

Lecture 21

Computational Methods for GPs

Colin Rundel

11/16/2018

GPs and Computational Complexity

The problem with GPs

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

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Update covariance parameter?

$$\{\boldsymbol{\Sigma}\}_{ij} = \sigma^2 \exp(-\{d\}_{ij}\phi) + \sigma_n^2 1_{i=j} \quad \mathcal{O}(n^2)$$

$\mathcal{O}(n)$ - Linear complexity

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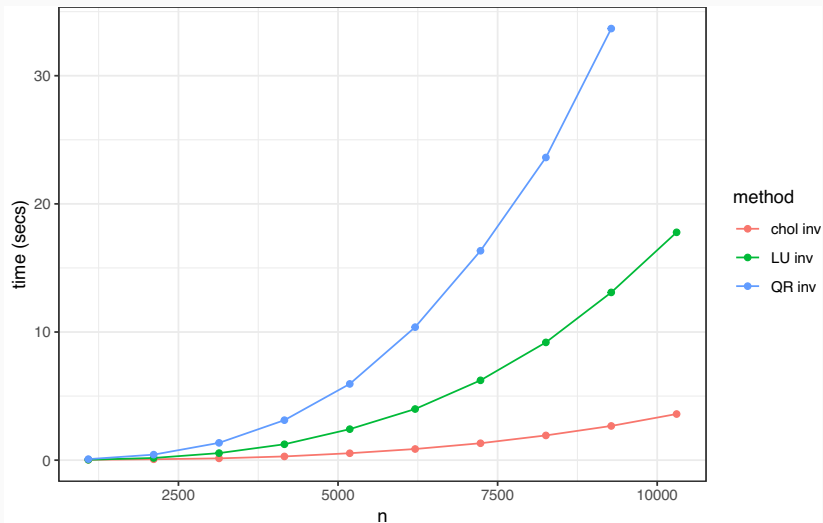
$\mathcal{O}(n^3)$ - Cubic complexity

$\mathcal{O}(n)$ - Linear complexity - Go for it

$\mathcal{O}(n^2)$ - Quadratic complexity - Pray

$\mathcal{O}(n^3)$ - Cubic complexity - Give up

How bad is the problem?



Practice - Migratory Model Prediction

After fitting the GP need to sample from the posterior predictive distribution at ~ 3000 locations

$$\mathbf{y}_p \sim \mathcal{N}(\mu_p + \Sigma_{po}\Sigma_o^{-1}(y_o - \mu_o), \Sigma_p - \Sigma_{po}\Sigma_o^{-1}\Sigma_{op})$$

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Step	CPU (secs)
1. Calc. $\Sigma_p, \Sigma_{po}, \Sigma_o$	1.080
2. Calc. $\text{chol}(\Sigma_p - \Sigma_{po}\Sigma_o^{-1}\Sigma_{op})$	0.467
3. Calc. $\mu_{p o} + \text{chol}(\Sigma_{p o}) \times Z$	0.049
4. Calc. Allele Prob	0.129
Total	1.732

Total run time for 1000 posterior predictive draws:

- CPU (28.9 min)

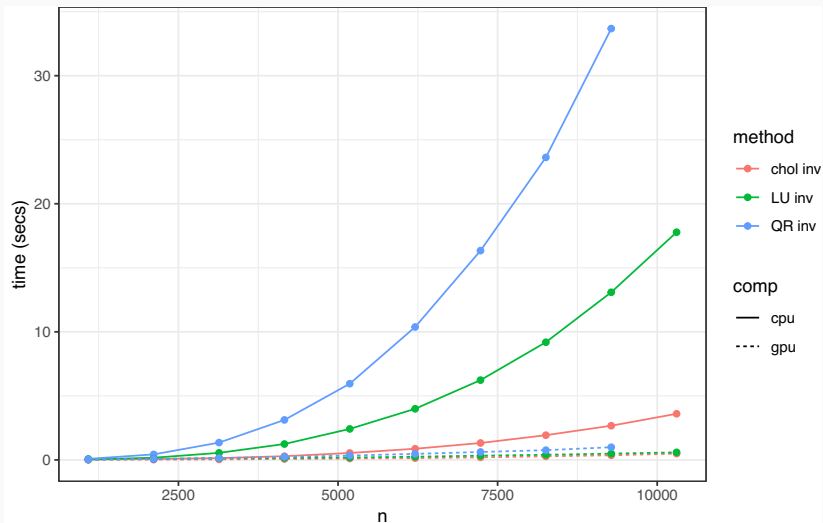
A bigger hammer?

