Lecture 22

Computational Methods for GPs

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GPs and Computational Complexity

The problem with GPs

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

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Evaluate the (log) likelihood?

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Update covariance parameter?

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

A simple guide to computational complexity

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

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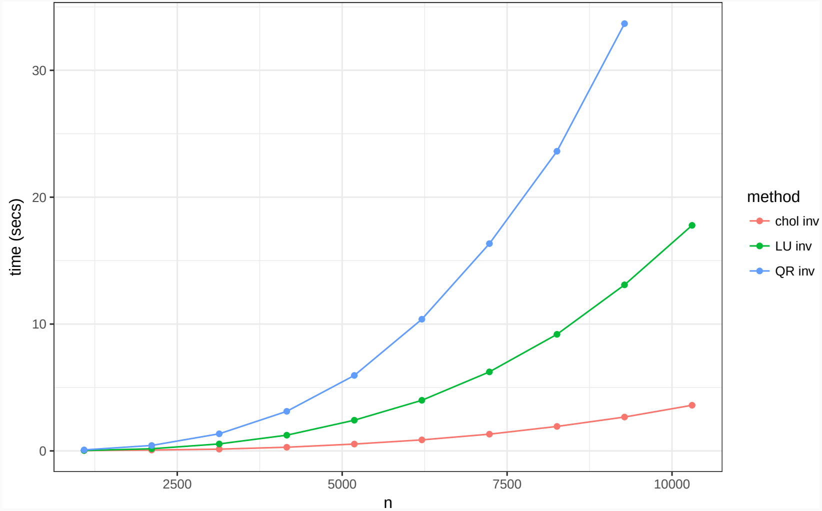
$\mathcal{O}(n^3)$ - Cubic complexity - Give up

How bad is the problem?



Practice - Migratory Model Prediction

After fitting the GP need to sample from the posterior predictive distribution at $\sim$ 3000 locations

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

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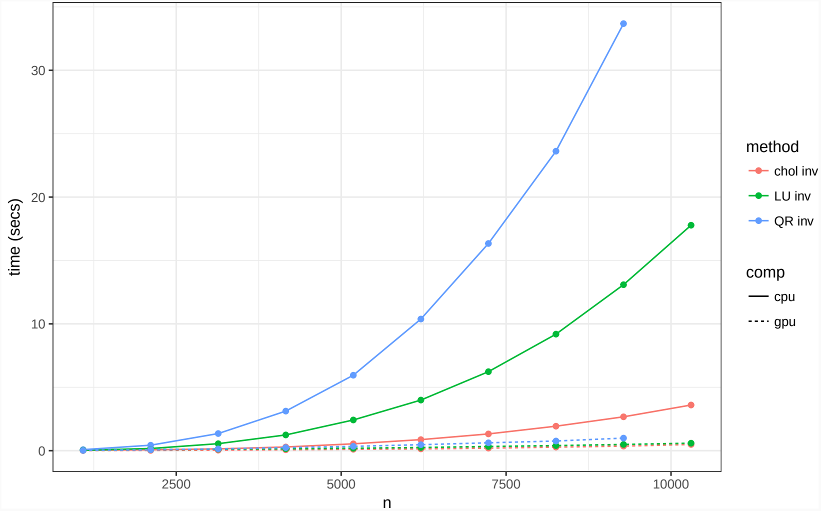
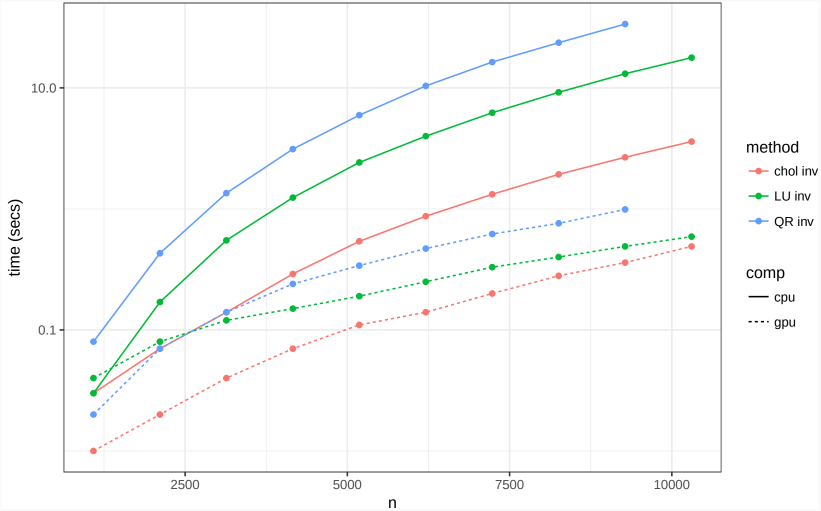
	Step	CPU (secs)	CPU+GPU (secs)	Rel. Performance
1.	Calc. Σ_p, Σ_{po}	1.080	0.046	23.0
2.	Calc. $\text{chol}(\Sigma_p - \Sigma_{po}\Sigma_o^{-1}\Sigma_{op})$	0.467	0.208	2.3
3.	Calc. $\mu_{p\|o} + \text{chol}(\Sigma_{p\|o}) \times Z$	0.049	0.052	0.9
4.	Calc. Allele Prob	0.129	0.127	1.0
	Total	1.732	0.465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

