Gaussian processes and modeling

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Background

Migratory Bird Spatial Assignment Model

Speciated $PM_{2.5}$ Modeling

Computing and GPs

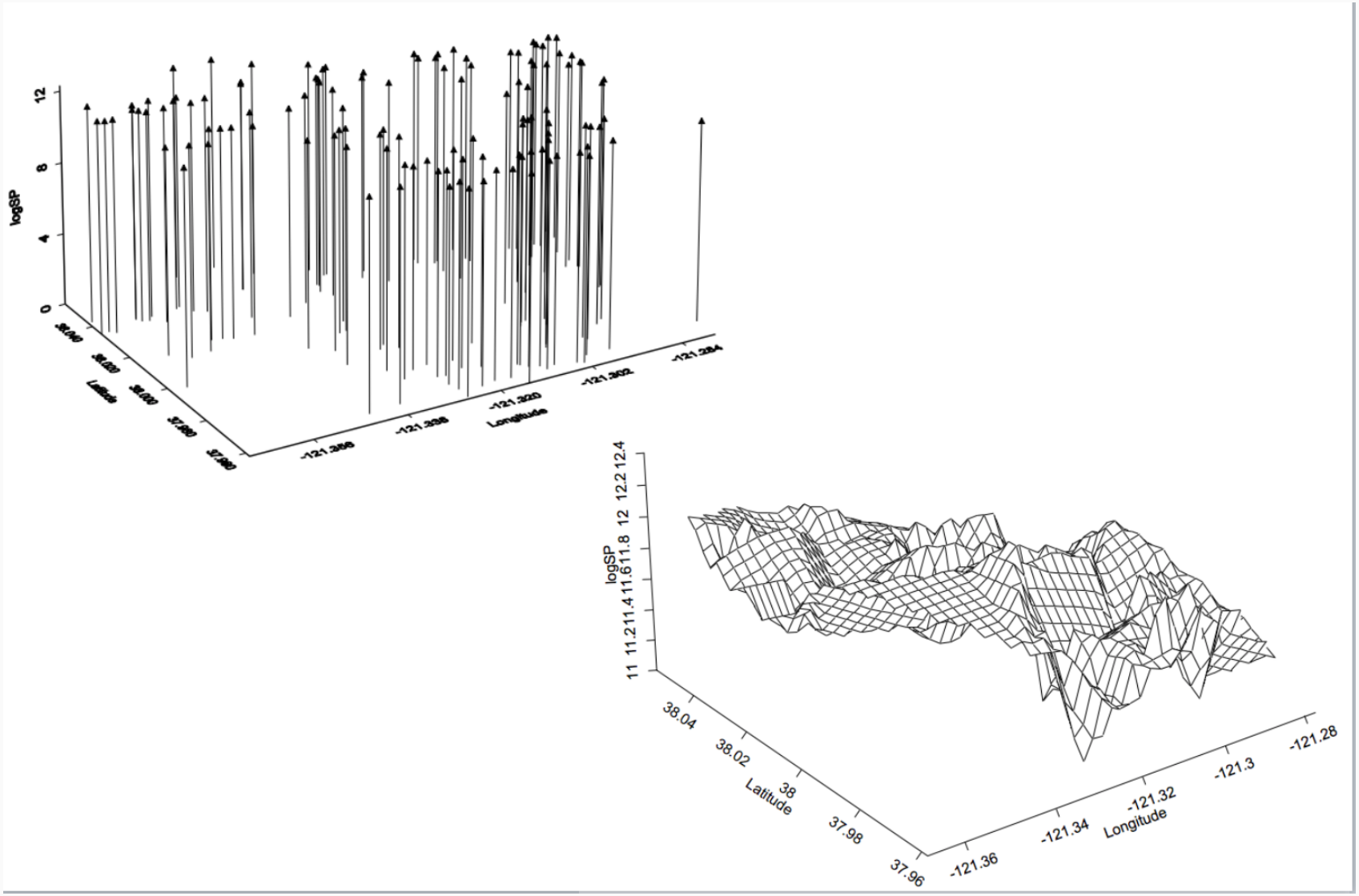
What is a Gaussian Process

A statistical distribution that describes observations that arise from a continuous domain (e.g. space, time, or both), whereby any subset of points within that domain have a multivariate normal distribution.

$$\underset{n\times 1}{X} \sim \mathcal{N}(\underset{n\times 1}{\mu}, \underset{n\times n}{\Sigma})$$

In general, we can think about the Gaussian process as a way of representing an infinite dimensional object (e.g. a smooth continuous surface over a region of space) that we observe at set of finite locations.

Gaussian Process as a Surface



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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 $\delta^2\mathrm{H}$

