Lecture 21

Computational Methods for GPs

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GPs and Computational Complexity

The problem with GPs

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Want to sample $\mathbf{y}$?

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

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Evaluate the (log) likelihood?

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

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Update covariance parameter?

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

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

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

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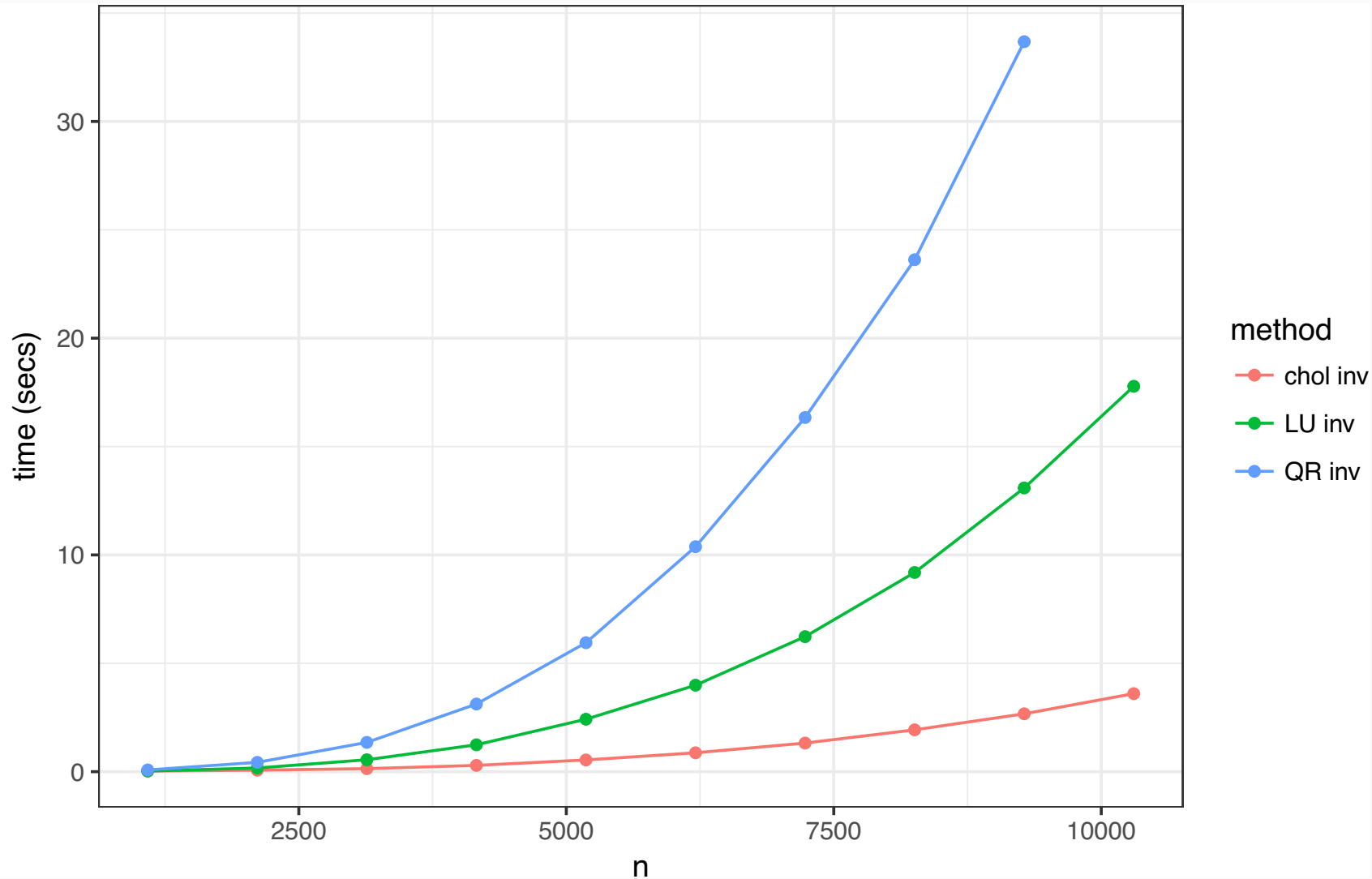
$\mathcal{O}\left(n^2\right)$ - Quadratic complexity - Pray

$\mathcal{O}\left(n^3\right)$ - 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

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

3000 × 3000 17×17

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Step	CPU (secs)
1. Calc. $\Sigma_p, \Sigma_{po},$ [illegible]	1.080
2. Calc. chol$(\Sigma_p - \Sigma_{po}\Sigma_o^{-1}\Sigma_{op})$	0.467
3. Calc. $\mu_{p\|o} +$ 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) $\times$ 150

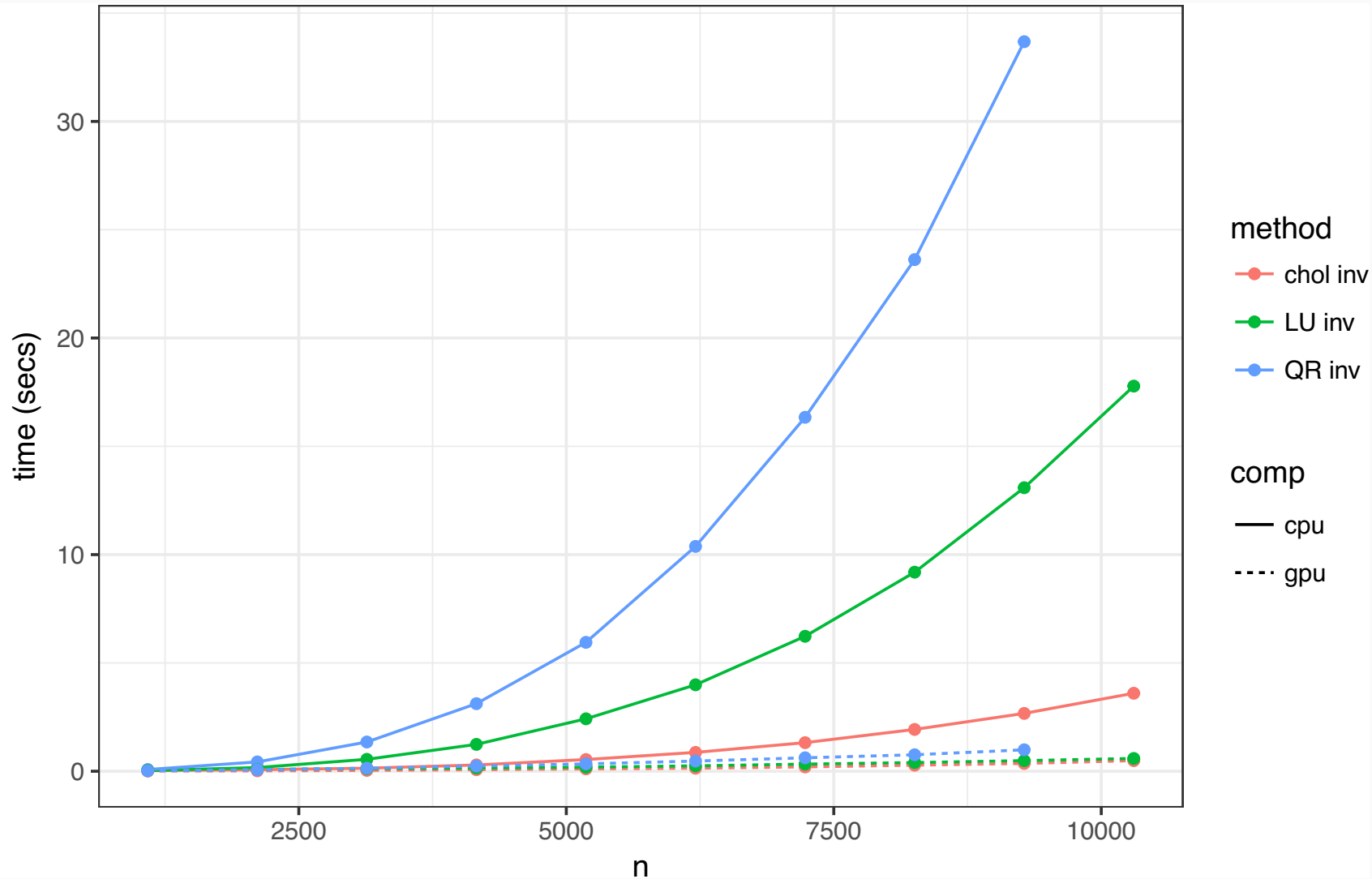
A bigger hammer?