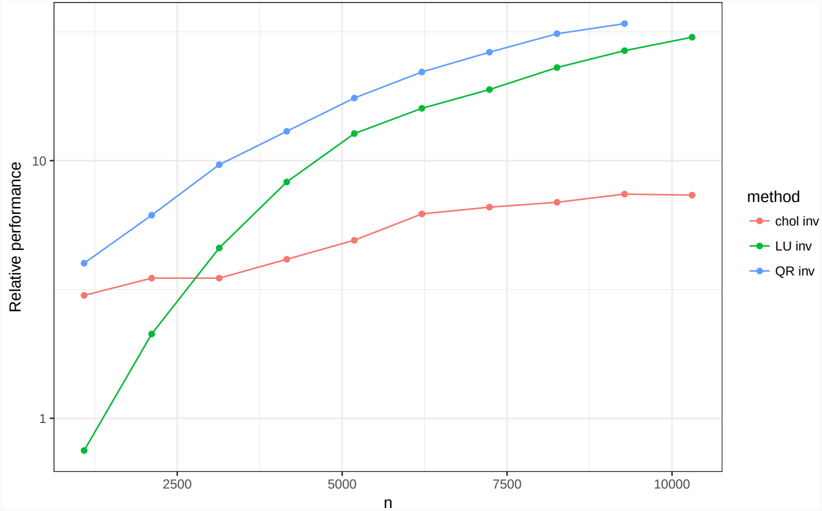
Total run time: CPU (28.9 min), CPU+GPU (7.8 min)

Cholesky CPU vs GPU (P100)

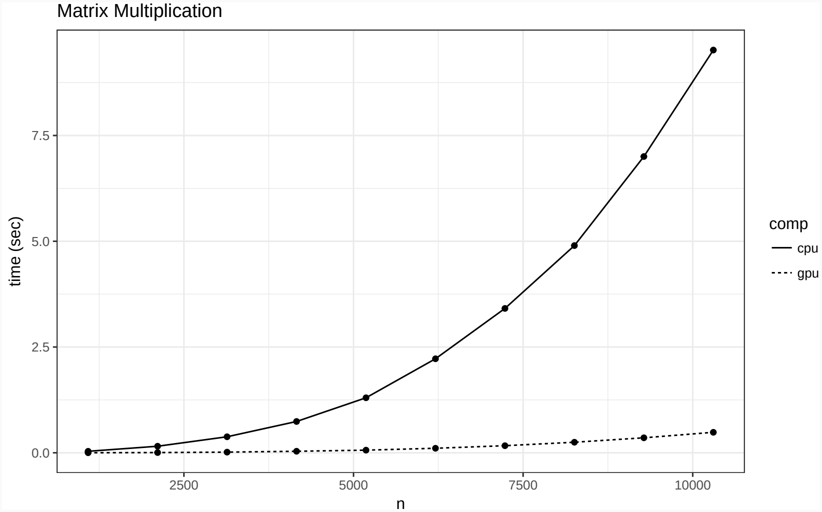



time (secs)
10.0
0.1
2500
5000
7500
10000
n
method
chol inv
LU inv
QR inv
comp
cpu
gpu

Relative Performance



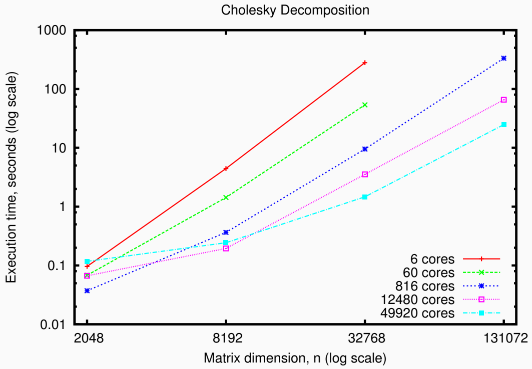
Aside - Matrix Multiplication



An even bigger hammer

`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 $n = 65$k (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,

$$\underset{n\times m}{M} = \underset{n\times n}{U} \underset{n\times m}{\mathrm{diag}(S)} \underset{m\times m}{V^t}$$

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 signular values are in descending order.