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

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

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

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

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

Genetic Assignment Model

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

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

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

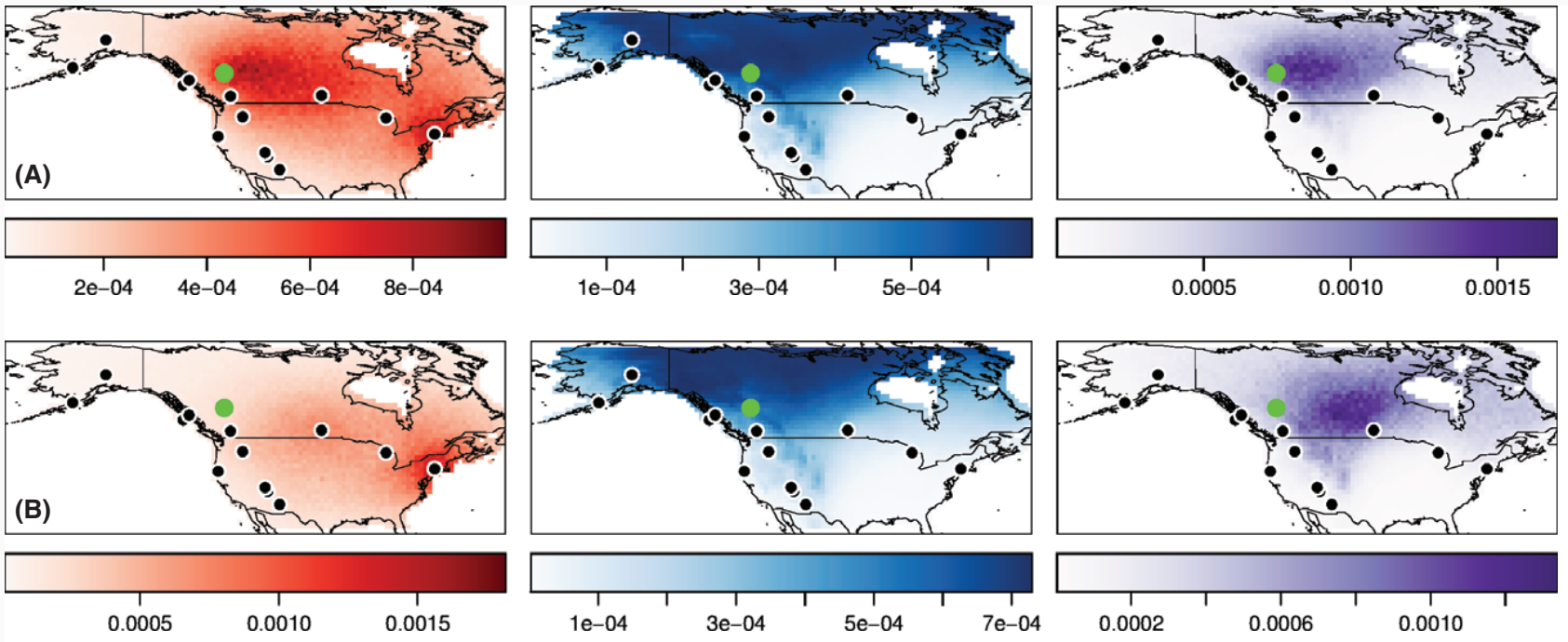
$$P(i_l|\boldsymbol{f}, k) = (1-\delta)f_{lik} + \delta/m_l$$

Combined Model

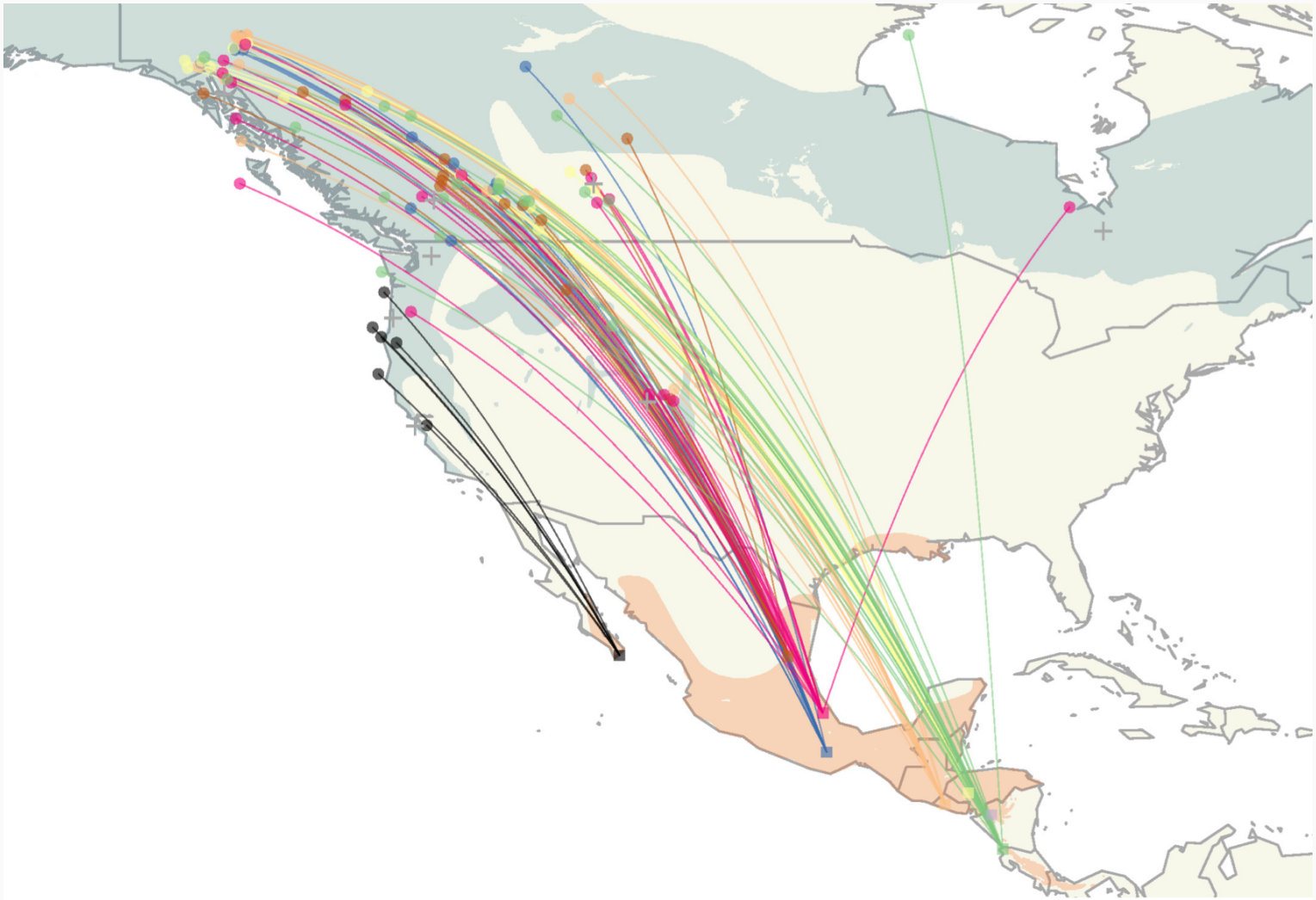
Genetic

Isotopic

Combined



Migratory Connectivity



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

- Classified based on particle size (< 2.5 μm 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