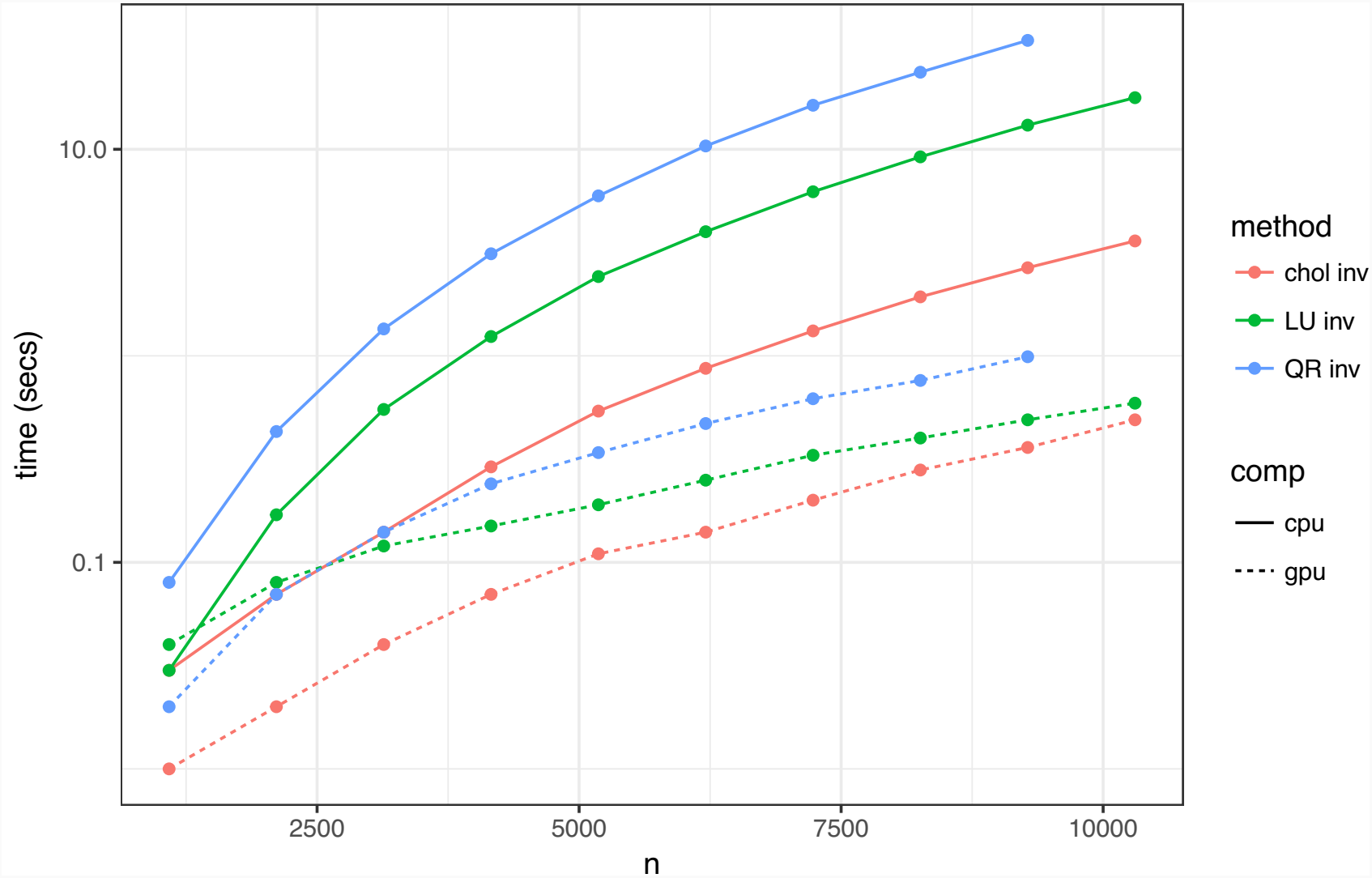
Step	CPU (secs)	CPU+GPU (secs)	Rel. Perf
1. Calc. $\Sigma_p, \Sigma_{po}, \Sigma_p$	1.080	0.046	23.0
2. Calc. chol$(\Sigma_p - \Sigma_{po}\Sigma_o^{-1}\Sigma_{op})$	0.467	0.208	2.3
3. Calc. $\mu_{p\|o} + \text{chol}(\Sigma_{p\|o}) \times Z$	0.049	0.052	0.9
4. Calc. Allele Prob	0.129	0.127	1.0
Total	1.732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

Total run time for 1000 posterior predictive draws:

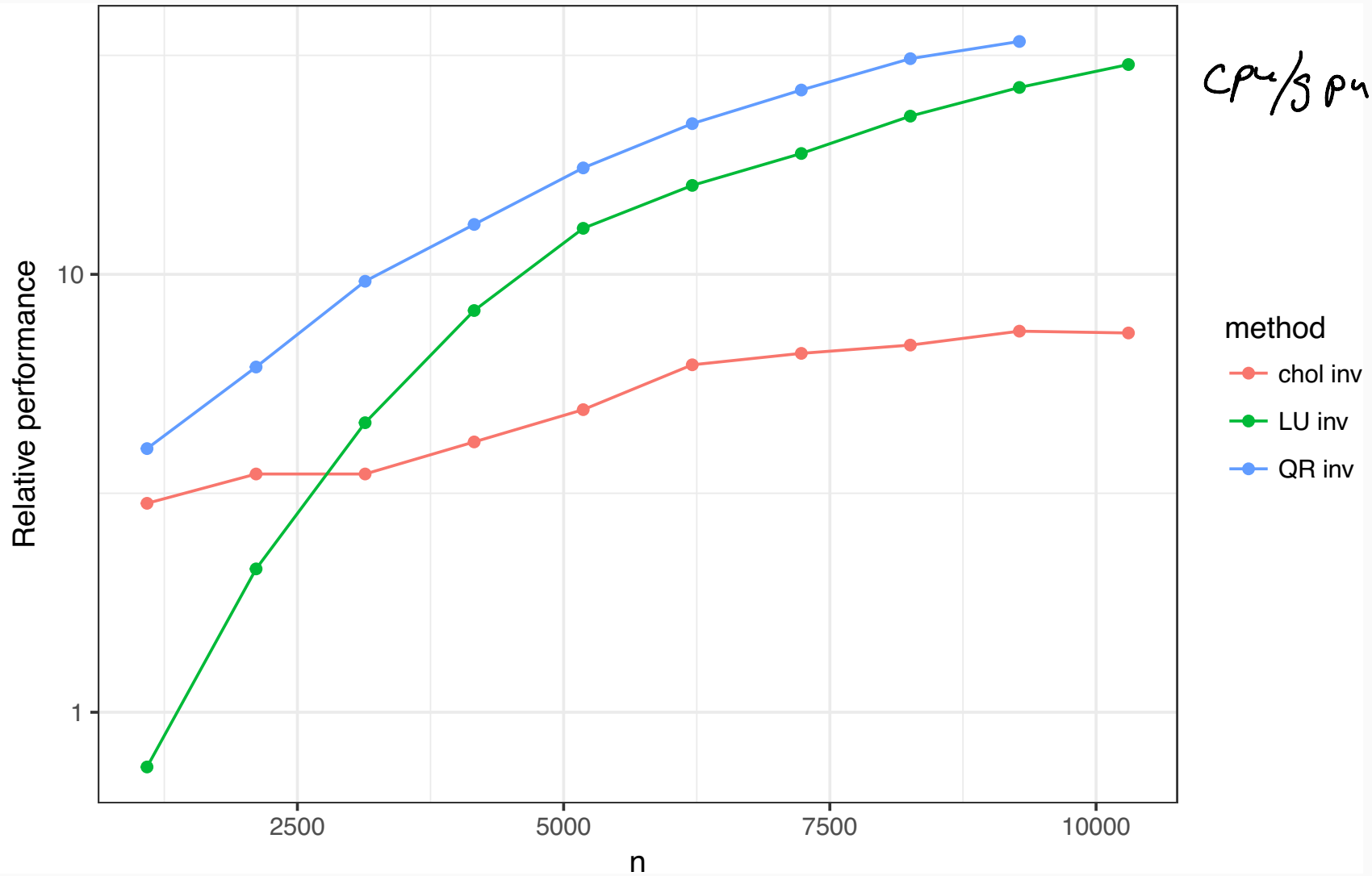
- CPU (28.9 min)
- CPU+GPU (7.8 min)