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It turns out (Eckart–Young theorem) that we can approximate M as having rank r by defining $\tilde{S}$ to only have the r largest singular values (others set to zero).

$$\underset{n\times m}{\tilde{M}} = \underset{n\times n}{U}\,\underset{n\times m}{\mathrm{diag}(\tilde{S})}\,\underset{m\times m}{V^t} \quad = \underset{n\times k}{\tilde{U}}\,\underset{k\times k}{\mathrm{diag}(\tilde{S})}\,\underset{k\times m}{\tilde{V}^t}$$

Example

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

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

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Rank 2 approximation:

$$\tilde{M} = \begin{pmatrix} -0.79 & 0.58 \\ -0.45 & -0.37 \\ -0.32 & -0.51 \\ -0.25 & -0.51 \end{pmatrix} \begin{pmatrix} 1.50 & 0.00 \\ 0.00 & 0.17 \end{pmatrix} \begin{pmatrix} -0.79 & -0.45 & -0.32 & -0.25 \\ 0.58 & -0.37 & -0.51 & -0.51 \end{pmatrix}$$

$$= \begin{pmatrix} 1.000 & 0.501 & 0.333 & 0.249 \\ 0.501 & 0.330 & 0.251 & 0.203 \\ 0.333 & 0.251 & 0.200 & 0.166 \\ 0.249 & 0.203 & 0.166 & 0.140 \end{pmatrix}$$

Approximation Error

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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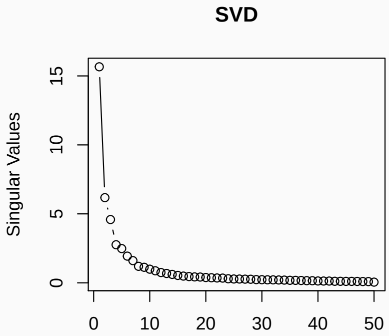
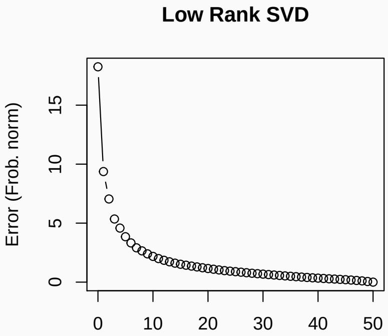
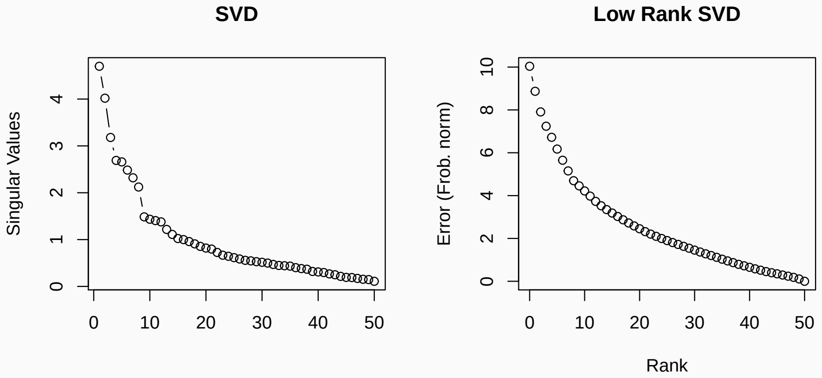
Strong dependence (large eff. range):





Weak dependence (short eff. range):



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,

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

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How does this help?

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

Aside - Determinant

Remember for any MVN distribution when evaluating the likelihood

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

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".