Data

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):

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

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

$$Z_t^i(\boldsymbol{s}) = \max\left(0,\ \widetilde{Z}_t^i(\boldsymbol{s})\right)$$
$$\widetilde{Z}_t^i(\boldsymbol{s}) = \beta_{0,t}^i + \beta_{0,t}^i(\boldsymbol{s}) + \beta_{1,t}^i\, Q_t^i(B_{\boldsymbol{s}})$$

Total $PM_{2.5}$ Model Details

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

$$C_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{C,t}^{tot}(\boldsymbol{s})$$
$$I_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{I,t}^{tot}(\boldsymbol{s})$$
$$F_t^{tot}(\boldsymbol{s}) = Z_t^{tot}(\boldsymbol{s}) + \epsilon_{F,t}^{tot}(\boldsymbol{s})$$

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

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

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

Spatial Dependence

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

$$\beta^i_{0,t}(\boldsymbol{s}) = \sigma^i_t \, w^i_t(\boldsymbol{s})$$

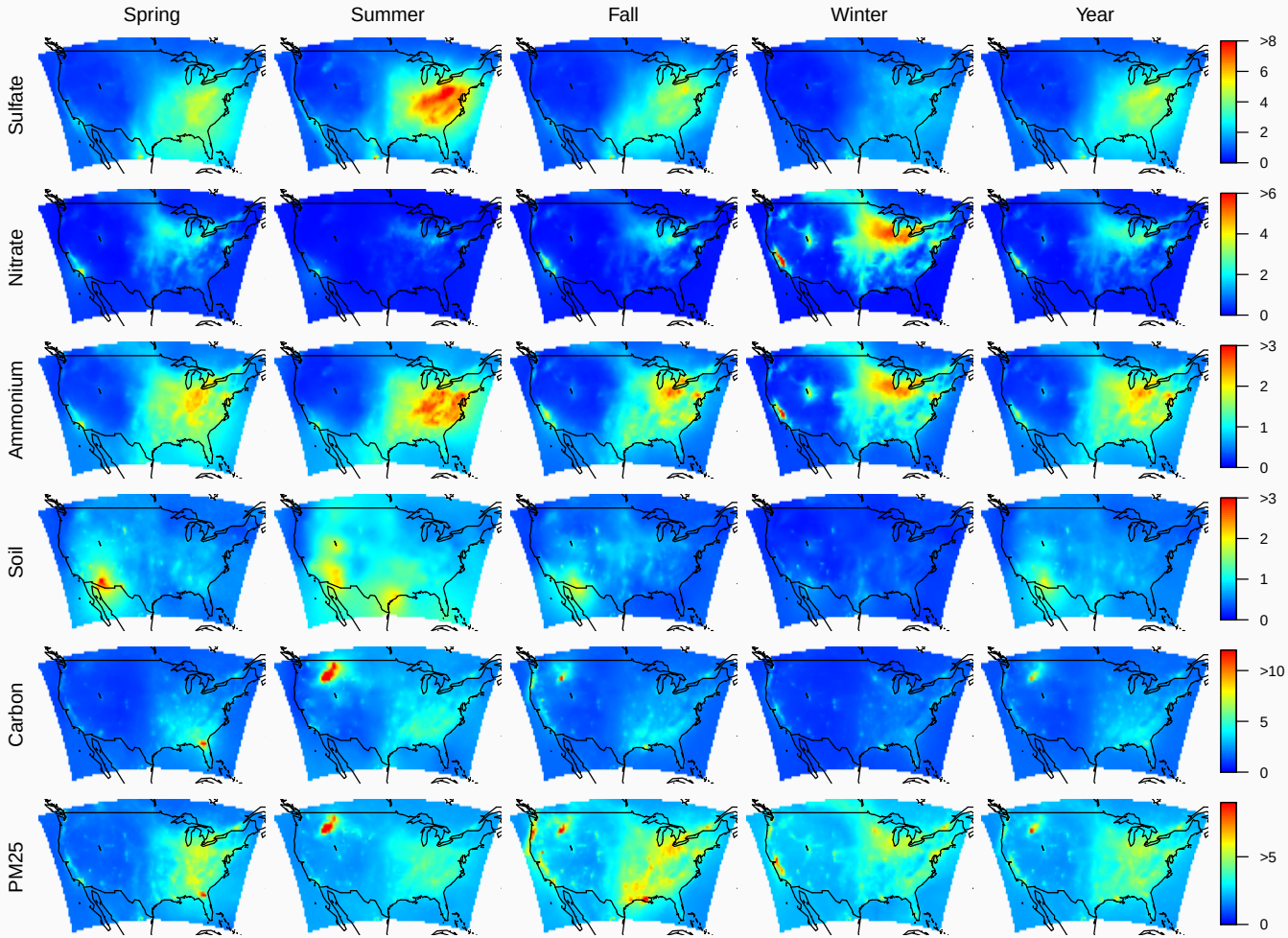
where $w^i_t(\boldsymbol{s})$ are zero mean, variance 1, Gaussian processes with exponential correlation given by

$$\text{corr}(w^i_t(\boldsymbol{s}), w^i_t(\boldsymbol{s}')) = \exp(-\phi^i_t |\boldsymbol{s} - \boldsymbol{s}'|)$$

Additional dependence between species is introduces via coregionalization,

$$\begin{pmatrix} \beta^i_{0,t}(\boldsymbol{s}) \\ \beta^j_{0,t}(\boldsymbol{s}) \end{pmatrix} = \boldsymbol{A}_t \begin{pmatrix} w^i_t(\boldsymbol{s}) \\ w^j_t(\boldsymbol{s}) \end{pmatrix}.$$