Cholesky CPU vs GPU (P100)

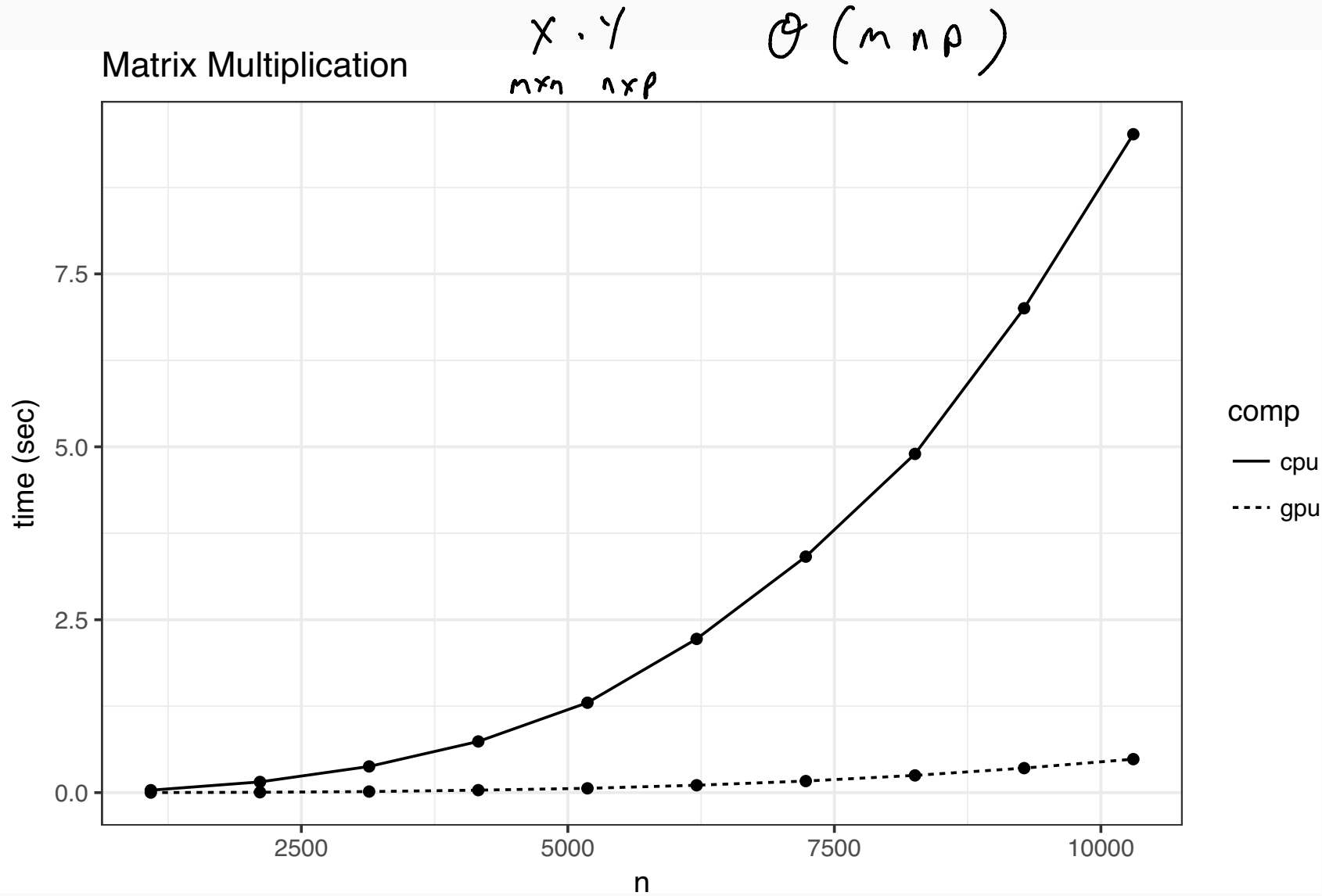


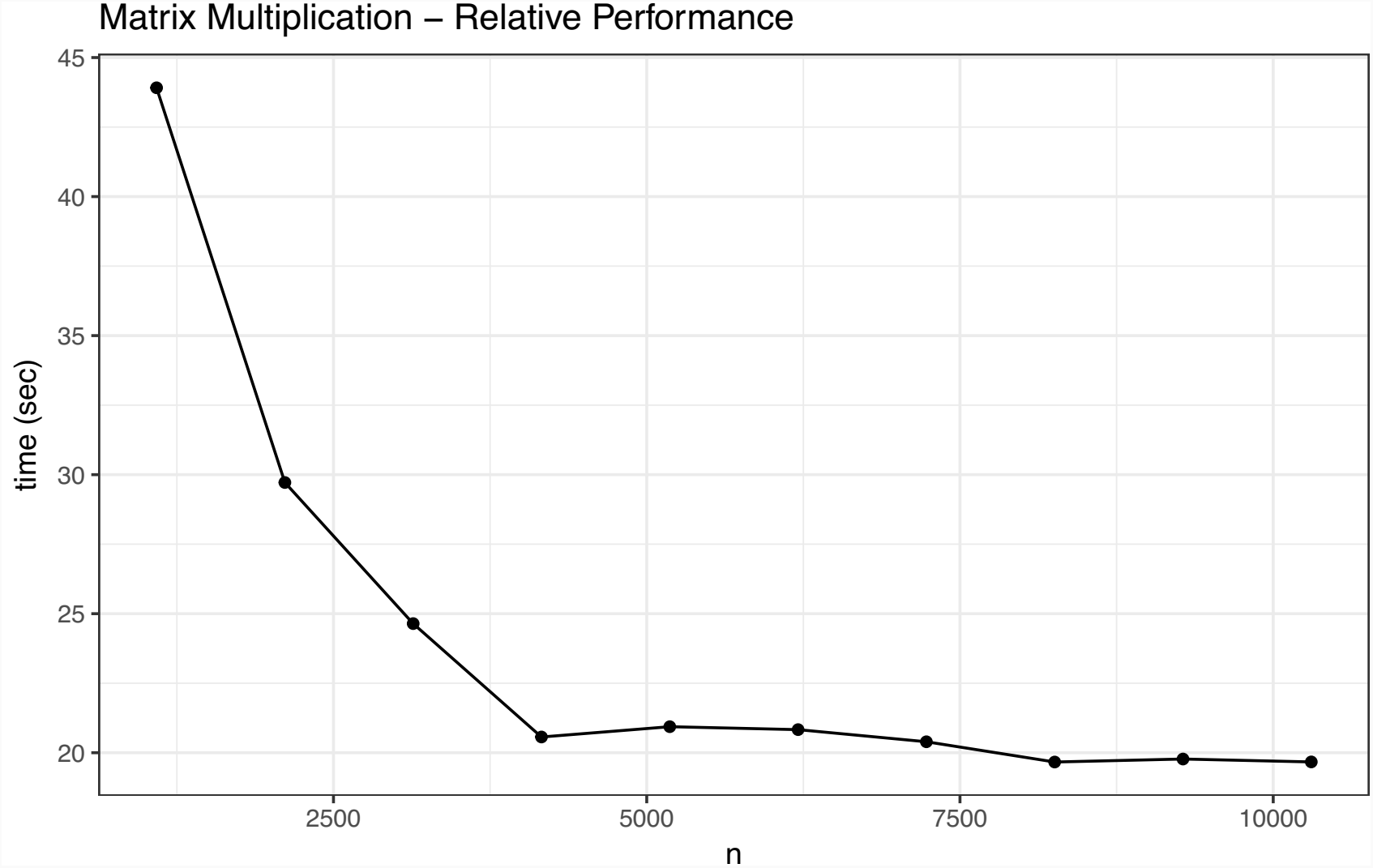

time (secs)
10.0
0.1
2500
5000
7500
10000
n
method
chol inv
LU inv
QR inv
comp
cpu
gpu

