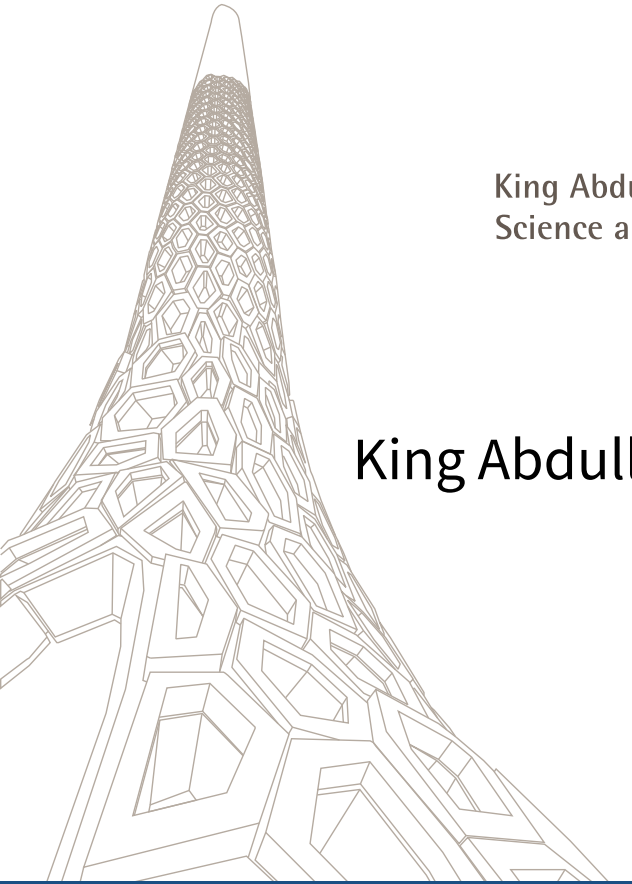
Scalable Bayesian inference for Latent Gaussian Models



King Abdullah University of Science and Technology

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Håvard Rue
King Abdullah University of Science and Technology
Saudi Arabia

June 2026

Outline

- Importance of GMRFs
- Latent Gaussian Models
- Bayesian Inference
- Key component: (a new) Sparse matrix solver

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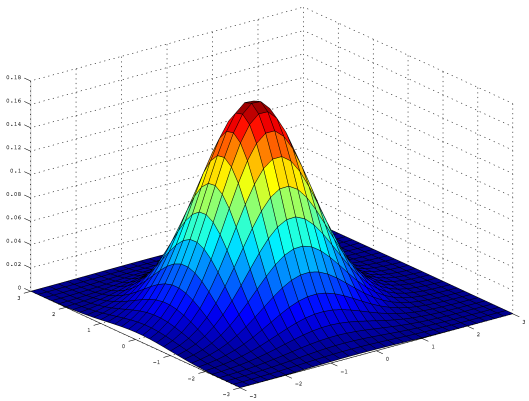
- Random vector $(x_1, \ldots, x_n)$
- (Scaled and centred) density

$$\pi(\boldsymbol{x}) \propto |\boldsymbol{\Sigma}|^{-1/2} \exp\left(-\frac{1}{2}\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}\right)$$

- $\boldsymbol{\Sigma}$ is the (SPD) covariance matrix
- $\Sigma_{ij} = \mathrm{E}(x_i x_j)$
- $\Sigma_{ij} = 0 \Leftrightarrow x_i \perp x_j \; (i \neq j)$



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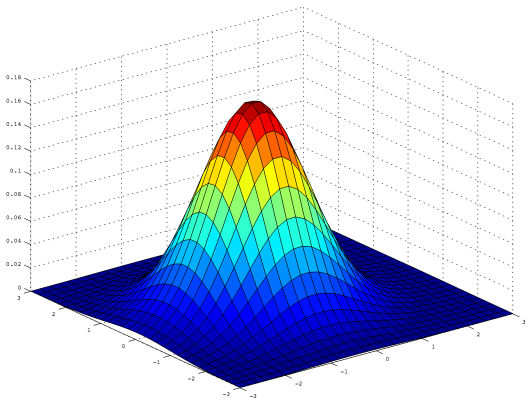

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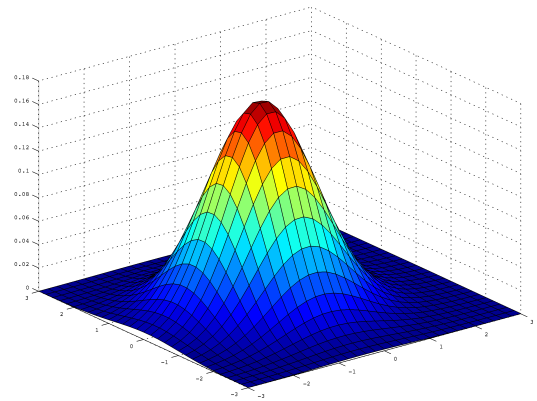

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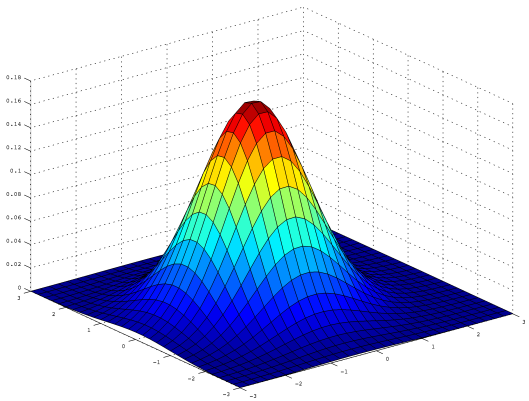

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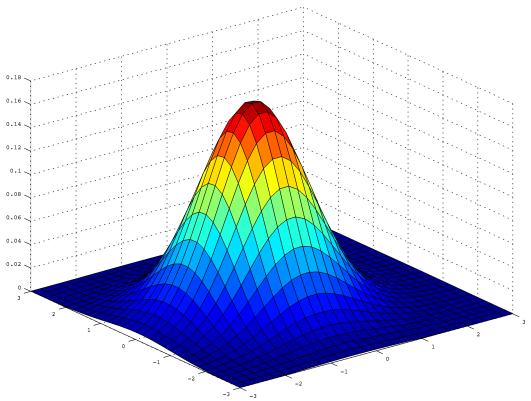

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Conditional independence and GMRFs