Model results



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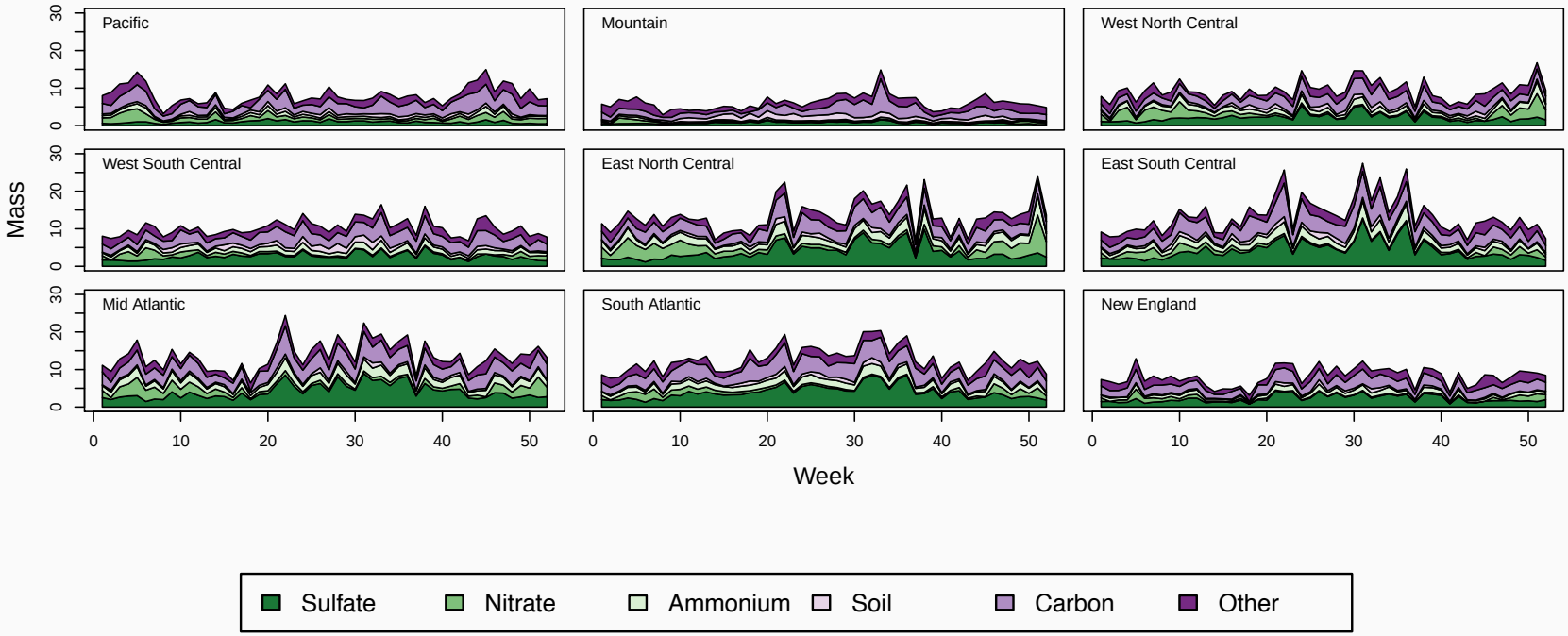

Lessons

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 are $\sim$ 20 desktops with GPUs available in the department (available via Condor)

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The problem with GPs ...

Gaussian process models are difficult to scale to large problems:

Evaluate the (log) likelihood?

$$-\frac{1}{2}\log|\Sigma| - \frac{1}{2}(x-\mu)'\Sigma^{-1}(x-\mu) - \frac{n}{2}\log 2\pi \quad \mathcal{O}\left(n^3\right)$$

Want a sample?

$$\mu + \text{Chol}(\Sigma) \times Z \text{ with } Z_i \sim \mathcal{N}(0,1) \quad \mathcal{O}\left(n^3\right)$$

Update covariance parameter?

$$\{\Sigma\}_{ij} = \sigma^2 \exp(-\{d\}_{ij}\phi) \quad \mathcal{O}\left(n^2\right)$$

Linear complexity?

Linear complexity? - Go for it

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Quadratic complexity?

Linear complexity? - Go for it

Quadratic complexity? - Pray

A simple guide to computational complexity

Linear complexity? - Go for it

Quadratic complexity? - Pray

Cubic complexity?