Relative Performance



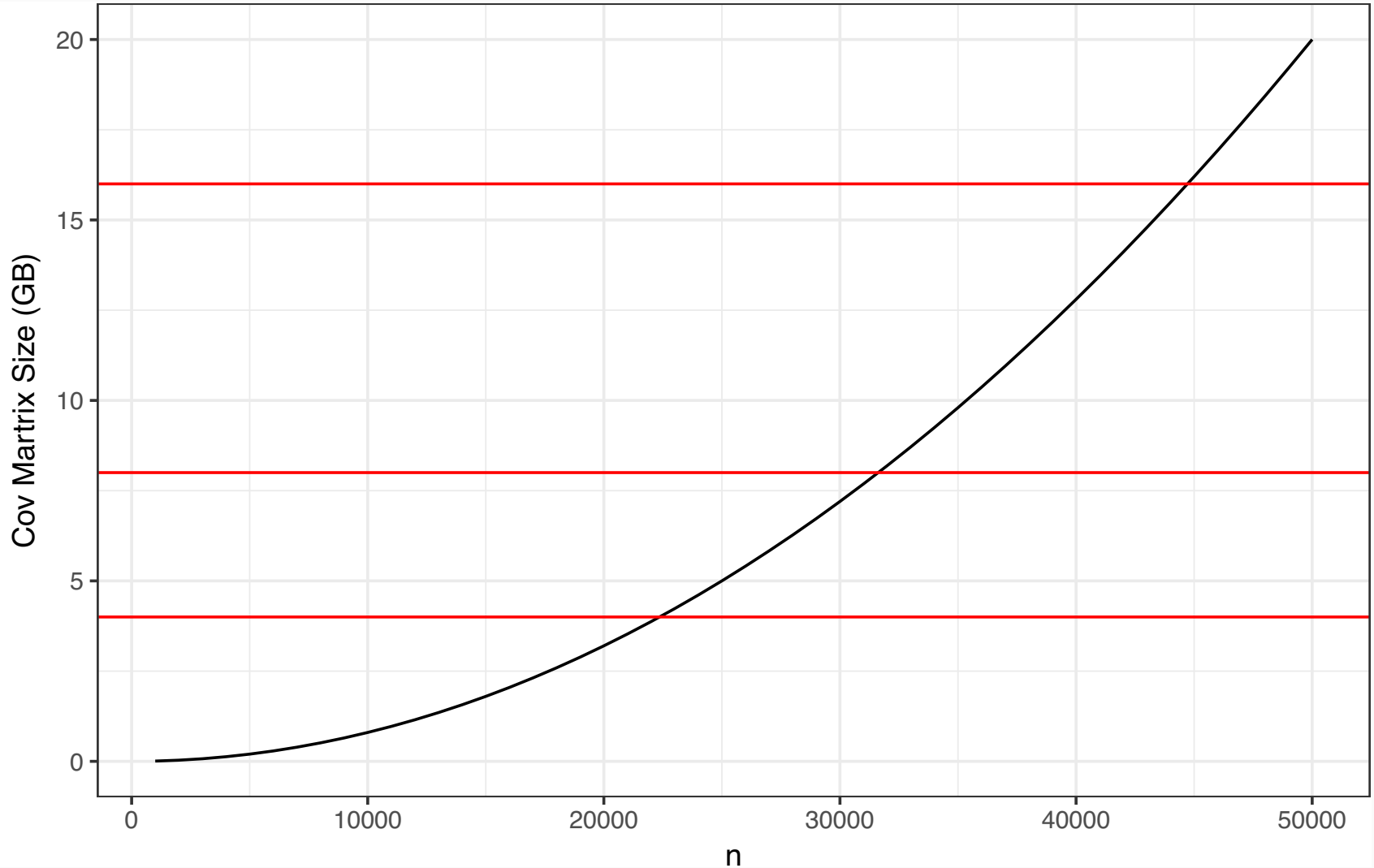
Aside (1) - Matrix Multiplication




Matrix Multiplication – Relative Performance
time (sec)
45
40
35
30
25
20
2500
5000
7500
10000
n

Aside (2) - Memory Limitations

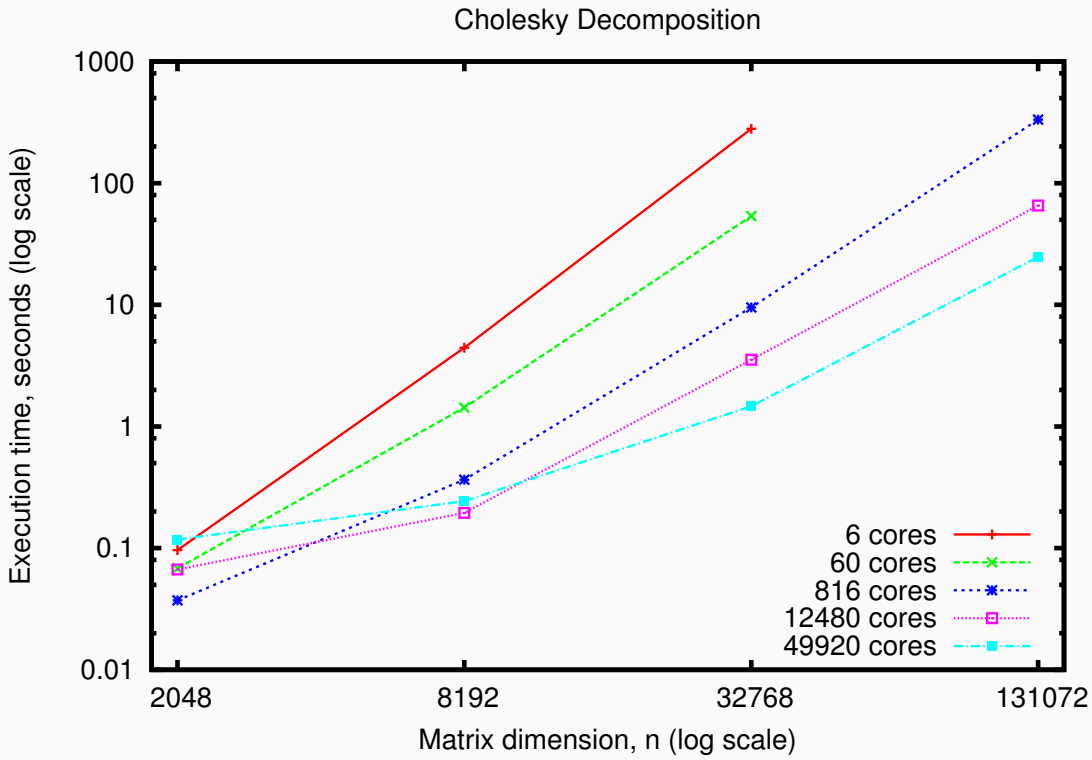
A general covariance is a dense $n \times n$ matrix, meaning it will require $n^2 \times$ 64-bits to store.



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 $n = 65$k (32 GB Cov. matrix)



More scalable solutions?

- Spectral domain / basis functions
- Covariance tapering
- GMRF approximations INLA
- Low-rank approximations PP Rand Proj
- Nearest-neighbor models $(x_1)\ (x_2|x)\ (x_3|x_2,x_1)\ \ldots$

Low Rank Approximations

Low rank approximations in general

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

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

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 singular values are in descending order.

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

$$\begin{aligned}\underset{n\times m}{\tilde{M}} &= \underset{n\times n}{U}\ \underset{n\times m}{\text{diag}(\tilde{S})}\ \underset{m\times m}{V^t} \\ &= \underset{n\times k}{\tilde{U}}\ \underset{k\times k}{\text{diag}(\tilde{S})}\ \underset{k\times m}{\tilde{V}^t}\end{aligned}$$