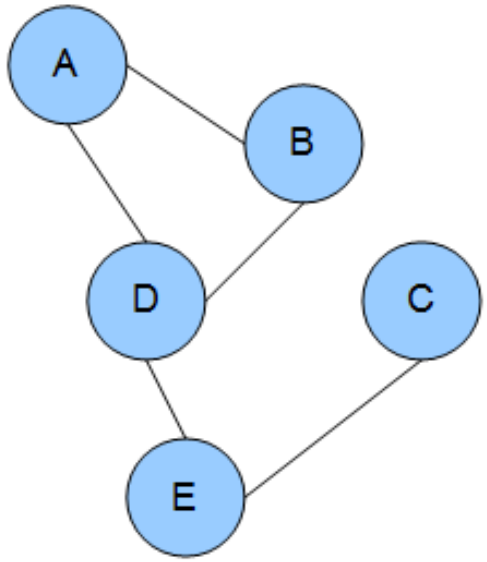
- Conditional independence of x_i and x_j, equals independence in

$$\pi(x_i, x_j \mid \boldsymbol{x}_{-ij})$$

- The result is, with $\boldsymbol{Q} = \boldsymbol{\Sigma}^{-1}$, that

$$Q_{ij} = 0 \Leftrightarrow x_i \perp x_j \mid \boldsymbol{x}_{-ij}$$

- This is potentially very very useful, as
  - If $\boldsymbol{Q}$ is fully connected then $\boldsymbol{\Sigma}$ is dense (Cayley–Hamilton thm)
  - Explain dependence by a sparse $\boldsymbol{Q}$
  - Sparse matrices: faster computations



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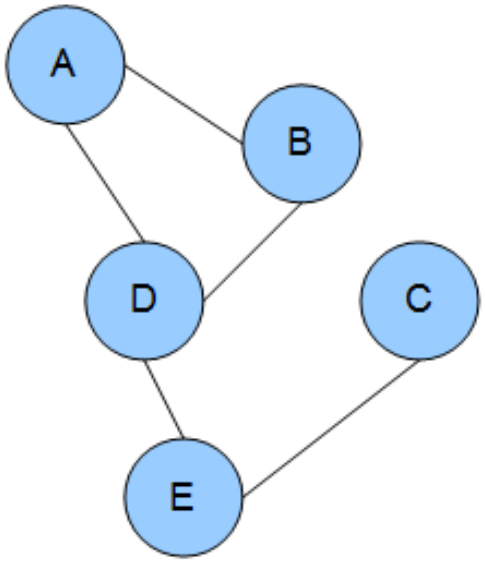

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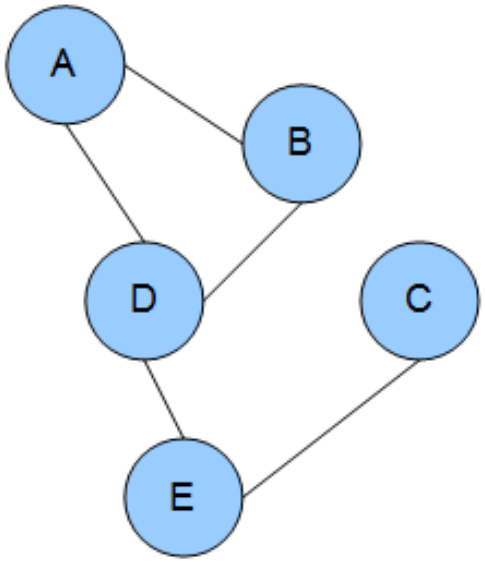

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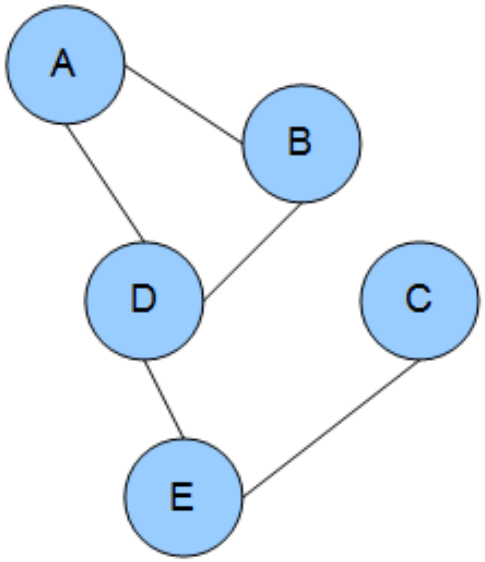

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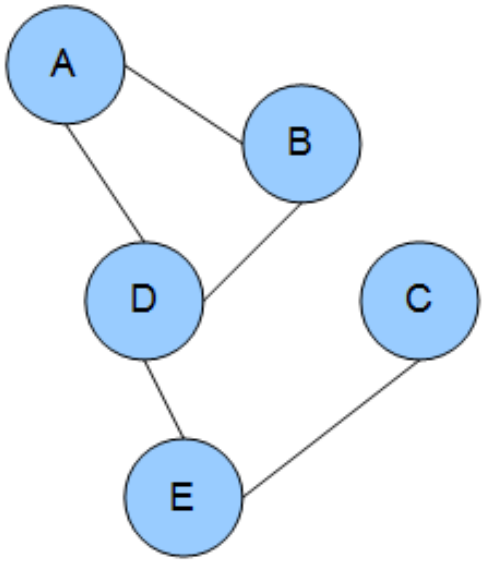

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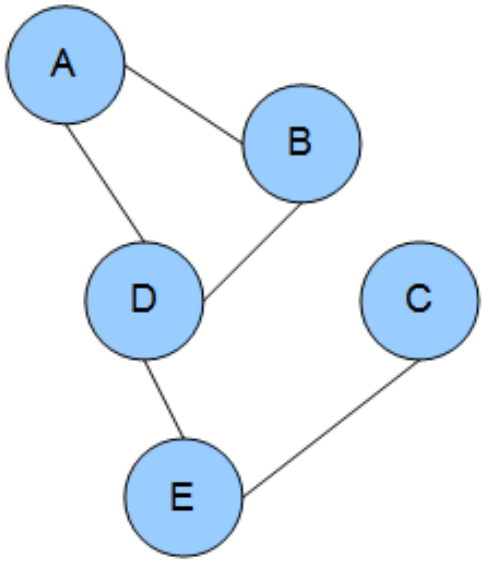