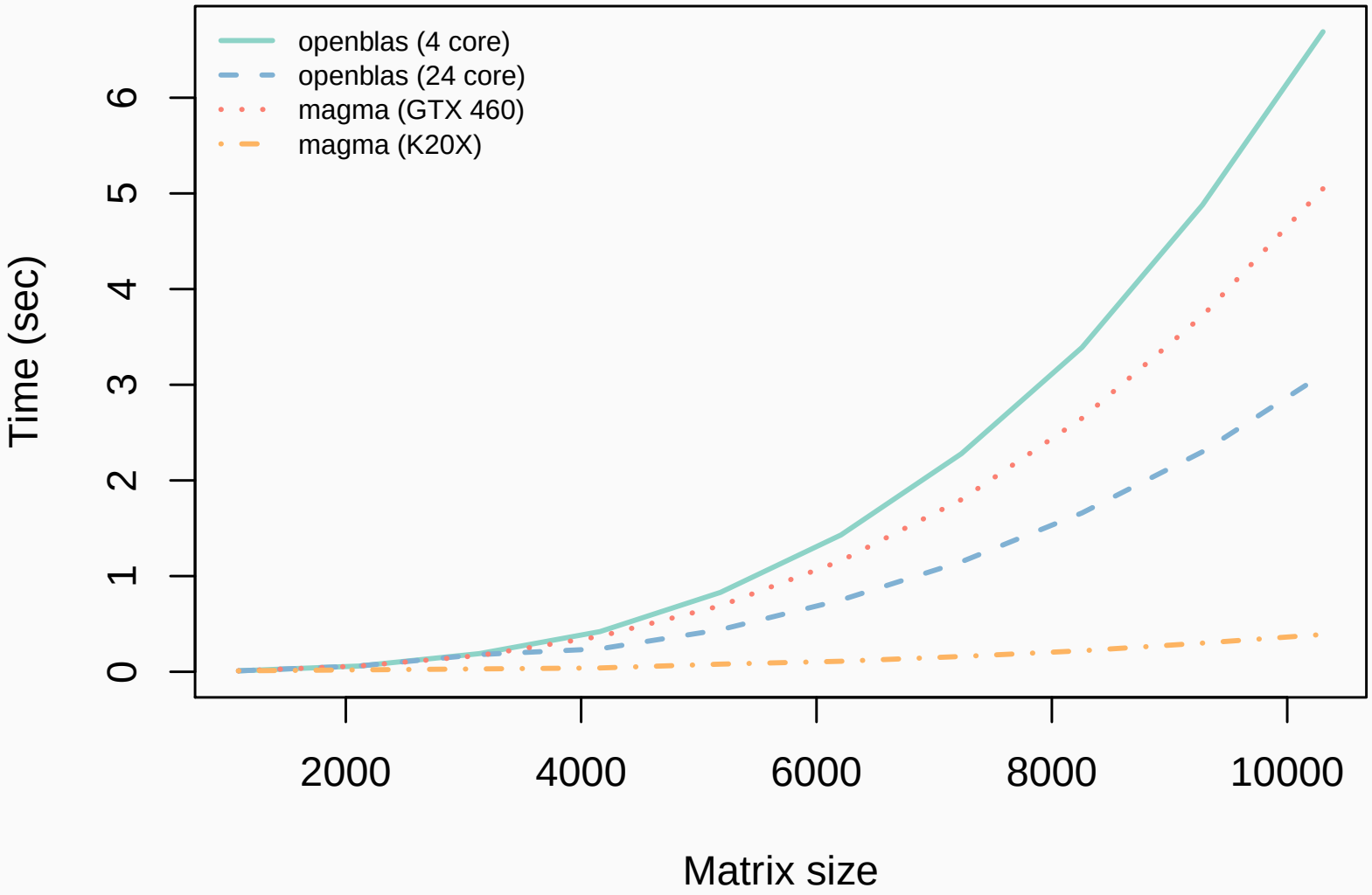
A simple guide to computational complexity

Linear complexity? - Go for it

Quadratic complexity? - Pray

Cubic complexity? - Give up

Improving Cholesky



PM Model run times

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

- CPU - 7.7 hours
- CPU+GPU - 4.8 hours

$\times$ 52 weeks

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$\times$ 3 model variants

$\times$ 10 for cross validation

Low rank approximations

For a Gaussian process

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

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

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

We can the use of the Sherman-Morrison-Woodbury formula for the inverse (and determinant),

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

Gaussian Predictive Processes

For a rank k approximation,

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

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

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

$$C(\boldsymbol{s}) \approx C(\boldsymbol{s}, \boldsymbol{s}^*)\, C(\boldsymbol{s}^*)^{-1}\, C(\boldsymbol{s}^*, \boldsymbol{s}) + \text{diag}\Big(C(\boldsymbol{s}) - C(\boldsymbol{s}, \boldsymbol{s}^*)\, C(\boldsymbol{s}^*)^{-1}\, C(\boldsymbol{s}^*, \boldsymbol{s})\Big).$$

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

Low Rank Approximations via Random Projections

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

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Resulting approximation has nicely bounded expected error,

$$\mathrm{E}\ \|\boldsymbol{A} - \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}'\| \leq \left[1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{\min(m,n)}\right]\sigma_{k+1}.$$

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

Once again we have a bound on the error,

$$\mathrm{E}\,\|\boldsymbol{A} - \boldsymbol{Q}(\boldsymbol{Q}'\boldsymbol{A}\boldsymbol{Q})\boldsymbol{Q}'\| = \mathrm{E}\,\|\boldsymbol{A} - \boldsymbol{U}\boldsymbol{S}\boldsymbol{U}'\| \lessapprox c \cdot \sigma_{k+1}.$$