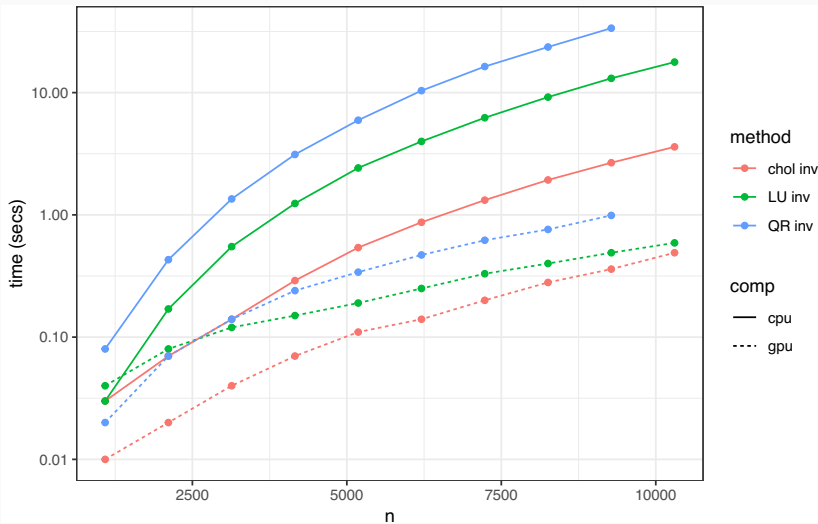
Step	CPU (secs)	CPU+GPU (secs)	Rel. Perf
1. Calc. $\Sigma_p, \Sigma_{p o}, \Sigma_p$	1.080	0.046	23.0
2. Calc. $\text{chol}(\Sigma_p - \Sigma_{p o} \Sigma_o^{-1} \Sigma_{op})$	0.467	0.208	2.3
3. Calc. $\mu_{p o} + \text{chol}(\Sigma_{p o}) \times Z$	0.049	0.052	0.9
4. Calc. Allele Prob	0.129	0.127	1.0
Total	1.732	0.465	3.7

Total run time for 1000 posterior predictive draws:

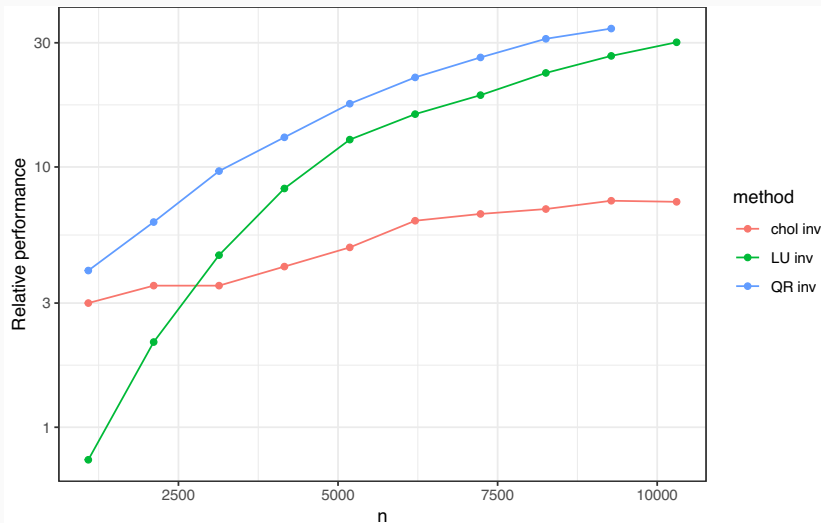
- CPU (28.9 min)
- CPU+GPU (7.8 min)

Cholesky CPU vs GPU (P100)