Example: Markov processes in time

- Auto-regressive process of order 1

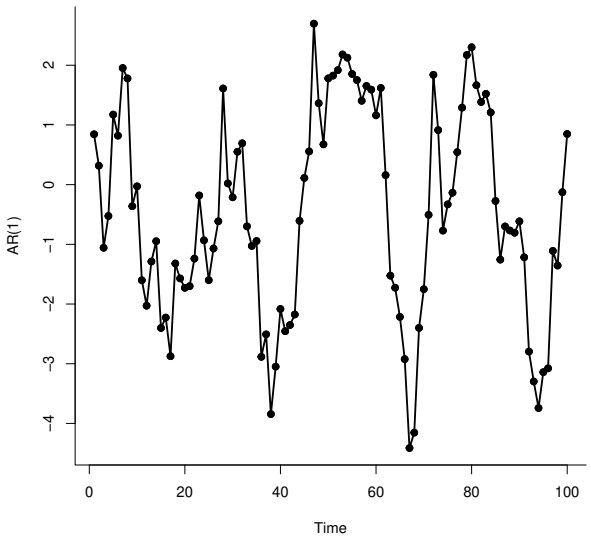
$$x_t = \phi x_{t-1} + \epsilon_t, \quad 0 \le \phi < 1, \quad t = 1, \ldots, n$$

with Gaussian noise ϵ_t

- Linear graph
- $\boldsymbol{Q}$ is tridiagonal (factorisation cost $\mathcal{O}(n)$)
- $\boldsymbol{\Sigma}$ is $\phi^{-|i-j|}$ (exp-correlation function)
- Cont.time: Ornstein-Uhlenbeck process

$$dx_t = -\theta\, x_t\, dt + dW_t,$$

Wiener process W_t



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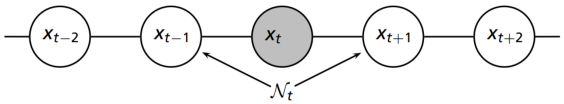

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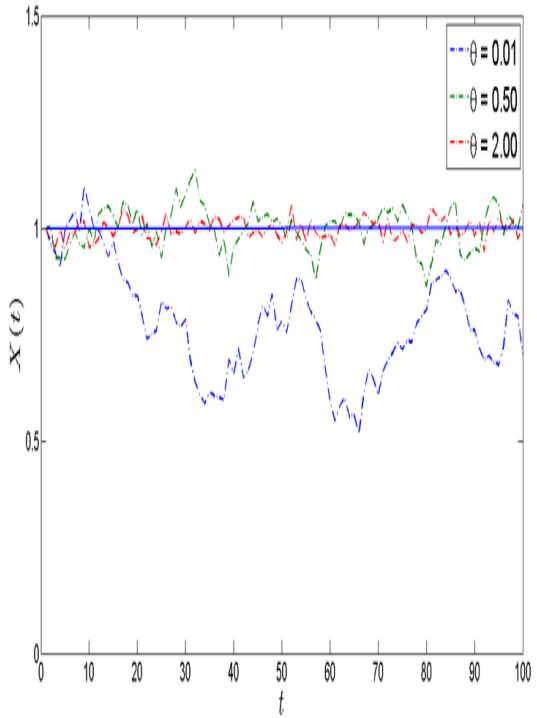

How does correlation work?

- Let

$$x_1 = z_1 + \mu$$

$$x_2 = z_2 + \mu$$

- z_1, z_2, μ are independent zero mean Gaussian's
- $\text{Var}(\mu) = \sigma^2$, $\text{Var}(z_i) = 1$
- Then

$$\text{Corr}(x_1, x_2) = \frac{\sigma^2}{\sigma^2 + 1}$$

- This is an constructive/intuitive way to introduce correlation (which is a 'consequence' of the construction)

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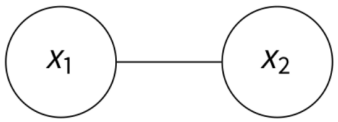

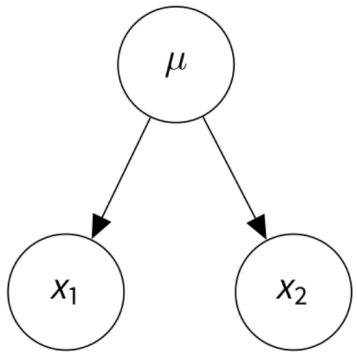

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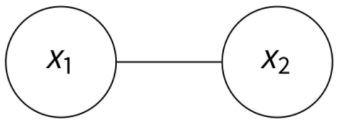

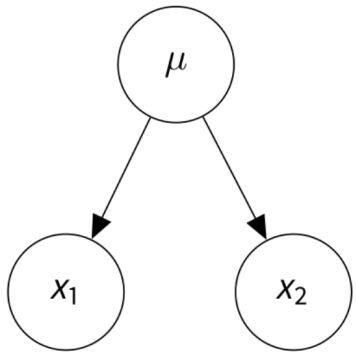

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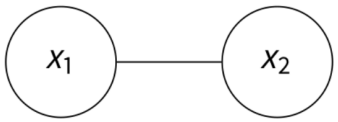

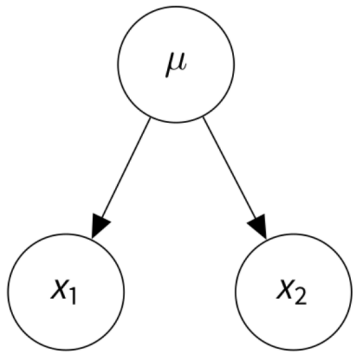

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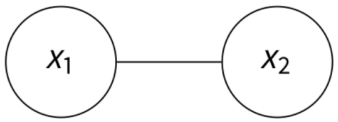

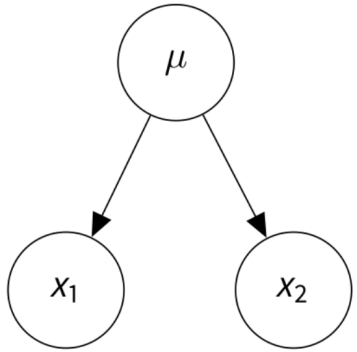

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What are good "operations" for GMRFs?