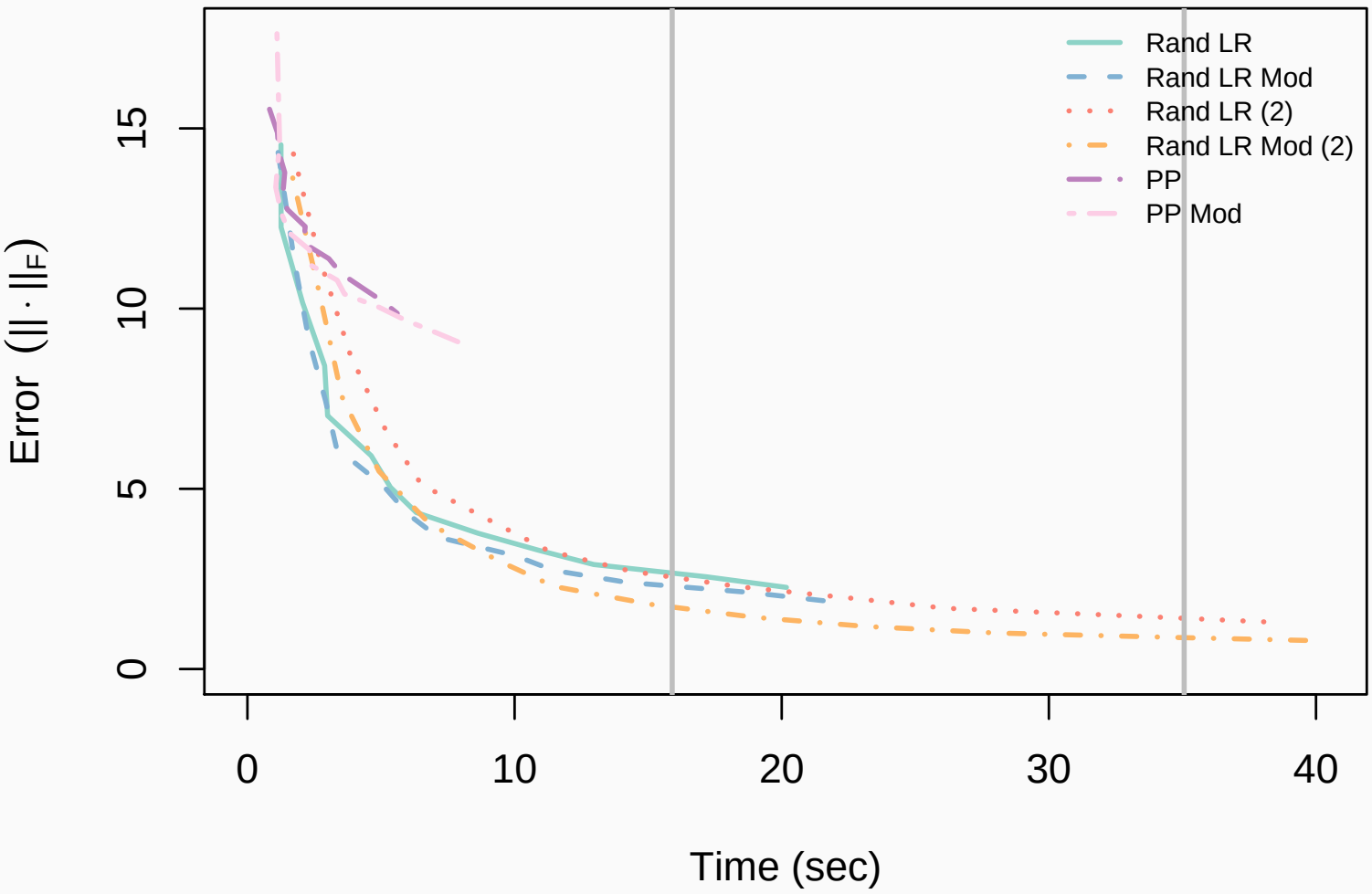
Halko, Martinsson, Tropp (2011), Banerjee, Dunson, Tokdar (2012)

Low Rank Approximations and GPUs

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

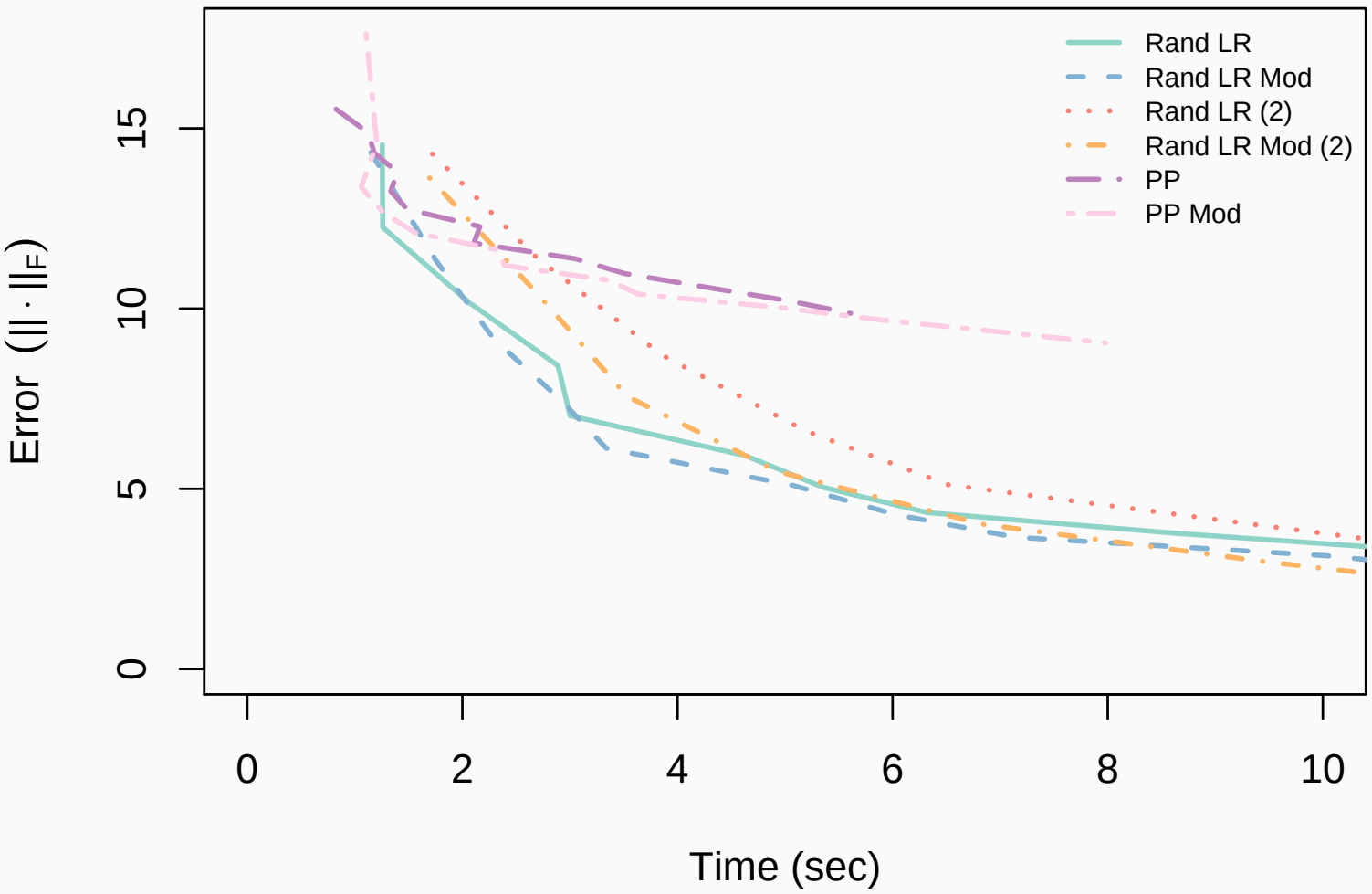
- Both use Sherman-Woodbury-Morrison to calculate the inverse (involves matrix multiplication, addition, and a small Matrix inverse).
- Predictive processes involves several covariance matrix calculations (knots and cross-covariance) and a small matrix inverse.
- Random matrix low rank involves a large matrix multiplication ($\boldsymbol{A\Omega}$) 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)