Example

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

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

$$S = \begin{pmatrix} 1.50 & 0.17 & 0.01 & 0.00 \end{pmatrix}$$

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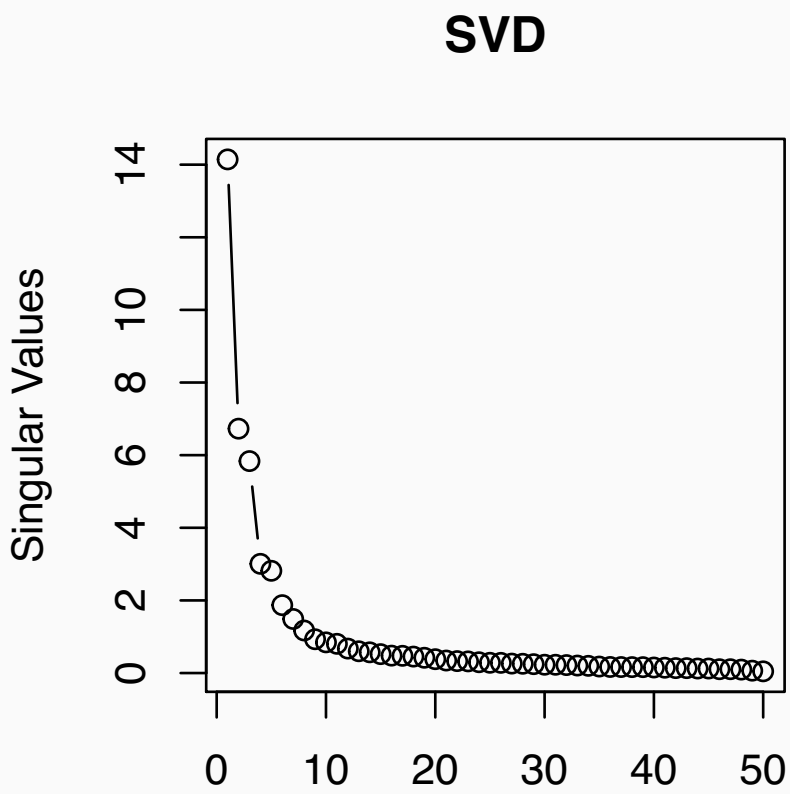
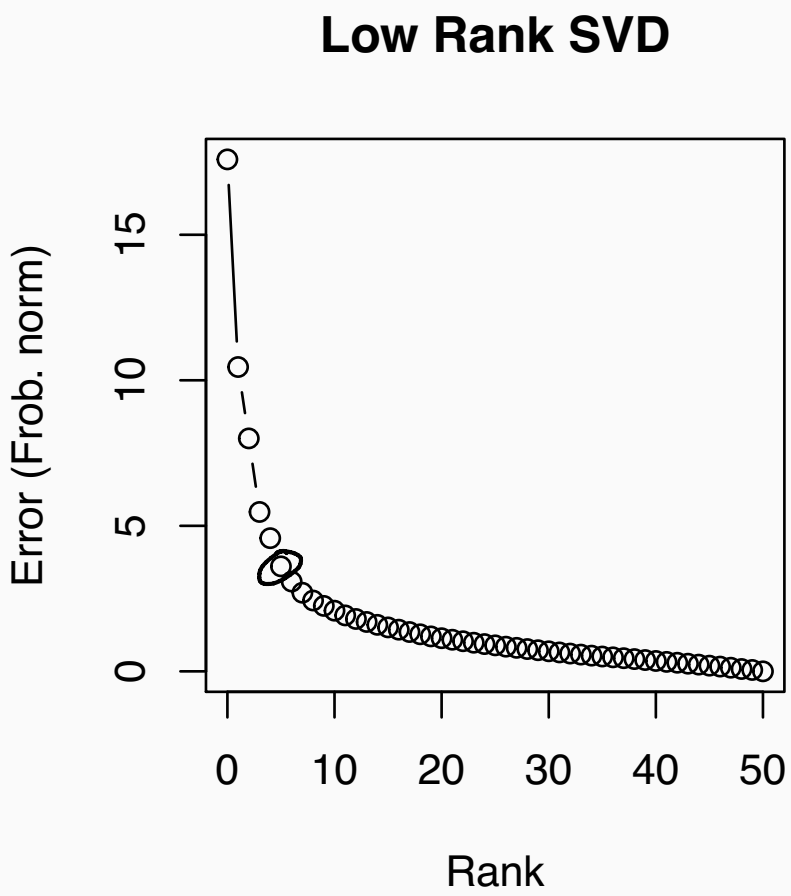
$$M - \tilde{M} = \begin{pmatrix} 0.00022 & -0.00090 & 0.00012 & 0.00077 \\ -0.00090 & 0.00372 & -0.00053 & -0.00317 \\ 0.00012 & -0.00053 & 0.00013 & 0.00039 \\ 0.00077 & -0.00317 & 0.00039 & 0.00277 \end{pmatrix}$$

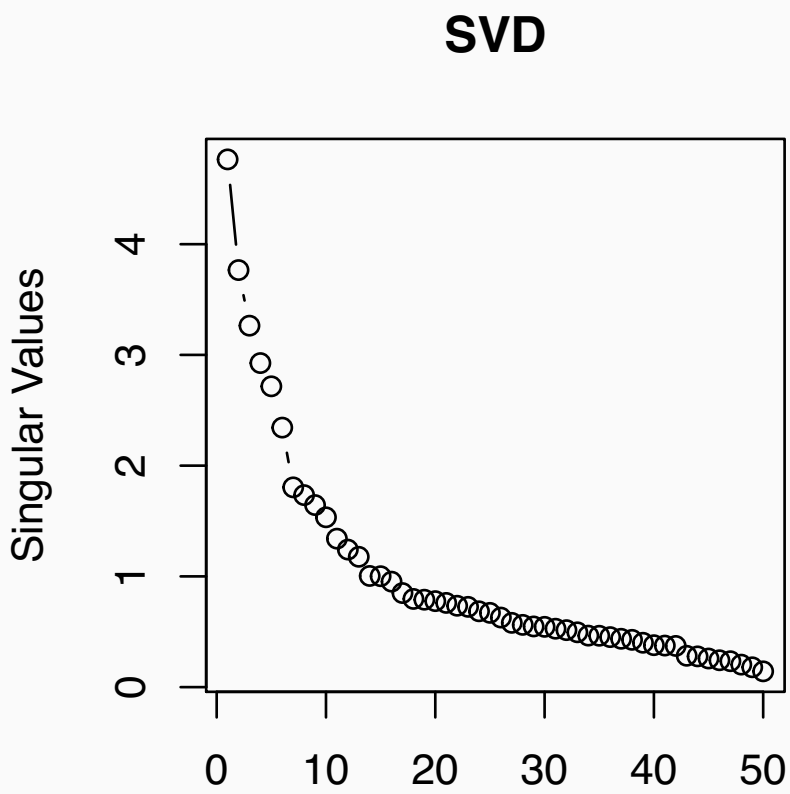
$$\|M - \tilde{M}\|_F = 0.00674$$

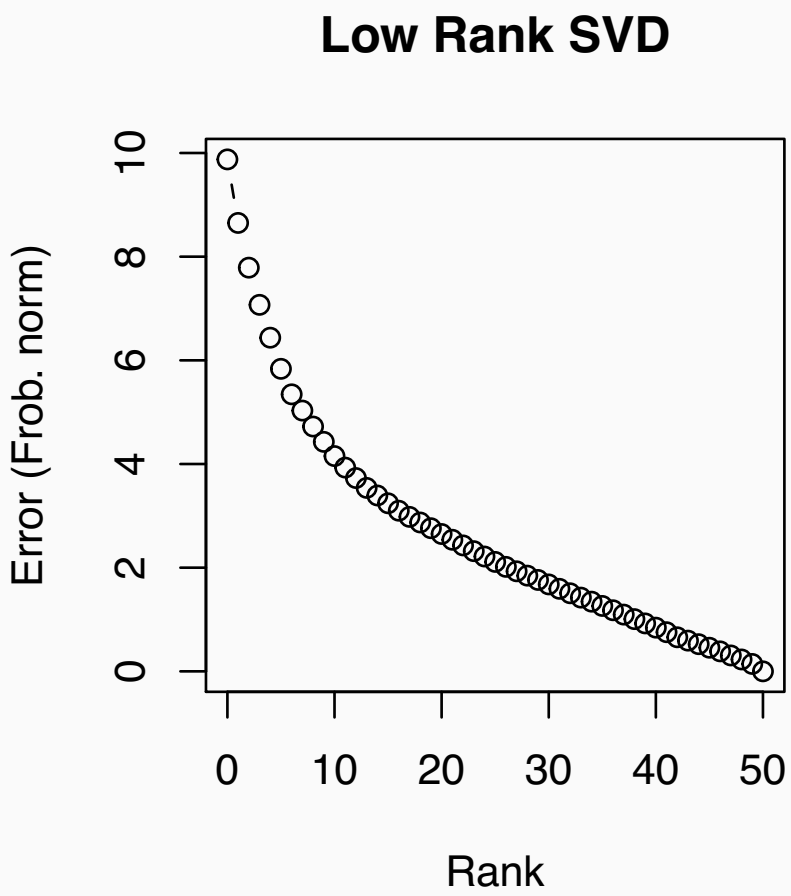
Cov Mat - Strong dependence (large eff. range):





Cov Mat - 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,

$A = \text{diag}$ $S = \text{diag}$

$k \ll n$ or n

$$\underset{n\times m}{\tilde{M}}^{-1} = \left(\underset{n\times m}{A} + \underset{n\times k}{U} \underset{k\times k}{S} \underset{k\times m}{V^t} \right)^{-1}$$

$$= A^{-1} - A^{-1}U\left(S^{-1} + V^t A^{-1} U\right)^{-1} V^t A^{-1}.$$

$k \times k$ $k \times k$

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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 $S = \text{diag}(S)$.
- $\left(S^{-1} + V^t A^{-1} U\right)$ is $k \times k$ which is also hopefully small.