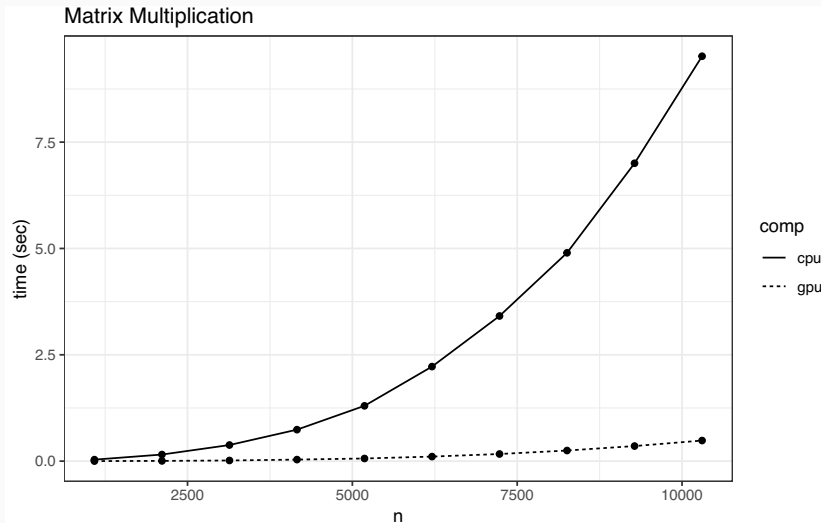




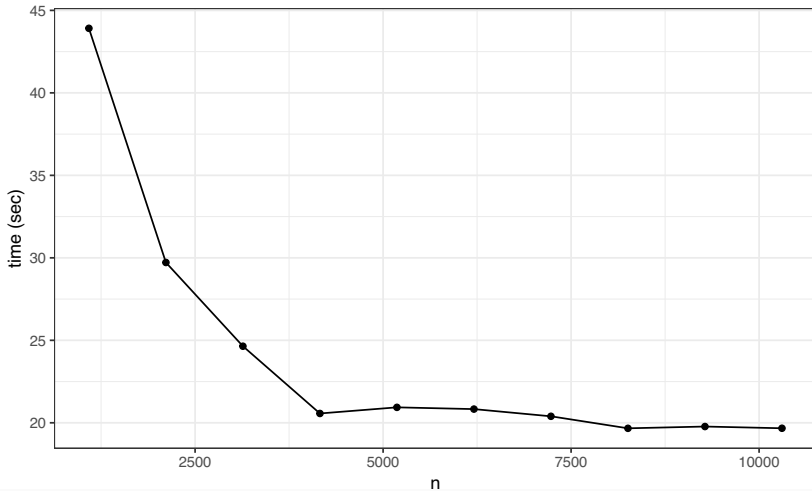
Relative Performance



Aside (1) - Matrix Multiplication

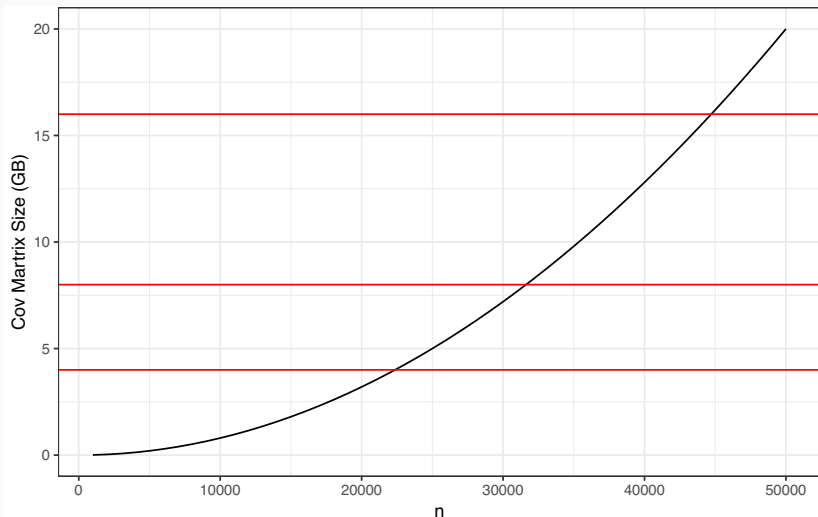


Matrix Multiplication – Relative Performance



Aside (2) - Memory Limitations

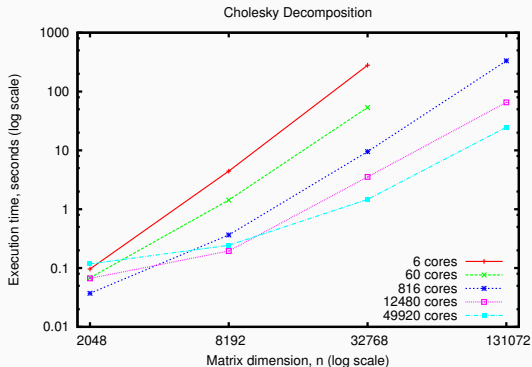
A general covariance is a dense $n \times n$ matrix, meaning it will require $n^2 \times 64$ -bits to store.



Other big hammers

bigGP is an R package written by Chris Paciorek (UC Berkeley), et al.

- Specialized distributed implementation of linear algebra 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)



More scalable solutions?

- Spectral domain / basis functions
- Covariance tapering
- GMRF approximations
- Low-rank approximations
- Nearest-neighbor models

Low Rank Approximations

Low rank approximations in general

Lets look at the example of the singular value decomposition of a matrix,

$$M = U \operatorname{diag}(S) V^t$$

$n \times m$ $n \times n$ $n \times m$ $m \times m$

where U are called the left singular vectors, V the right singular vectors, and S the singular values. Usually the singular values and vectors are ordered such that the singular values are in descending order.