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

Matrix inverse (fixed rank, strong dependence)



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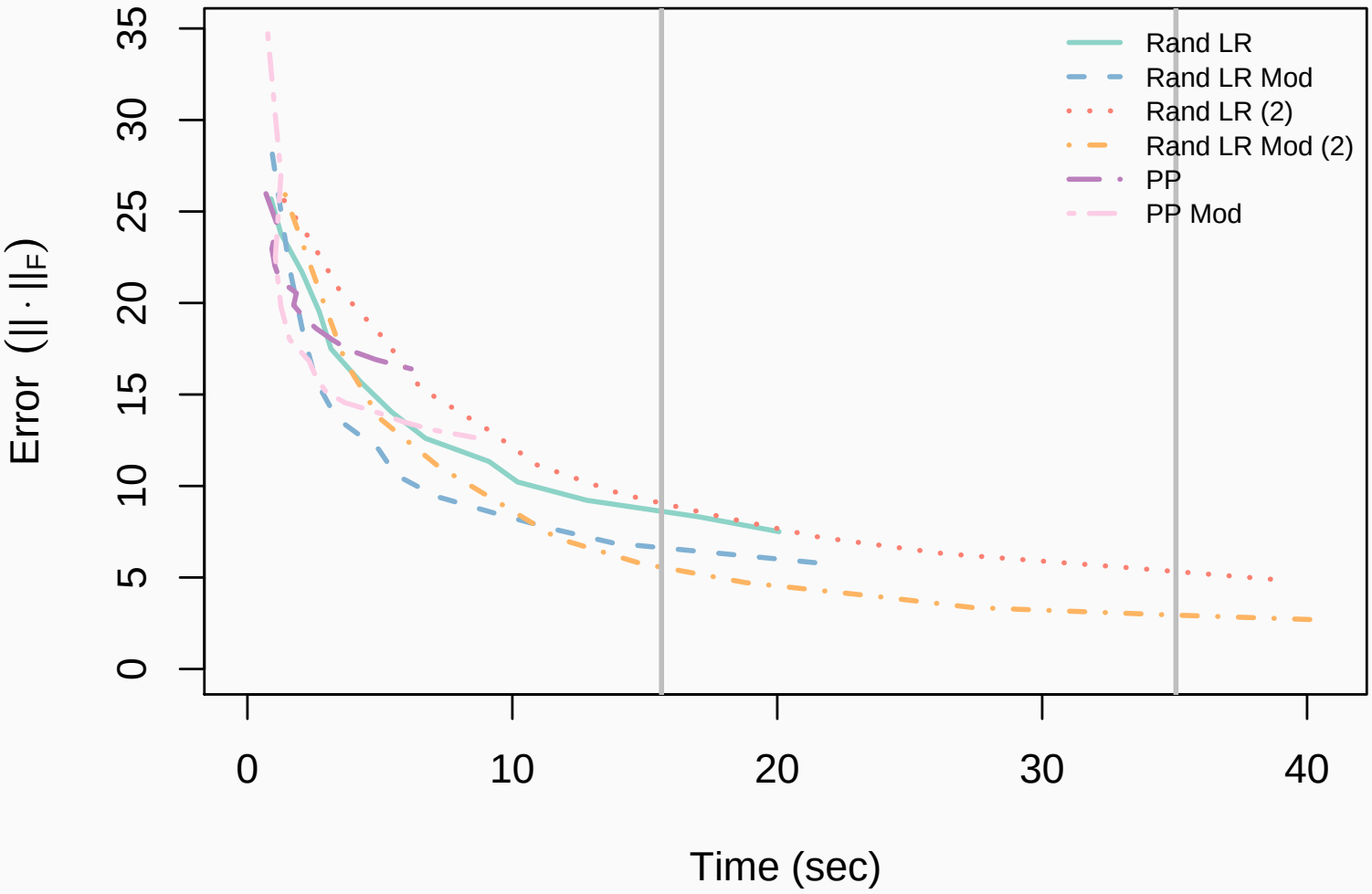