Conditioning $\boldsymbol{x}_1|\boldsymbol{x}_2$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{pmatrix} \qquad \boldsymbol{Q} = \begin{pmatrix} \boldsymbol{Q}_{11} & \boldsymbol{Q}_{12} \\ \boldsymbol{Q}_{12}^T & \boldsymbol{Q}_{22} \end{pmatrix}$$

$$\text{Var}(\boldsymbol{x}_1|\boldsymbol{x}_2) = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T \qquad \text{Prec}(\boldsymbol{x}_1|\boldsymbol{x}_2) = \boldsymbol{Q}_{11}$$

What are good "operations" for GMRFs?

Updating/Learning:

$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_{\boldsymbol{x}}^{-1})$$

then we observe

$$\boldsymbol{y}|\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{x}, \boldsymbol{Q}_{\boldsymbol{y}}^{-1})$$

$$\text{Var}(\boldsymbol{x}|\boldsymbol{y}) = \left(\boldsymbol{\Sigma}_{\boldsymbol{x}}^{-1} + \boldsymbol{\Sigma}_{\boldsymbol{y}}^{-1}\right)^{-1} \qquad \text{Prec}(\boldsymbol{x}|\boldsymbol{y}) = \boldsymbol{Q}_{\boldsymbol{x}} + \boldsymbol{Q}_{\boldsymbol{y}}$$

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Distribution of sums:

$$\eta = \boldsymbol{x} + \boldsymbol{y} + \boldsymbol{z}$$

where $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_{\boldsymbol{x}}^{-1})$, $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_{\boldsymbol{y}}^{-1})$ and $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_{\boldsymbol{z}}^{-1})$.

$$\boldsymbol{Q}_\eta = \left(\boldsymbol{Q}_{\boldsymbol{x}}^{-1} + \boldsymbol{Q}_{\boldsymbol{y}}^{-1} + \boldsymbol{Q}_{\boldsymbol{z}}^{-1}\right)^{-1}$$

$\boldsymbol{Q}_\eta$ is (in general) dense and it is costly to update $\boldsymbol{Q}_\eta$

The covariance formulation is easy

$$\boldsymbol{\Sigma}_\eta = \boldsymbol{\Sigma}_{\boldsymbol{x}} + \boldsymbol{\Sigma}_{\boldsymbol{y}} + \boldsymbol{\Sigma}_{\boldsymbol{z}}$$

Marginalisation destroy sparsity...

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$\boldsymbol{Q}_\eta$ is (in general) dense and it is costly to update $\boldsymbol{Q}_\eta$

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- Using "ϵ" with high precision τ

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- Then

$$\text{Var}\begin{pmatrix} \eta \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \tau I & -\tau I & -\tau I & -\tau I \\ & Q_x + \tau I & \tau I & \tau I \\ & & Q_y + \tau I & \tau I \\ & & & Q_z + \tau I \end{pmatrix}$$

- Good practical solution unless choice of τ becomes an issue

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Additive regression models/GLM++

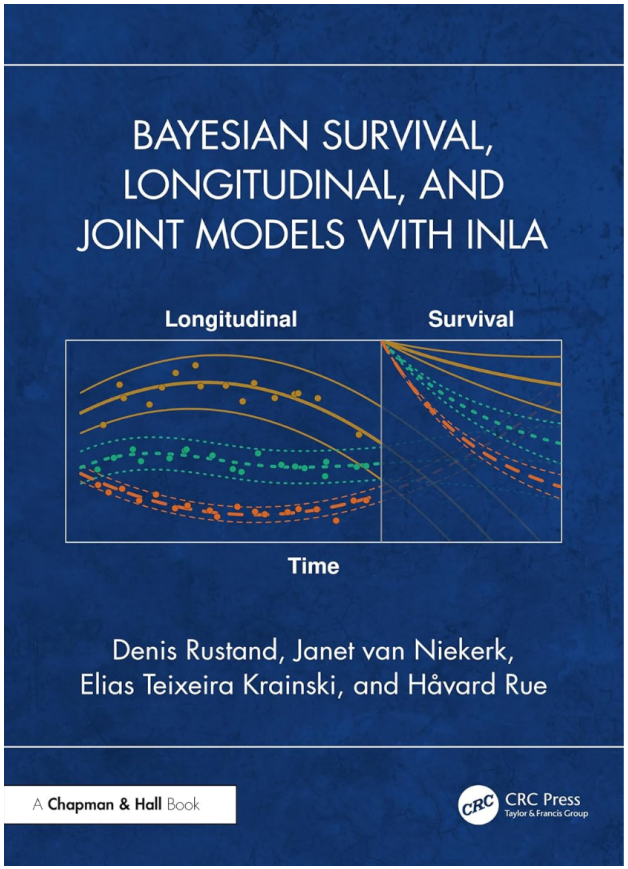
- Linear predictor

$$\eta_i = \mu + \sum_j \beta_j z_{ij} + \boldsymbol{f}_{1i} + \boldsymbol{f}_{2i} + \cdots$$

with observations

$$y_i | \ldots \sim \pi(y_i | \eta_i, \ldots)$$

- $\boldsymbol{f}_k$ is a Gaussian process, think times-series, spatial-model, spline, some kind of dependent 'random effect', measurement error model, etc...



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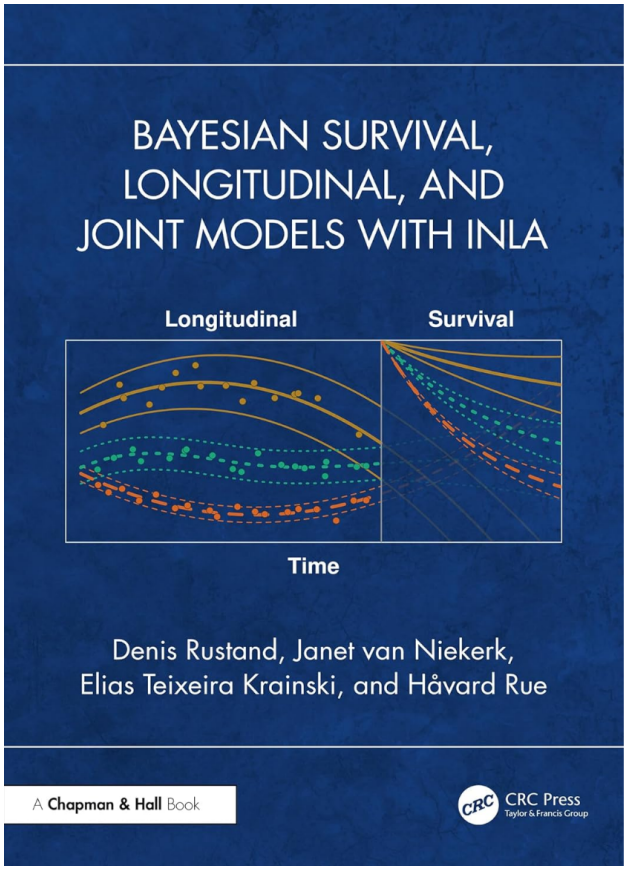