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The Eckart–Young theorem states that we can construct an approximation of M with rank k by setting \tilde{S} to contain only the k largest singular values and all other values set to zero.

$$\begin{aligned} \tilde{M} &= U \operatorname{diag}(\tilde{S}) V^t \\ &= \tilde{U} \operatorname{diag}(\tilde{S}) \tilde{V}^t \end{aligned}$$

$n \times m$ $n \times n$ $n \times m$ $m \times m$
 $n \times k$ $k \times k$ $k \times m$

Example

$$M = \begin{pmatrix} 1.000 & 0.500 & 0.333 & 0.250 \\ 0.500 & 0.333 & 0.250 & 0.200 \\ 0.333 & 0.250 & 0.200 & 0.167 \\ 0.250 & 0.200 & 0.167 & 0.143 \end{pmatrix} = U \operatorname{diag}(S) V^t$$

$$U = V = \begin{pmatrix} -0.79 & 0.58 & -0.18 & -0.03 \\ -0.45 & -0.37 & 0.74 & 0.33 \\ -0.32 & -0.51 & -0.10 & -0.79 \\ -0.25 & -0.51 & -0.64 & 0.51 \end{pmatrix}$$

$$S = (1.50 \quad 0.17 \quad 0.01 \quad 0.00)$$

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Rank 2 approximation:

$$\begin{aligned} \tilde{M} &= \begin{pmatrix} -0.79 & 0.58 \\ -0.45 & -0.37 \\ -0.32 & -0.51 \\ -0.25 & -0.51 \end{pmatrix} \begin{pmatrix} 1.50 & 0.00 \\ 0.00 & 0.17 \end{pmatrix} \begin{pmatrix} -0.79 & -0.45 & -0.32 & -0.25 \\ 0.58 & -0.37 & -0.51 & -0.51 \end{pmatrix} \\ &= \begin{pmatrix} 1.000 & 0.501 & 0.333 & 0.249 \\ 0.501 & 0.330 & 0.251 & 0.203 \\ 0.333 & 0.251 & 0.200 & 0.166 \\ 0.249 & 0.203 & 0.166 & 0.140 \end{pmatrix} \end{aligned}$$

We can measure the error of the approximation using the Frobenius norm,

$$\|M - \tilde{M}\|_F = \left(\sum_{i=1}^m \sum_{j=1}^n (M_{ij} - \tilde{M}_{ij})^2 \right)^{1/2}$$

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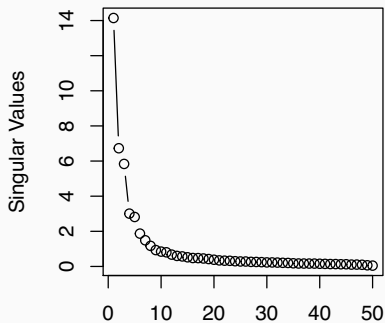
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$$M - \tilde{M} = \begin{pmatrix} 0.00022 & -0.00090 & 0.00012 & 0.00077 \\ -0.00090 & 0.00372 & -0.00053 & -0.00317 \\ 0.00012 & -0.00053 & 0.00013 & 0.00039 \\ 0.00077 & -0.00317 & 0.00039 & 0.00277 \end{pmatrix}$$

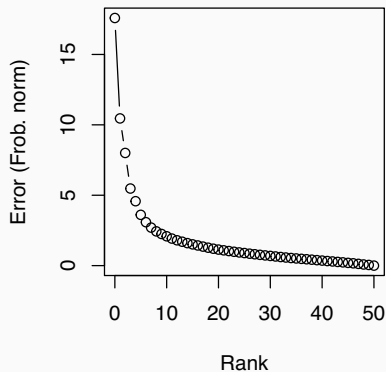
$$\|M - \tilde{M}\|_F = 0.00674$$

Cov Mat - Strong dependence (large eff. range):

SVD

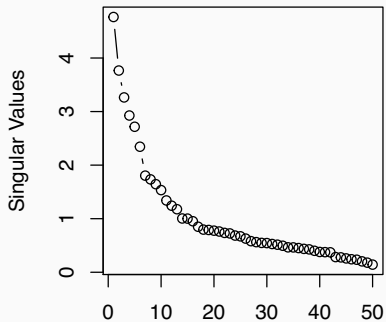


Low Rank SVD

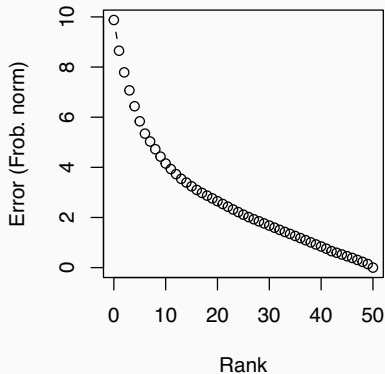


Cov Mat - Weak dependence (short eff. range):

