aligned} &\prod_l \prod_k \frac{n_{lk}!}{\prod_i y_{lik}!} \textstyle\prod_i (f_{lik})^{y_{lik}} \\ \times &\prod_l \prod_i 2\pi^{-r/2} |\boldsymbol{\Sigma}|^{-1/2} \exp\left[-\frac{1}{2}(\boldsymbol{X_{li}} - \boldsymbol{M}_{li})' \boldsymbol{\Sigma}^{-1} (\boldsymbol{X_{li}} - \boldsymbol{M}_{li})\right] \\ \times &\ \pi(\boldsymbol{\theta}) \end{aligned}$$

Implementation

Model fitting and prediction is done via MCMC

- Original implementation in pure C++ with minimal dependencies
- Rewritten using R / C++ via Rcpp(Armadillo)
  - Code closer to matrix notation (and R)
  - Transparent use of high performance LAPACK implementations (ATLAS, OpenBLAS, Intel MKL)
- GPU based optimizations were added using CUDA, CUBLAS, and MAGMA libraries
- Cross platform R package scatR (hopefully added to CRAN soon)

Performance

System specs - 4 core Intel i5-2500K, GeForce GTX 460

Software specs - Ubuntu 12.04, ATLAS 3.8.4, Cuda 4.2, Magma 1.1

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(predictions calculated every 100 iterations)

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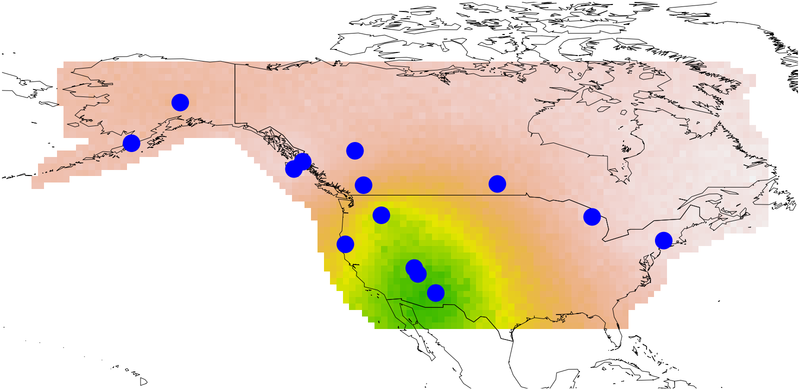
Not too bad in the greater scheme of things, but we would really like to be able to do cross validation (~ 200 runs per species) ...

Prediction Example



Prediction algorithm details

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To do so we need to draw samples from:

$$\boldsymbol{X_p}|\boldsymbol{X_m} \sim \mathcal{N}(\boldsymbol{\mu_p} + \boldsymbol{\Sigma}_{pm}\boldsymbol{\Sigma}_m^{-1}(\boldsymbol{X_m} - \boldsymbol{\mu}_m),\ \boldsymbol{\Sigma}_p - \boldsymbol{\Sigma}_{pm}\boldsymbol{\Sigma}_m^{-1}\boldsymbol{\Sigma}_{mp})$$

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Algorithm steps

1. Calculate $\boldsymbol{\Sigma}_{pm}$ and $\boldsymbol{\Sigma}_p$
2. Calculate $\boldsymbol{\Sigma}_{pm}\boldsymbol{\Sigma}_m^{-1}$
3. Calculate Chol$(\boldsymbol{\Sigma}_p - \boldsymbol{\Sigma}_{pm}\boldsymbol{\Sigma}_m^{-1}\boldsymbol{\Sigma}_{mp})$
4. Sample from MVN
5. Calculate allele frequencies
6. Output results

Prediction algorithm timings

	Step	CPU Timing (secs)
1.	Covariances	1.02
2.	$\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}$	0
3.	Cholesky	1.15
4.	Sample from MVN	0.23
5.	Allele Freq	0.14
6.	Output	0
	Total	2.54

Prediction algorithm timings

	Step	CPU Timing (secs)	CPU+GPU (secs)
1.	Covariances	1.02	0.05
2.	$\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}$	0	0
3.	Cholesky	1.15	0.23
4.	GP Sample	0.23	0.06
5.	Allele Freq	0.14	0.14
6.	Write	0	0
	Total	2.54	0.48

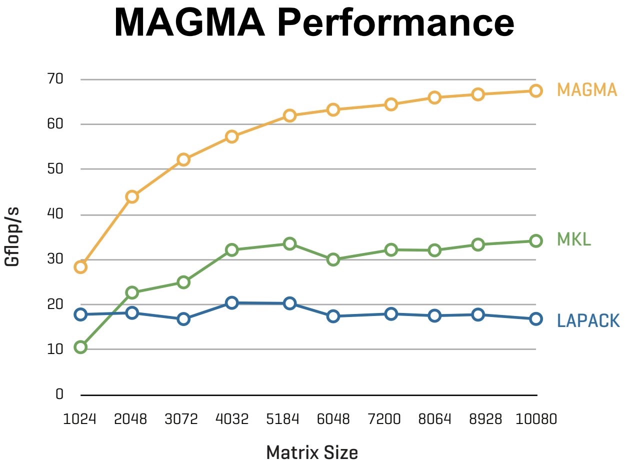
Improving the Cholesky step

Not surprising given Cholesky factorization is $\mathcal{O}(n^3)$ and $n = 3318$.

There isn't a magical solution to this, so we just want to use the fastest possible implementation of the Cholesky decomposition.

- **Intel MKL / OpenBLAS / Eigen** - all (multicore) CPU based with very marginal improvement
- **CUBLAS** - part of NVidia's CUDA toolkit, implements core BLAS functions (but not cholesky)
- **CULA** - proprietary / closed source (dense and sparse) GPU linear algebra library with an expensive license
- **MAGMA** - open source Multicore+GPU dense linear algebra library (CUDA and OpenCL implementations)

Cholesky GPU



Ltaief, H. "A Scalable High Performant Cholesky Factorization for Multicore with GPU Accelerators"

VECTAR'10 Presentation, Berkeley, CA, June 22-25, 2010.

Additional Considerations

- There are costs for moving data on to and off of the GPU
- Once the data is there, may as well do as many calculations as possible
  - Drawing sample from the GP is sped up by performing the matrix multiplication on the GPU
- GPU code is much more verbose / dense

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Armadillo

```
arma::mat tmp = cov12.t() * p.Sinv
```

GPU (CUBLAS)

```
cublasDgemm_v2(
    p.handle, CUBLAS_OP_T, CUBLAS_OP_N,
    n_pred, n_known, n_known,
   &one,
    p.d_cov12, n_known,
    p.d_invcov11, n_known,
   &zero,
    p.d_tmp, n_pred
)
```

Improving Covariance calculations

Covariance in our model is assumed to be stationary and isotropic (depend only on distance between locations)

- Elements of the covariance matrix can be calculated independently
- Small scale “embarrassingly parallel” ⇒ good candidate for the GPU.
- Implementation is straight forward

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```
__global__ void powered_exponential_kernel(double* dist, double* cov,
                                           const int n, const int nm,
                                           const double sigma2, const double phi,
                                           const double kappa, const double nugget)
{
    int n_threads = gridDim.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)) + nugget*(i%n == i/n);
}
```

Summary

Relatively small changes in one function resulted in ~ 5x improvement

- Cross validation results in days and not weeks
- Started with trying to find an improved Cholesky decomposition, other optimizations followed
- GPU implementation was relatively painless
- Libraries are under active development (read: things can and will break)
- External libraries make package development non-trivial

Questions, Comments?

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presentation	:	*http://github.com/rundel/Presentations/*