Key observation

- If each $\boldsymbol{f}_k$ is a GMRF, then

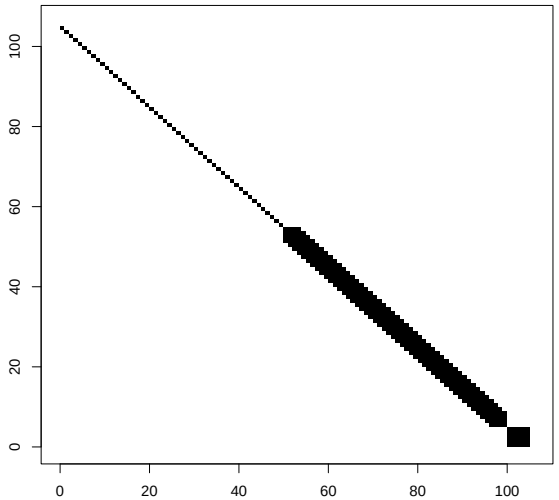
$$\boldsymbol{x} = (\beta_1, \beta_2, \ldots, \boldsymbol{f}_1, \boldsymbol{f}_2, \ldots)$$

  is also a GMRF with precision matrix $\boldsymbol{Q}$

- Let $\eta = \boldsymbol{A}\boldsymbol{x}$. Assume Gaussian data with unit variance, then $\boldsymbol{x}|\boldsymbol{y}$ is a GMRF with precision matrix

$$\boldsymbol{Q} + \boldsymbol{A}^T\boldsymbol{A}$$

- Non-Gaussian data: "sequence of Gaussian-data"



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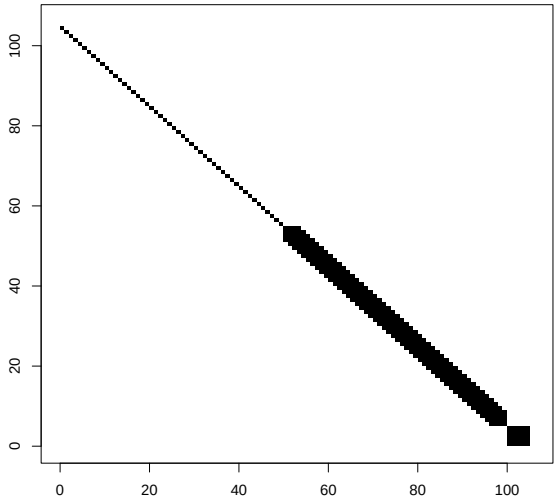

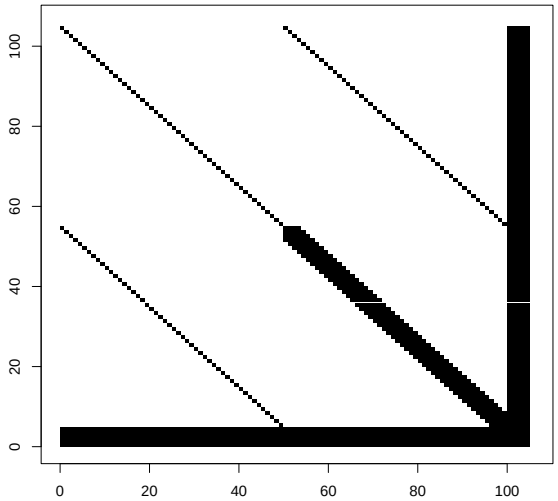

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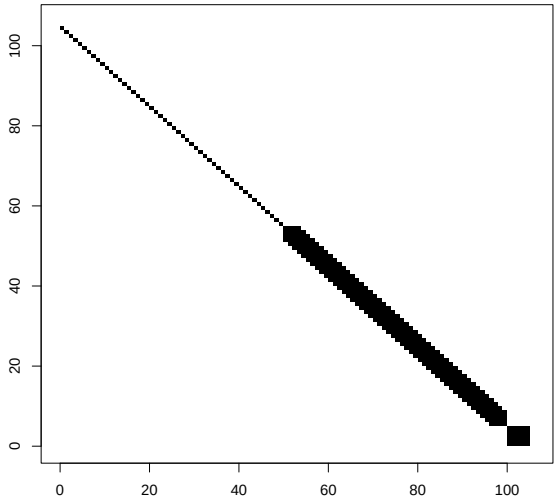

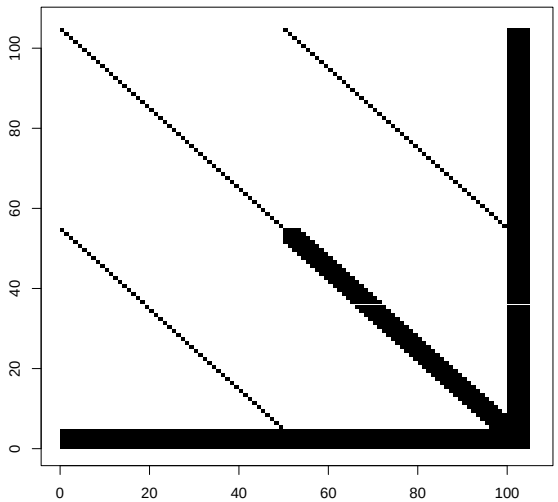

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GMRFs is closed

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- conditioning

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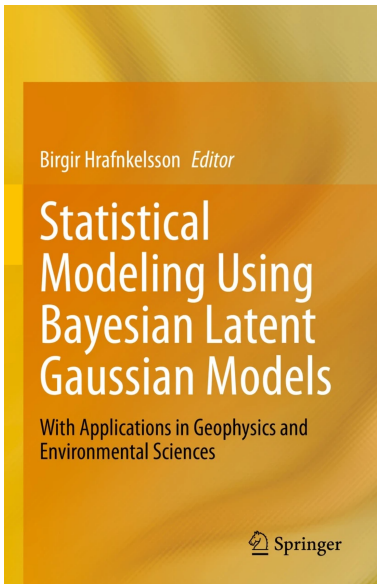
Bayesian inference: Latent Gaussian models (LGMs)

The most important class of models...