SVD



Low Rank SVD



How does this help? (Sherman-Morrison-Woodbury)

There is an immensely useful linear algebra identity, the Sherman-Morrison-Woodbury formula, for the inverse (and determinant) of a decomposed matrix,

$$\begin{aligned} M_{n \times m}^{-1} &= \left(A_{n \times m} + \begin{matrix} U_{n \times k} & S_{k \times k} & V^t_{k \times m} \end{matrix} \right)^{-1} \\ &= A^{-1} - A^{-1} U \underbrace{\left(S^{-1} + \underbrace{V^t A^{-1} U}_{\text{diag}} \right)^{-1}}_{k \times k} V^t A^{-1}. \end{aligned}$$

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$$\begin{aligned} M^{-1} &= \begin{pmatrix} A & U & S & V^t \\ n \times m & n \times k & k \times k & k \times m \end{pmatrix}^{-1} \\ &= A^{-1} - A^{-1}U(S^{-1} + V^tA^{-1}U)^{-1}V^tA^{-1}. \end{aligned}$$

How does this help?

- Imagine that $A = \text{diag}(A)$, then it is trivial to find A^{-1} .
- S^{-1} is $k \times k$ which is hopefully small, or even better $S = \text{diag}(S)$.
- $(S^{-1} + V^tA^{-1}U)$ is $k \times k$ which is also small.

Aside - Determinant

Remember for any MVN distribution when evaluating the likelihood

$$-\frac{1}{2} \log |\Sigma| - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) - \frac{n}{2} \log 2\pi$$

we need the inverse of Σ as well as its *determinant*.

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- For a full rank Cholesky decomposition we get the determinant for “free”.

$$|M| = |LL^t| = \prod_{i=1}^n (\text{diag}(L)_i)^2$$

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- The Sherman-Morrison-Woodbury Determinant lemma gives us,

$$\begin{aligned} \det(M) &= \det(A + USV^t) \\ &= \det(S^{-1} + V^t A^{-1} U) \det(S) \det(A) \end{aligned}$$

Low rank approximations for GPs

For a standard spatial random effects model,

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

if we can replace $\boldsymbol{\Sigma}(\mathbf{s})$ with a low rank approximation of the form

- $\boldsymbol{\Sigma}(\mathbf{s}) \approx \mathbf{U} \mathbf{S} \mathbf{V}^t$ where
- \mathbf{U} and \mathbf{V} are $n \times k$,
- \mathbf{S} is $k \times k$, and
- $A = \sigma^2 I$ or a similar diagonal matrix

Predictive Processes

For a rank k approximation,

- Pick k knot locations \mathbf{s}^*

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Gaussian Predictive Processes

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- Approximate full covariance using

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$\mathbf{u} \times \mathbf{S} \times \mathbf{u}^T$

Gaussian Predictive Processes

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- PPs systematically underestimates variance (σ^2) and inflate τ^2 , Modified predictive process corrects this using

$$\begin{aligned} \Sigma(\mathbf{s}) \approx & \Sigma(\mathbf{s}, \mathbf{s}^*) \Sigma(\mathbf{s}^*)^{-1} \Sigma(\mathbf{s}^*, \mathbf{s}) \\ & + \text{diag}\left(\Sigma(\mathbf{s}) - \Sigma(\mathbf{s}, \mathbf{s}^*) \Sigma(\mathbf{s}^*)^{-1} \Sigma(\mathbf{s}^*, \mathbf{s})\right). \end{aligned}$$

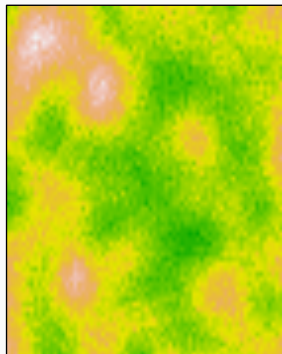
Example

Below we have a surface generate from a squared exponential Gaussian Process where