Aside - Determinant

Remember for any MVN distribution when evaluating the likelihood

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

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".

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

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

- 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,

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

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
- $A = \tau^2 I$ or a similar diagonal matrix

Predictive Processes

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For a rank k approximation,

- Pick k knot locations $\mathbf{s}^\star$

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- Pick k knot locations $\mathbf{s}^\star$
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- Approximate full covariance using

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

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

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

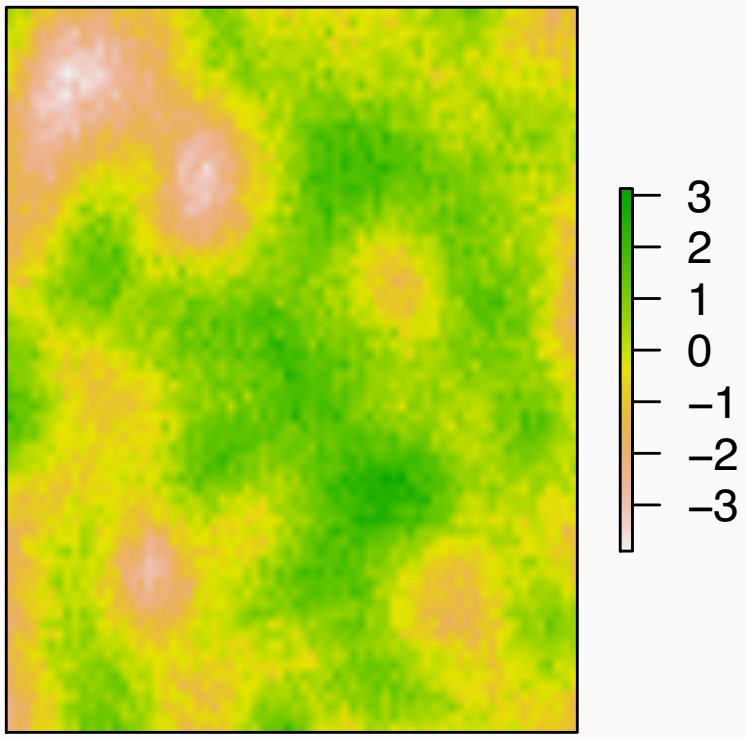
Example

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

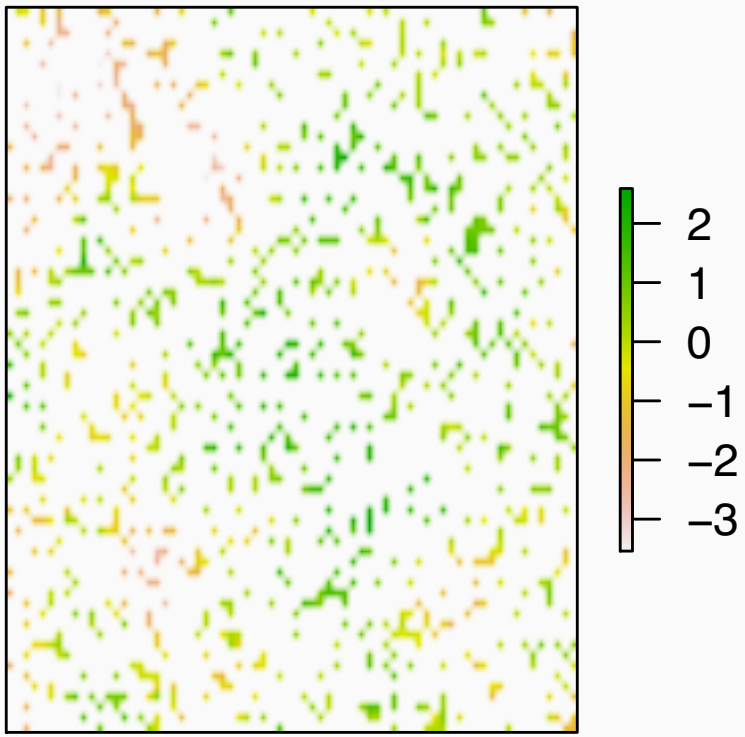
$$\{\Sigma\}_{ij} = \sigma^2 \exp\left(-(\phi\, d)^2\right) + \tau^2 I$$

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

True Surface

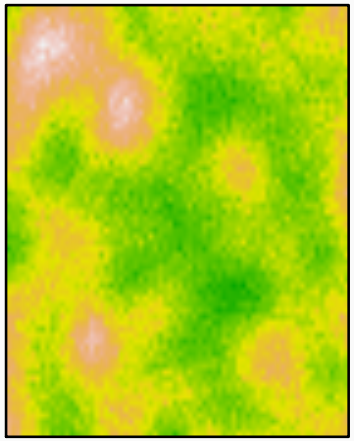


Observed Data

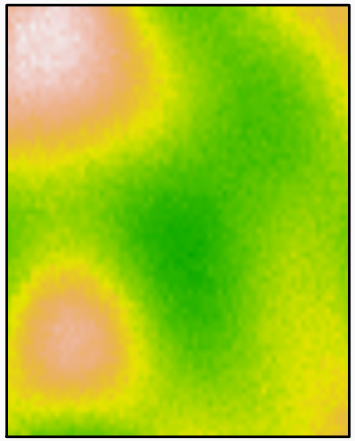


Predictive Process Model Results

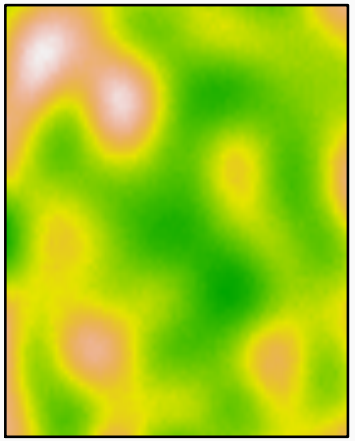
True Field



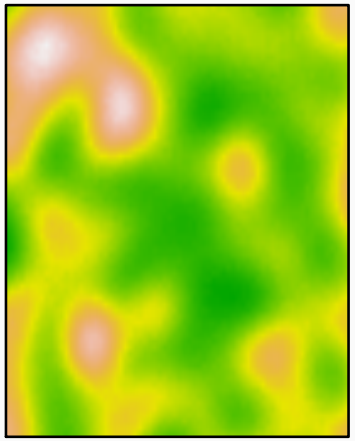
PP – 5 x 5 knots



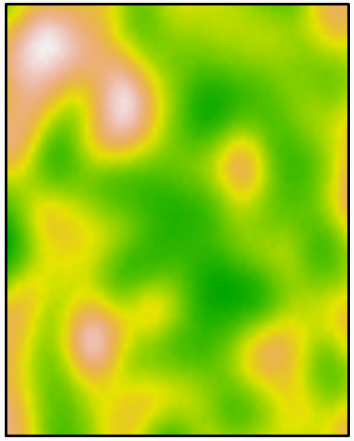
PP – 10 x 10 knots



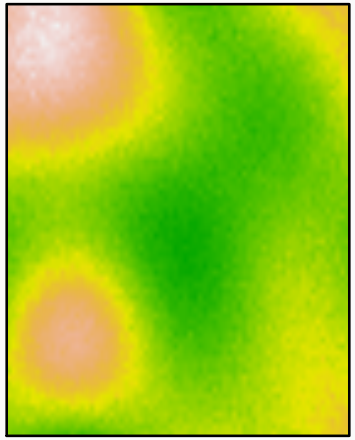
PP – 15 x 15 knots



Full GP



Mod. PP – 5 x 5 knots



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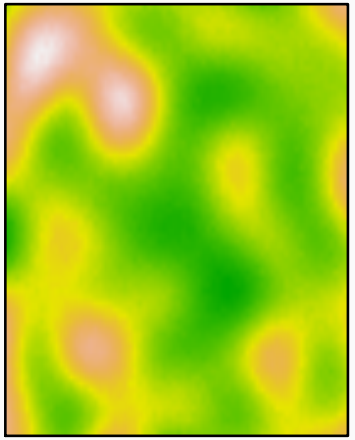