- Conditionally independent data $y_i|\eta_i, \theta$
- Latent

$$\eta_i = \sum_j \beta_j c_{ij} + \sum_k f_{ki}$$

- Hyperparameters θ (latent and/or likelihood)
- Each component is a GMRF (or a "small" dense)
- Covariance is a property, not a defining quantity



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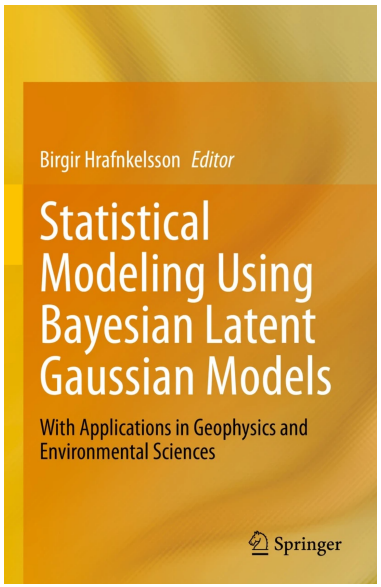

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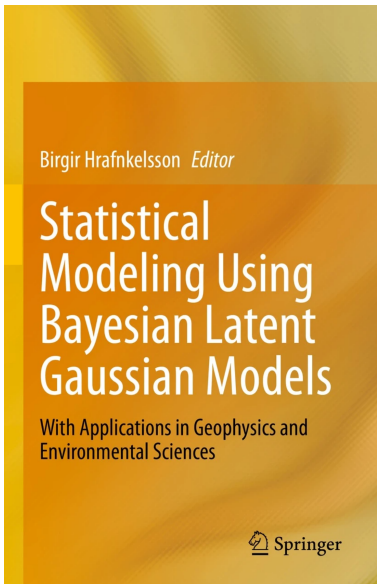

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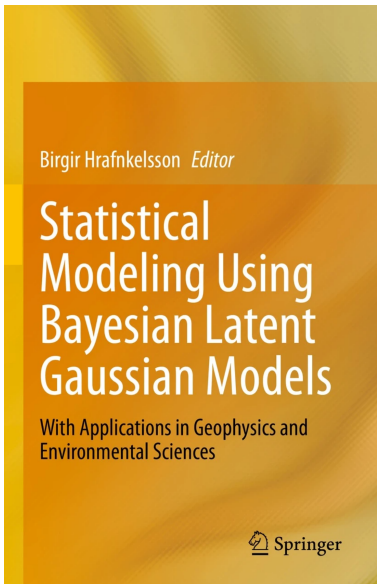

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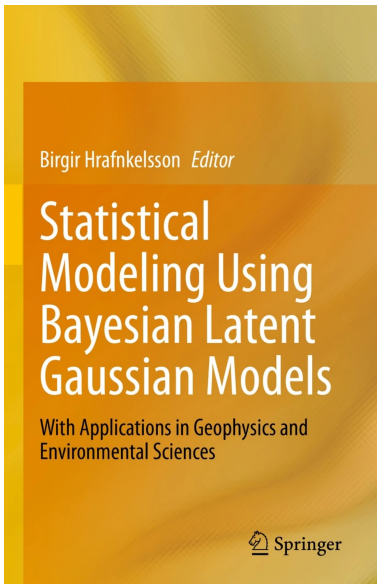
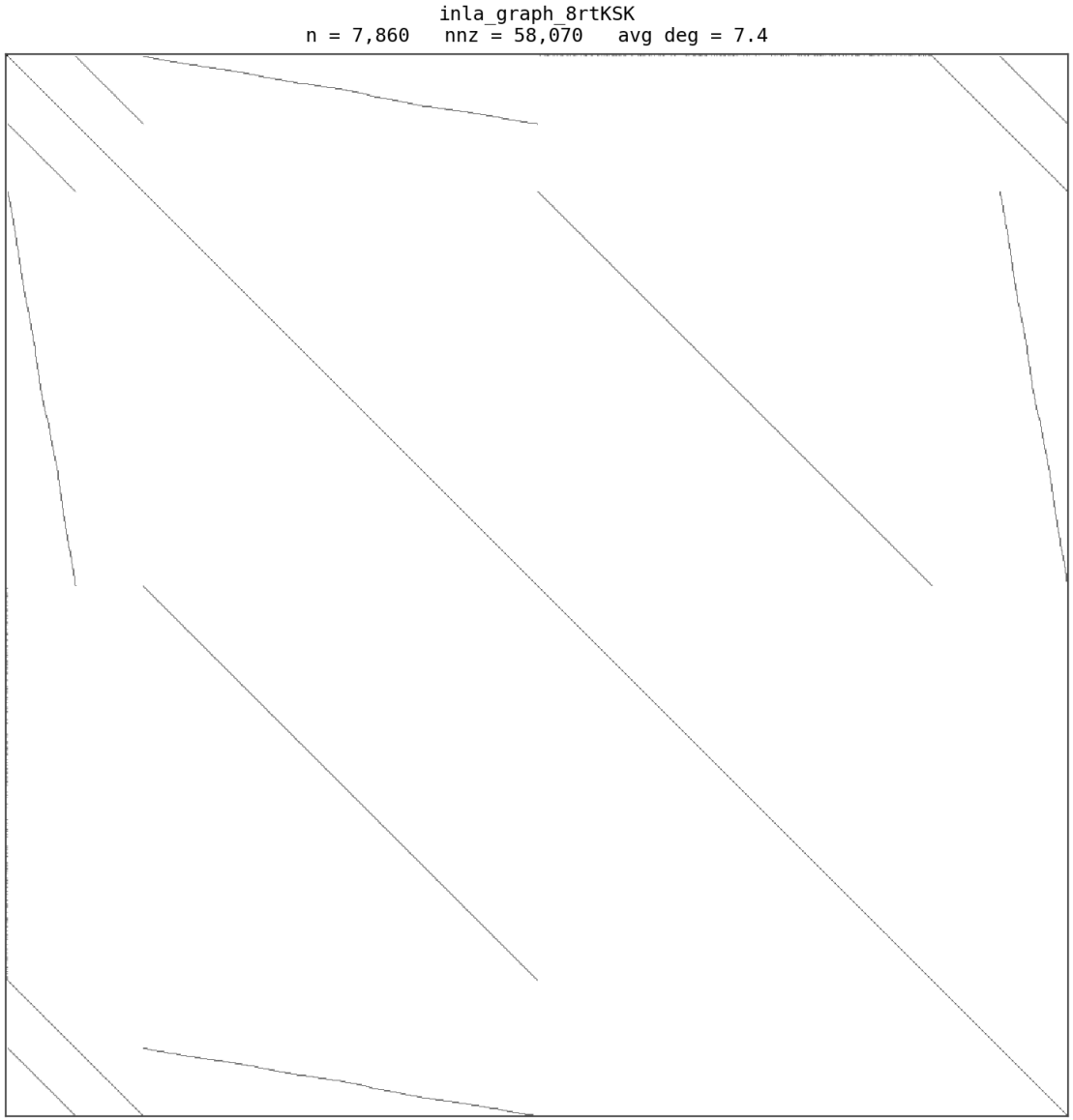