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

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- For a low rank approximation the Sherman-Morrison-Woodbury / Determinant lemma gives us,

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

Low rank approximations for GPs

For a standard spatial random effects model,

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

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

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

Predictive Processes

Gaussian Predictive Processes

For a rank k approximation,

- Pick k knot locations $s^\star$
- Calculate knot covariance, $\boldsymbol{\Sigma}(s^\star)$, and knot cross-covariance, $\boldsymbol{\Sigma}(s, s^\star)$
- Approximate full covariance using

$$\boldsymbol{\Sigma}(s) \approx \underset{n\times k}{\boldsymbol{\Sigma}(s, s^\star)}\, \underset{k\times k}{\boldsymbol{\Sigma}(s^\star)^{-1}}\, \underset{k\times n}{\boldsymbol{\Sigma}(s^\star, s)}.$$

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

$$\begin{aligned}\boldsymbol{\Sigma}(s) \approx & \boldsymbol{\Sigma}(s, s^\star)\, \boldsymbol{\Sigma}(s^\star)^{-1}\, \boldsymbol{\Sigma}(s^\star, s) \\ & + \operatorname{diag}\Big(\boldsymbol{\Sigma}(s) - \boldsymbol{\Sigma}(s, s^\star)\, \boldsymbol{\Sigma}(s^\star)^{-1}\, \boldsymbol{\Sigma}(s^\star, s)\Big).\end{aligned}$$

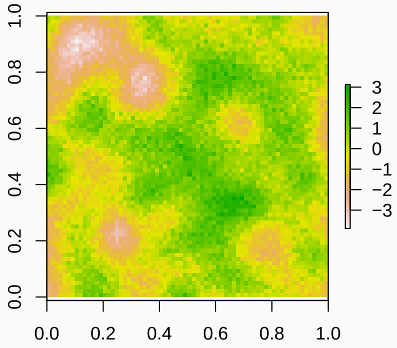
Banerjee, Gelfand, Finley, Sang (2008) Finley, Sang, Banerjee, Gelfand (2008)

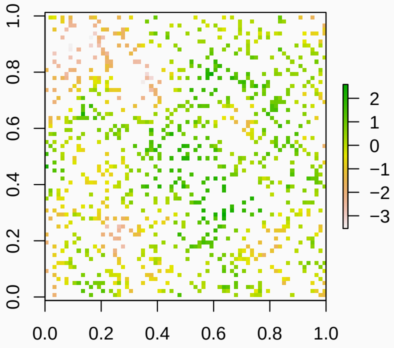
Example

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

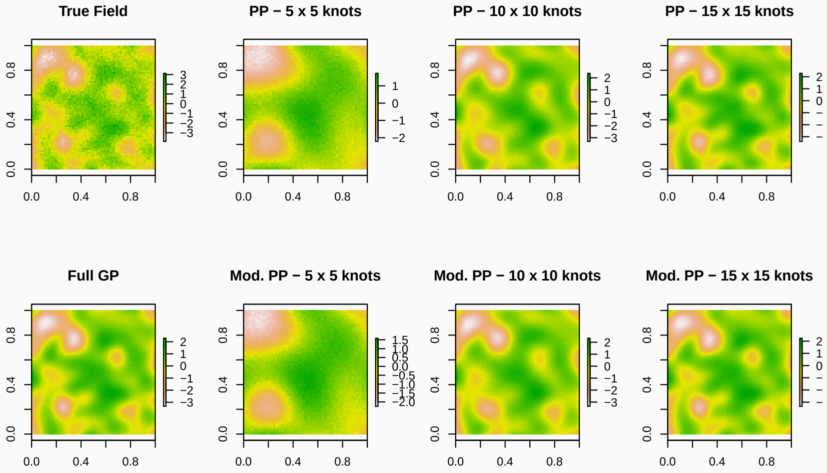
$$\{\Sigma\}_{ij} = \sigma^2 \exp\left(-(\phi\, d)^2\right) + \tau^2 I$$