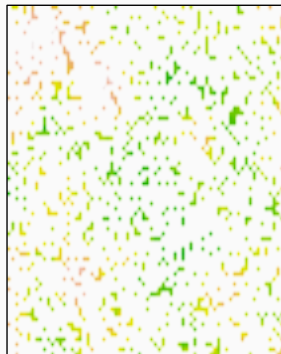
$$\{\Sigma\}_{ij} = \sigma^2 \exp(-(\phi d)^2) + \tau^2 I$$

$$\sigma^2 = 1 \quad \phi = 9 \quad \tau^2 = 0.1$$

True Surface

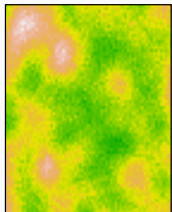


Observed Data

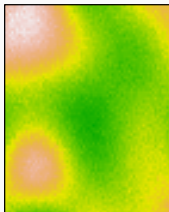


Predictive Process Model Results

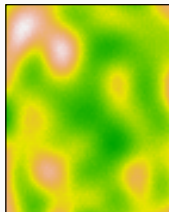
True Field



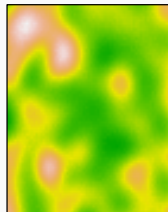
PP – 5 x 5 knots



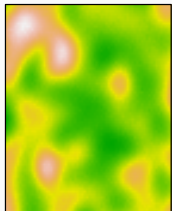
PP – 10 x 10 knots



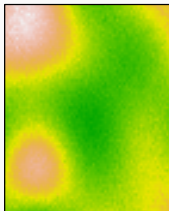
PP – 15 x 15 knots



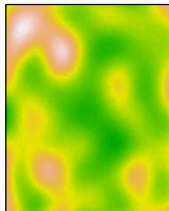
Full GP



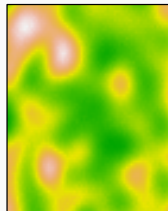
Mod. PP – 5 x 5 knots



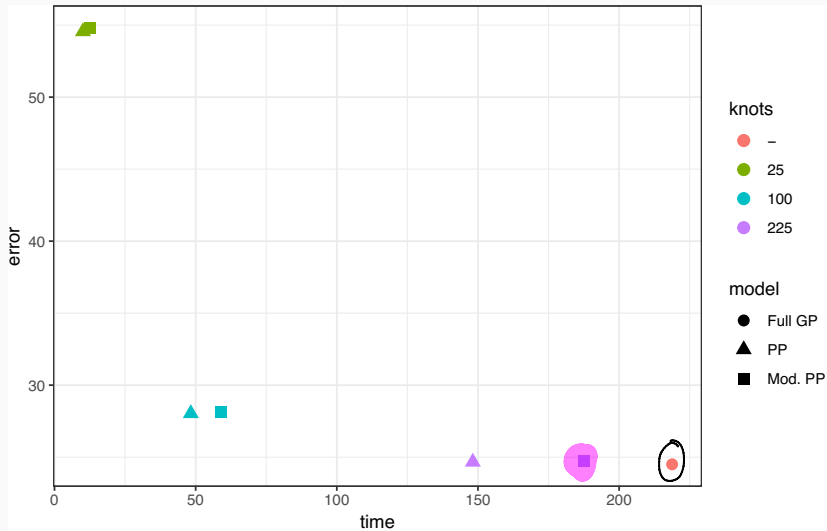
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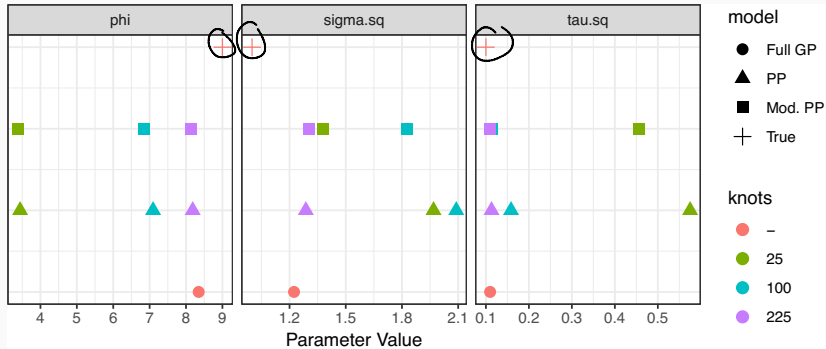
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Performance



Parameter Estimates



Random Projections

Low Rank Approximations via Random Projections

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 $m \times n$

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Low Rank Approximations via Random Projections

1. Starting with an matrix \mathbf{A} $m \times n$.
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3. Form $\mathbf{Y} = \mathbf{A} \mathbf{\Omega}$ and compute its QR factorization $\mathbf{Y} = \mathbf{Q} \mathbf{R}$.

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6. Form the matrix $\mathbf{U} = \mathbf{Q} \hat{\mathbf{U}}$.
7. Form $\tilde{\mathbf{A}} = \mathbf{U} \mathbf{S} \mathbf{V}'$.