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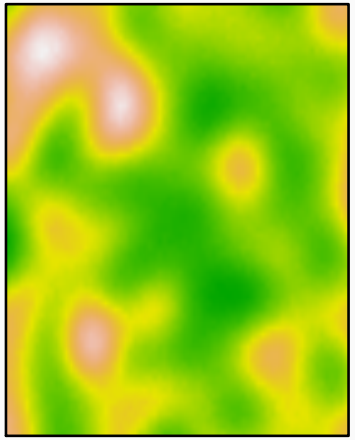
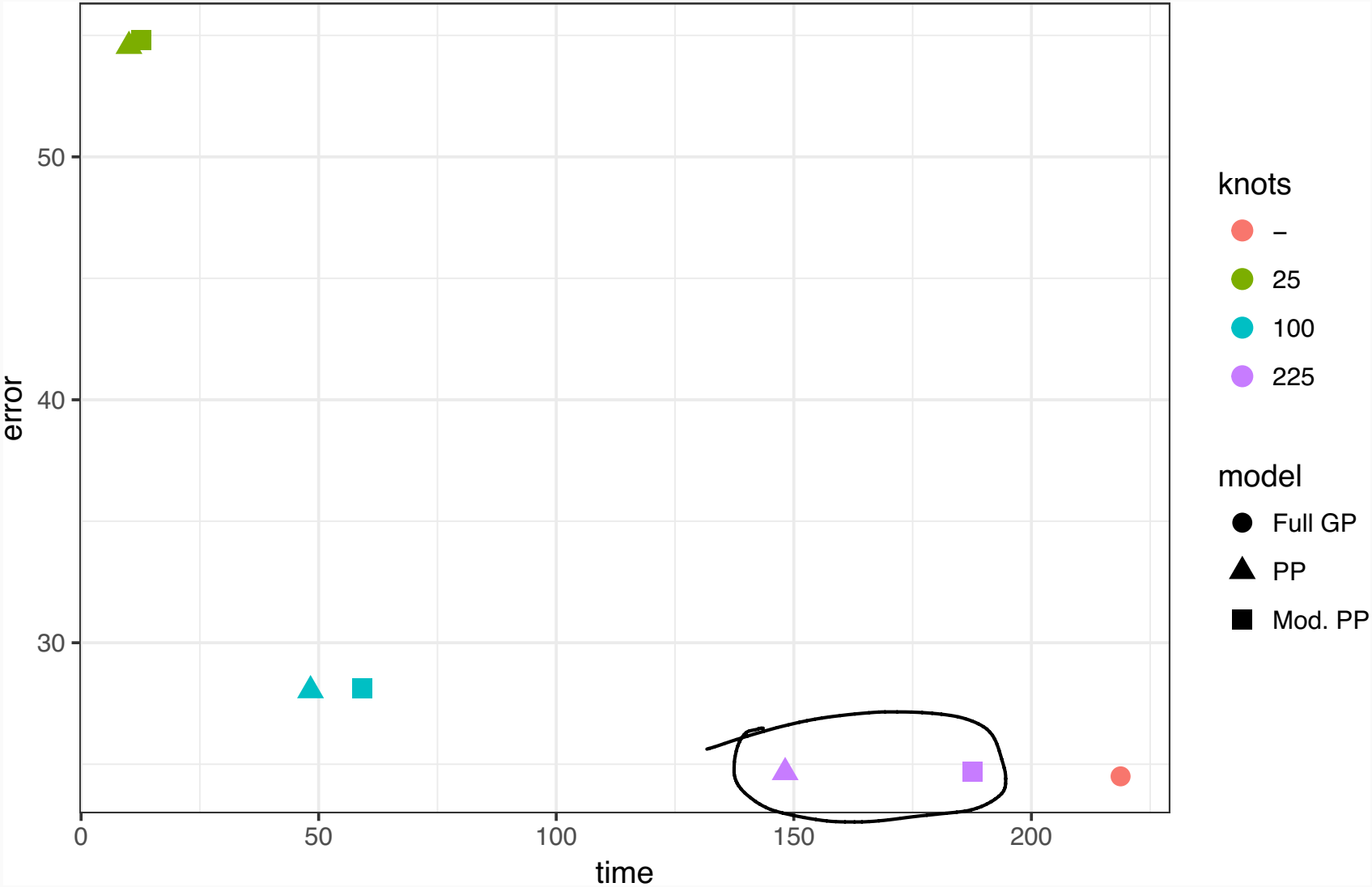
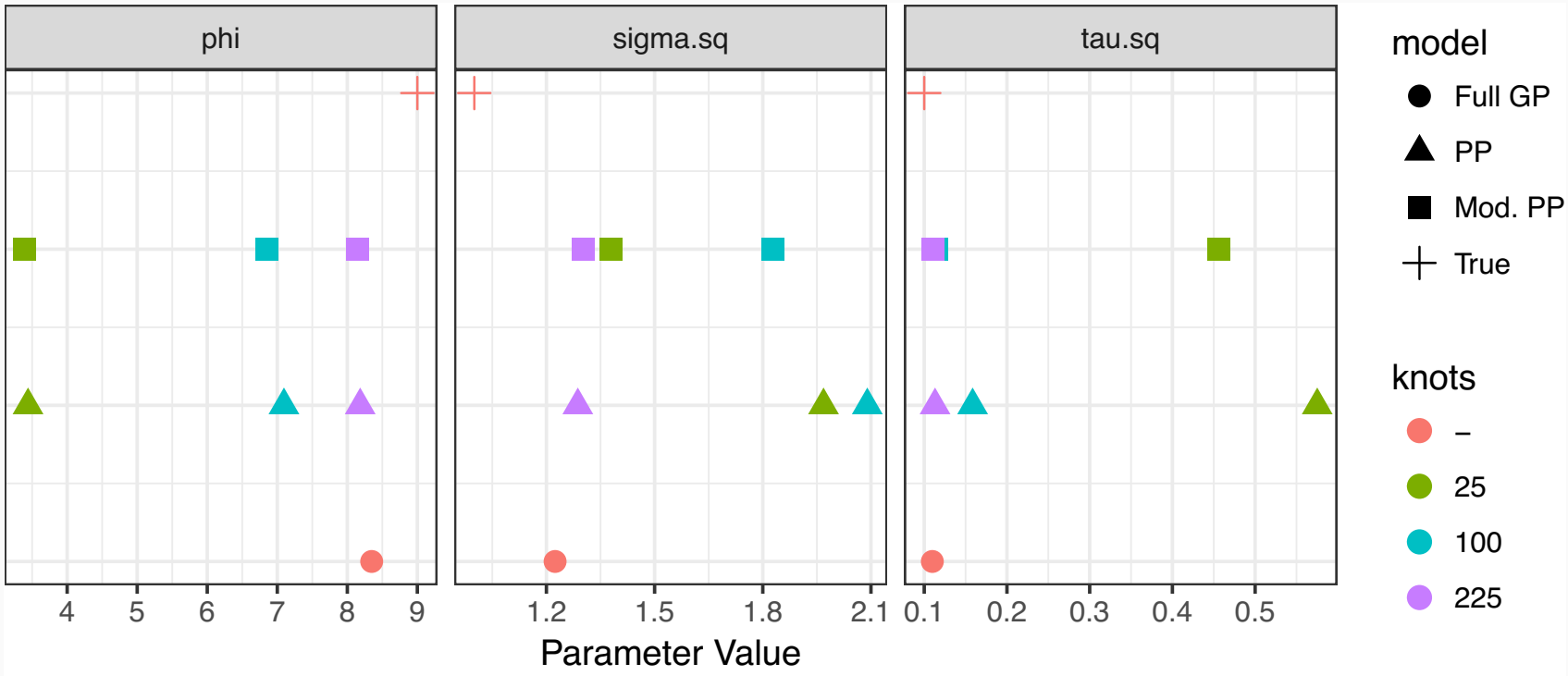


Performance



Parameter Estimates



Random Projections

Low Rank Approximations via Random Projections

1. Starting with an matrix $\underset{m \times n}{\mathbf{A}}$.

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

Resulting approximation has a bounded expected error,

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

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

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Random Matrix Low Rank Approximations and GPs