Examples



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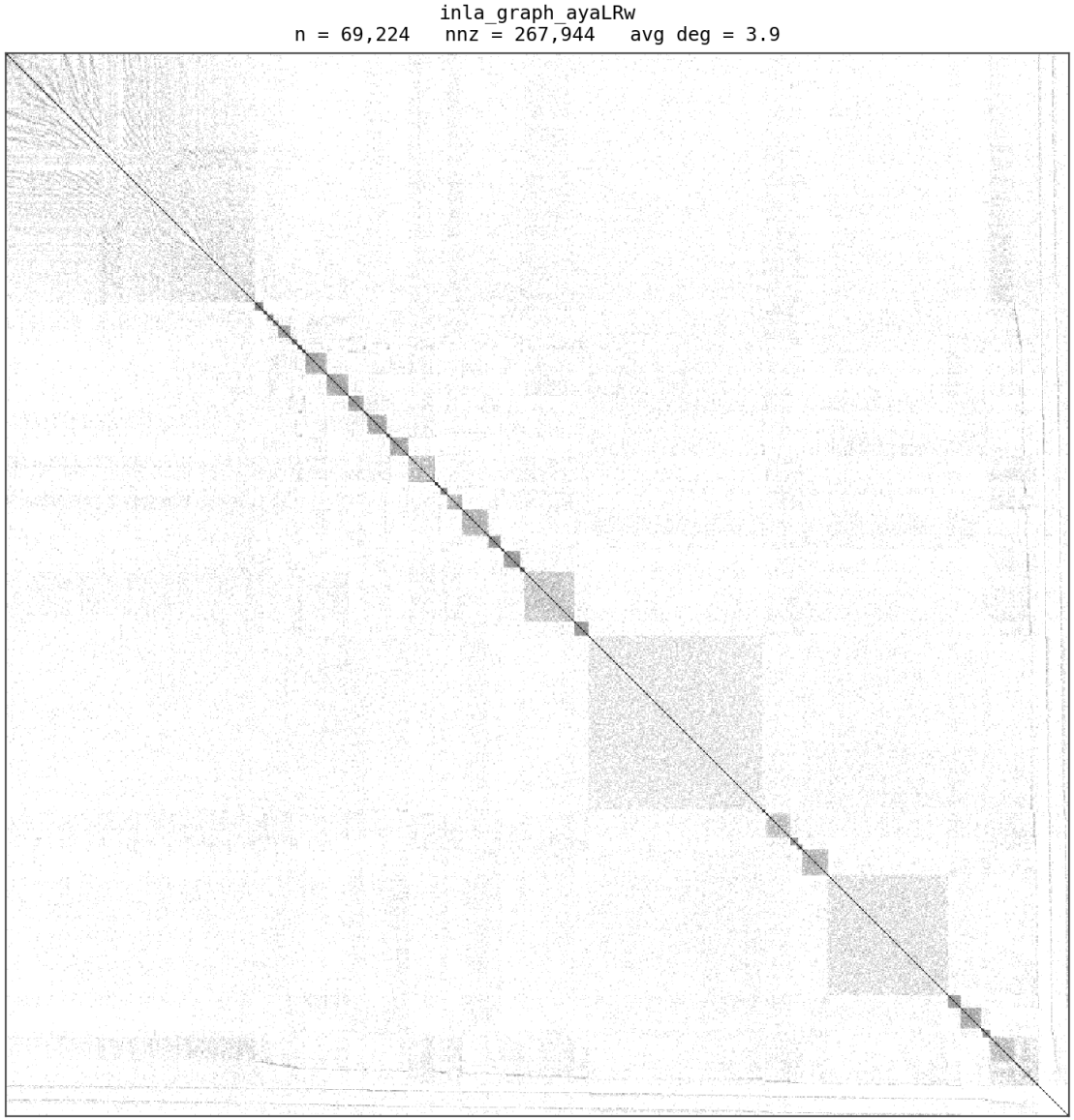