σ_k is the k th
smallest eigenvalue

Resulting approximation has a bounded expected error,

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

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3. Form $\mathbf{Y} = \mathbf{A} \mathbf{\Omega}$ and compute its QR factorization $\mathbf{Y} = \mathbf{Q} \mathbf{R}$.
4. Form the $\mathbf{B} = \mathbf{Q}' \mathbf{A} \mathbf{Q}$.
5. Compute the eigen decomposition of $\mathbf{B} = \hat{\mathbf{U}} \mathbf{S} \hat{\mathbf{U}}'$.

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

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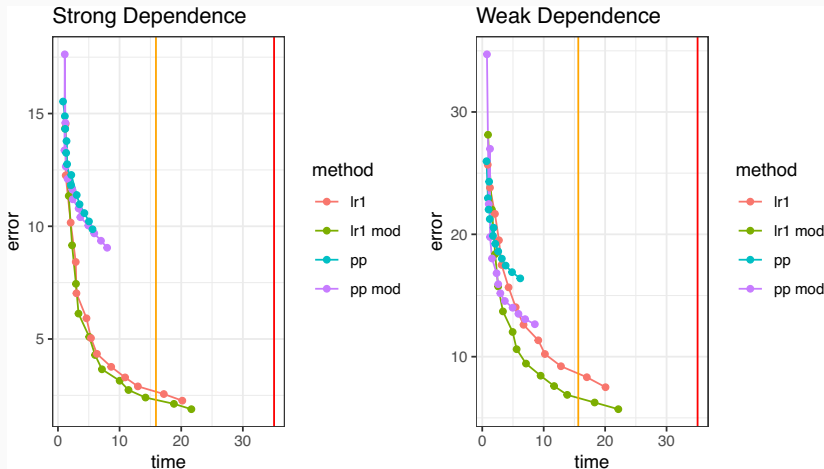
Once again we have a bound on the error,

$$E \|\mathbf{A} - \mathbf{U} \mathbf{S} \mathbf{U}'\|_F \lesssim c \cdot \sigma_{k+1}$$

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 approximations involves a large matrix multiplication ($\mathbf{A} \mathbf{\Omega}$) and several small matrix decompositions (QR, eigen).

Comparison ($n = 15,000, k = \{100, \dots, 4900\}$)



Rand. Projection LR Depositions for Prediction

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

$$\text{chol}(\Sigma) = L$$

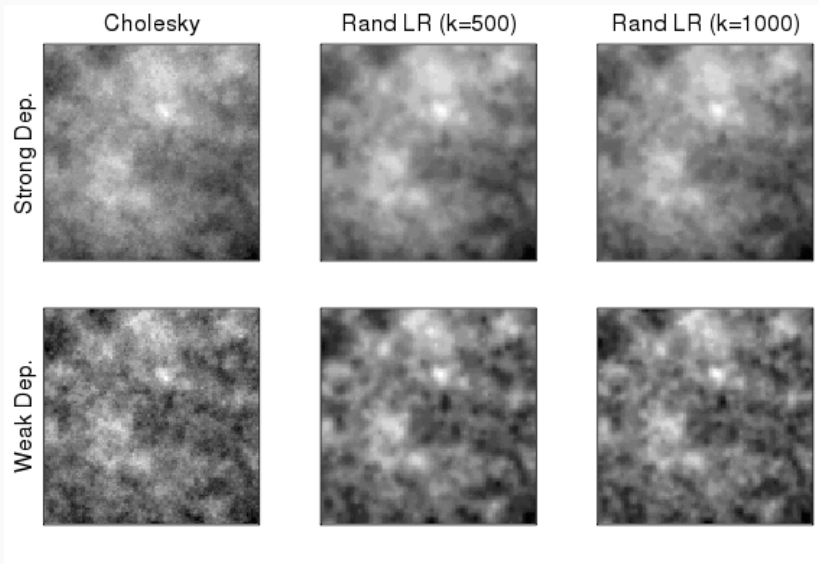
$$\mathbf{y} \sim \mathcal{N}(0, \Sigma)$$

$$\Sigma \approx \mathbf{U}\mathbf{S}\mathbf{U}^t = (\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}^t)(\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}^t)^t$$