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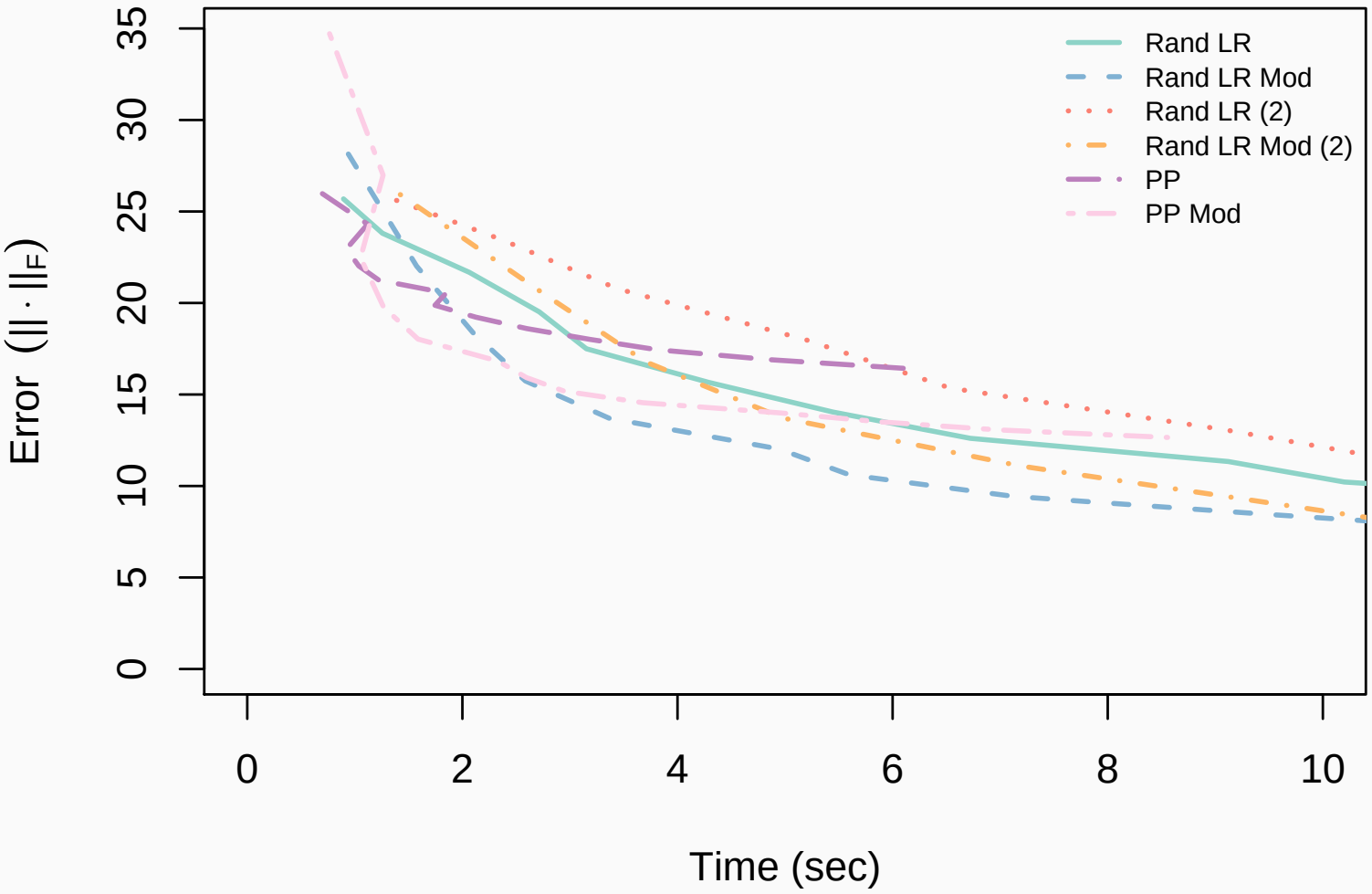

$$n = 15000, \quad k = \{100, \ldots, 4900\}$$

Rand. Matrix Low Rank Decompositions for Prediction

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

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

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

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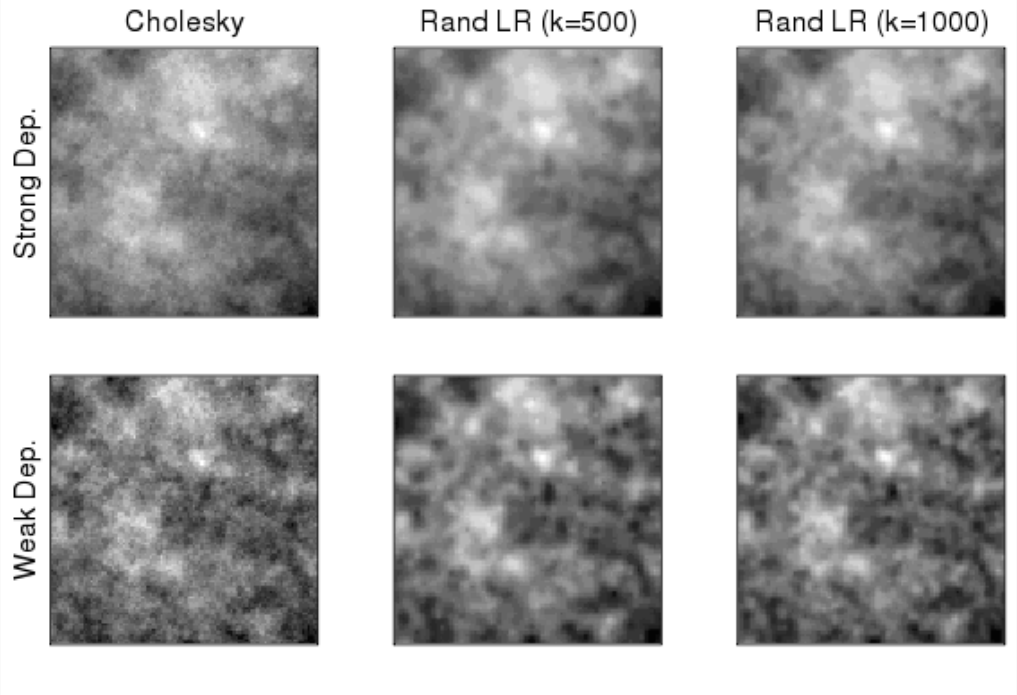
$$\mathcal{N}(0, \Sigma) \text{ with } \Sigma \approx USU' = (US^{1/2}U')(US^{1/2}U')'$$

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



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

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 - Missouri

RcppGP `https://github.com/rundel/RcppGP`