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Once again we have a bound on the error,

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

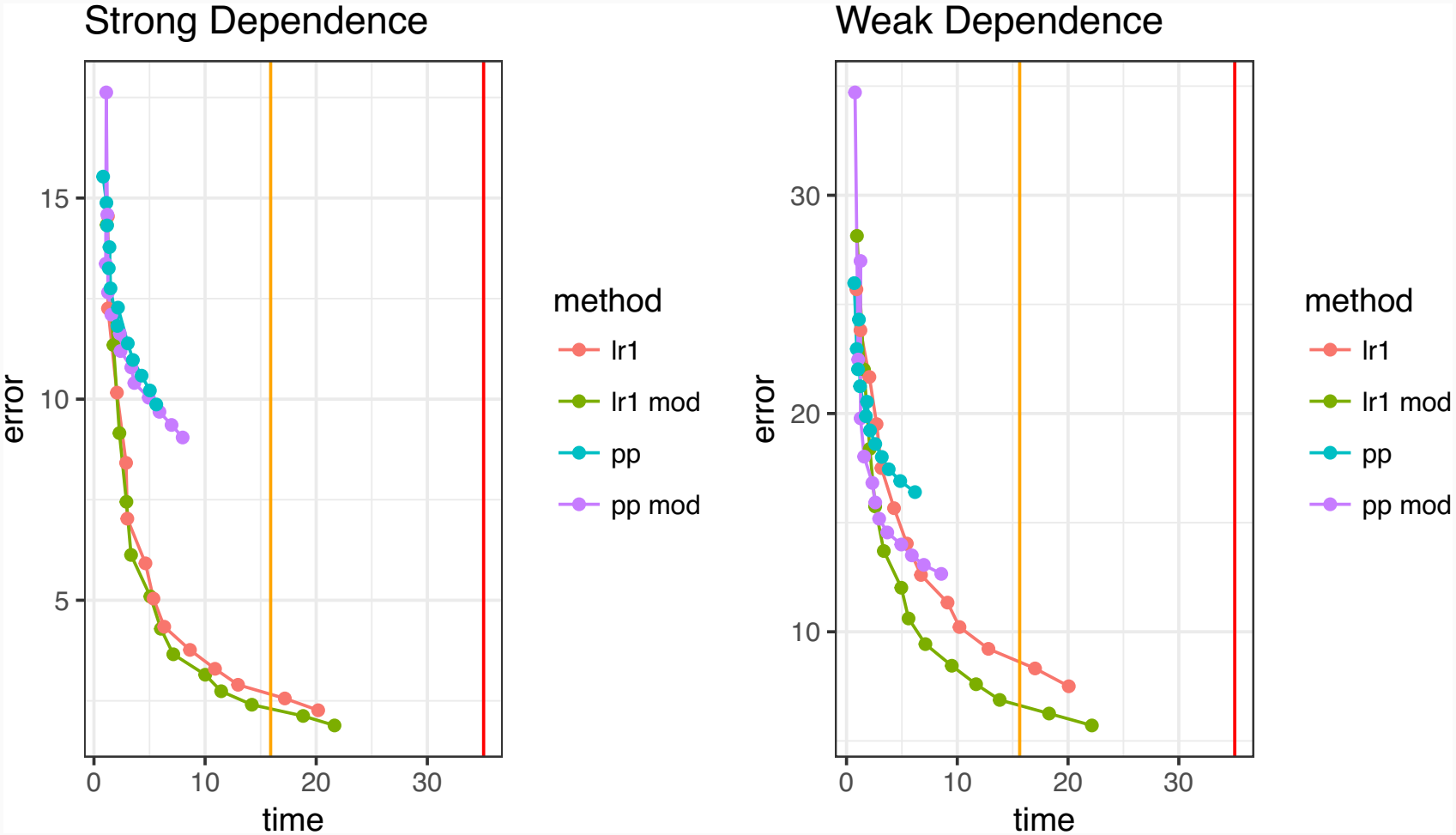
Halko, Martinsson, Tropp (2011), Banerjee, Dunson, Tokdar (2012)

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 ($\mathbf{A}\,\mathbf{\Omega}$) and several small matrix decompositions (QR, eigen).

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



Rand. Projection LR Depositions for Prediction

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

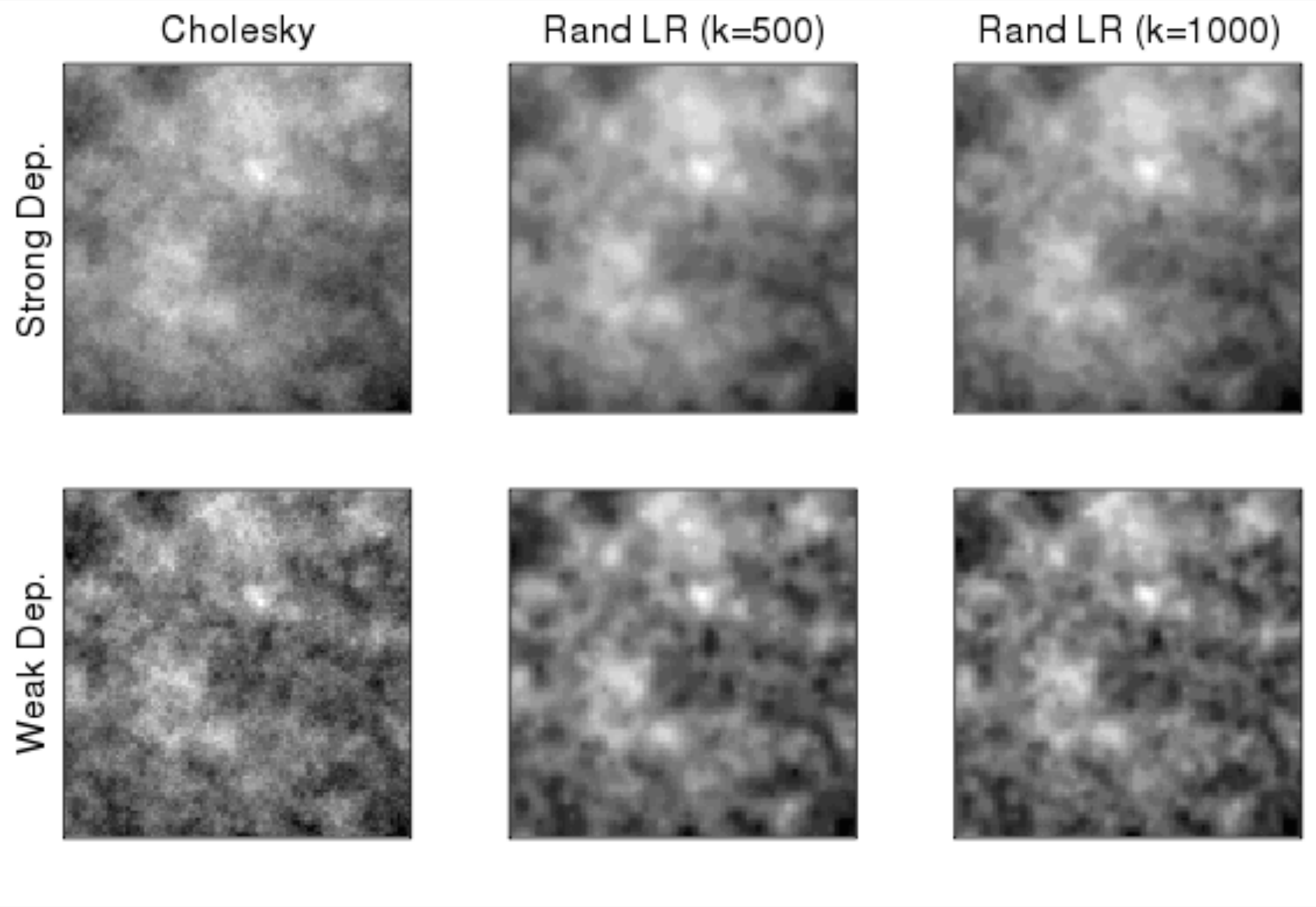
$$\mathbf{y} \sim \mathcal{N}(0, \mathbf{\Sigma})$$
$$\Sigma \approx \mathbf{USU}^t = (\mathbf{US}^{1/2}\mathbf{U}^t)(\mathbf{US}^{1/2}\mathbf{U}^t)^t$$

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.

Dehdari, Deutsch (2012)



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