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

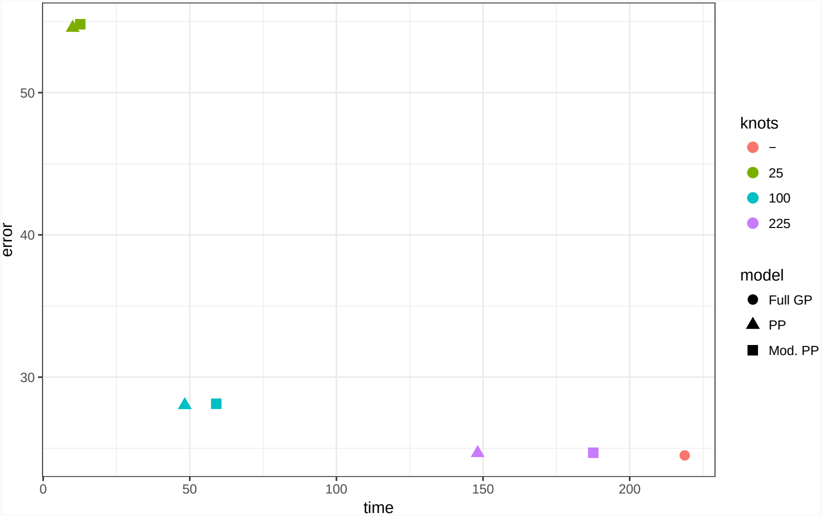




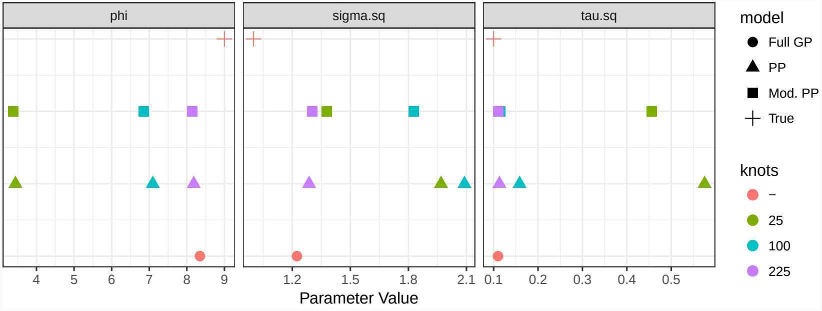
Predictive Process Model Results



Performance



Parameter Estimates



Random Projections

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 $\boldsymbol{U} = \boldsymbol{Q}\,\hat{\boldsymbol{U}}$.

Resulting approximation has a 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 Approximations and GPs

Preceeding 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,

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

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

Low Rank Approximations and GPUs

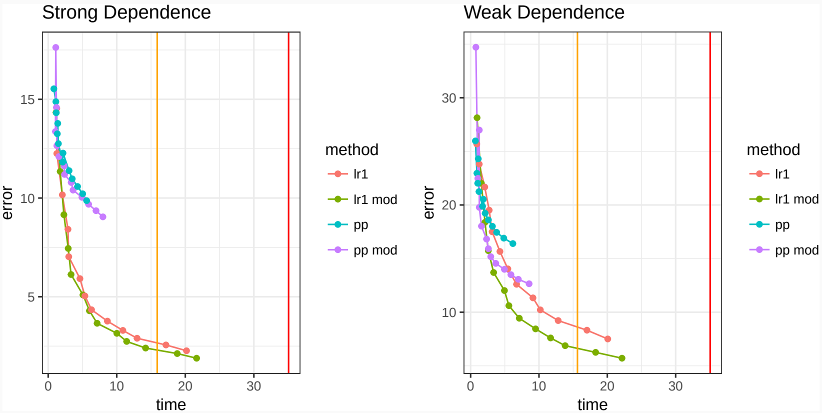
Both predictive process and random matrix low rank approximations are good candidates for acceleration using GPUs.

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

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



Rand. Projection LR Decompositions for Prediction

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

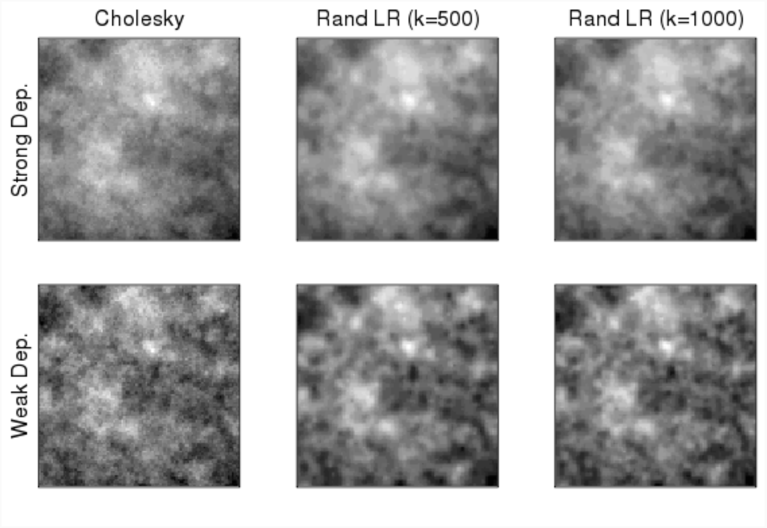
$$y \sim \mathcal{N}(0, \boldsymbol{\Sigma})$$
$$\Sigma \approx \boldsymbol{U}\boldsymbol{S}\boldsymbol{U}^t = (\boldsymbol{U}\boldsymbol{S}^{1/2}\boldsymbol{U}^t)(\boldsymbol{U}\boldsymbol{S}^{1/2}\boldsymbol{U}^t)^t$$

then

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

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

Dehdari, Deutsch (2012)



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