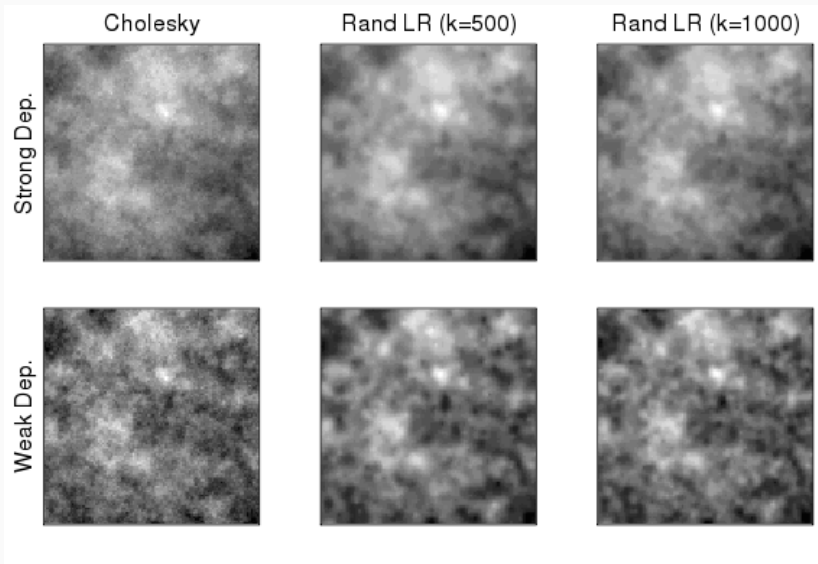
then

$$y_{\text{pred}} = (\mathbf{U}\mathbf{S}^{1/2}\mathbf{U}^t) \times \mathbf{Z} \text{ where } Z_i \sim \mathcal{N}(0, 1)$$

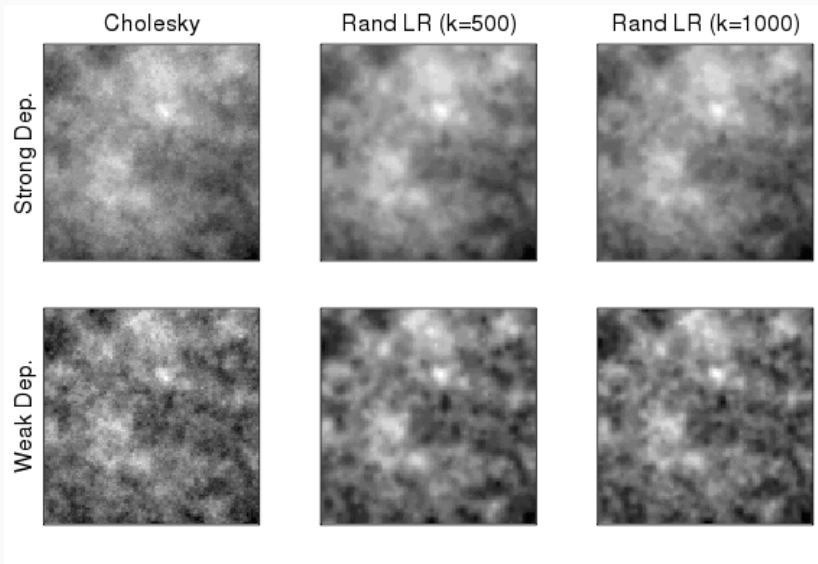
because $\mathbf{U}^t \mathbf{U} = I$ since \mathbf{U} is an orthogonal matrix.



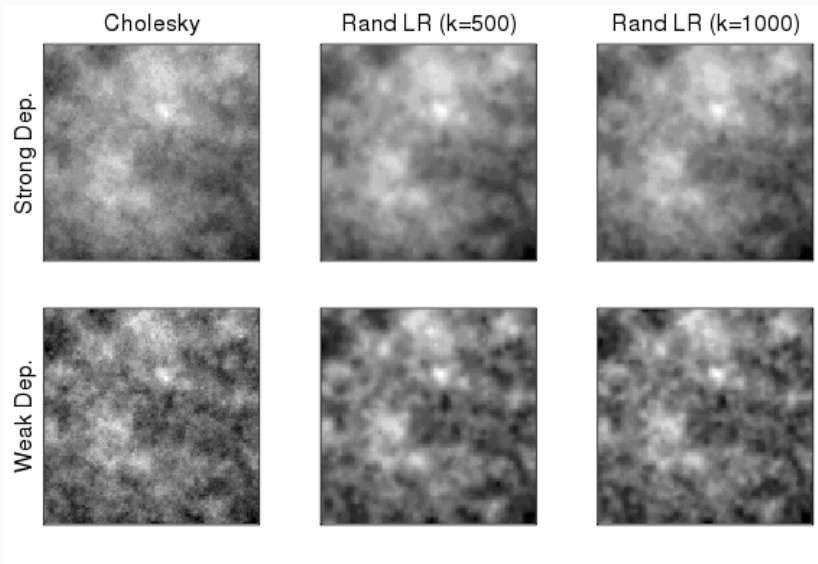
$$n = 1000, \quad p = 10000$$



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