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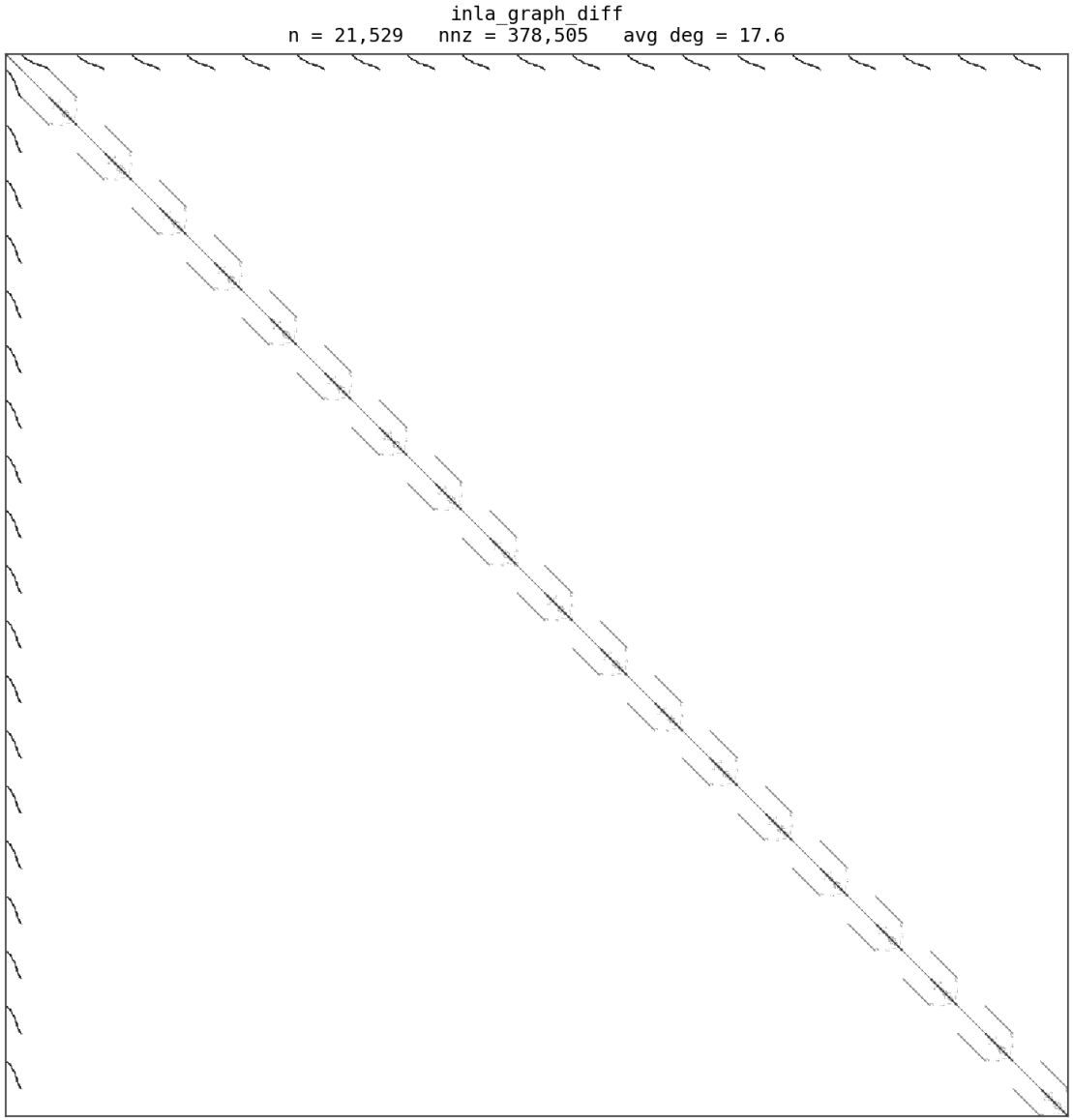

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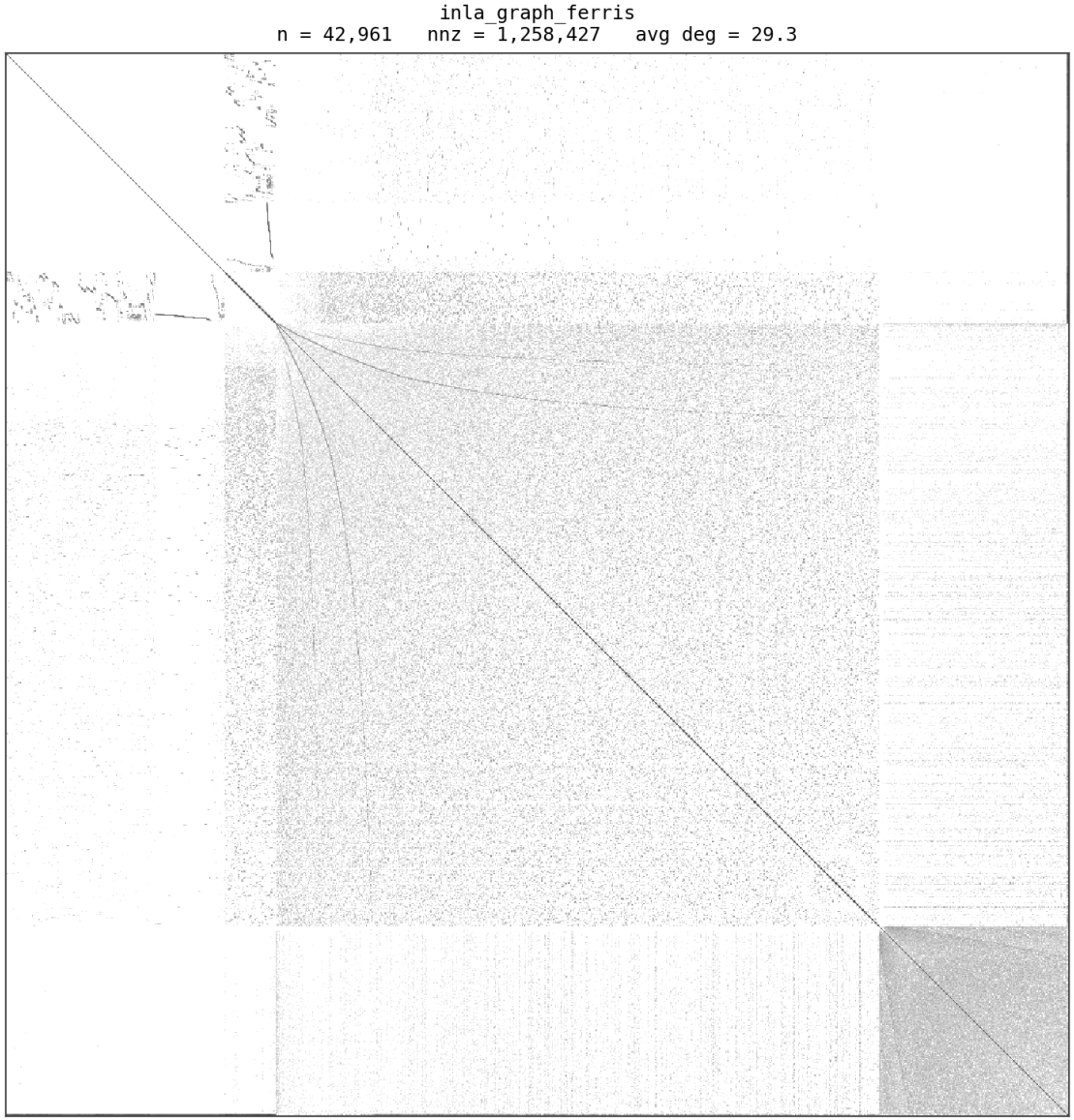

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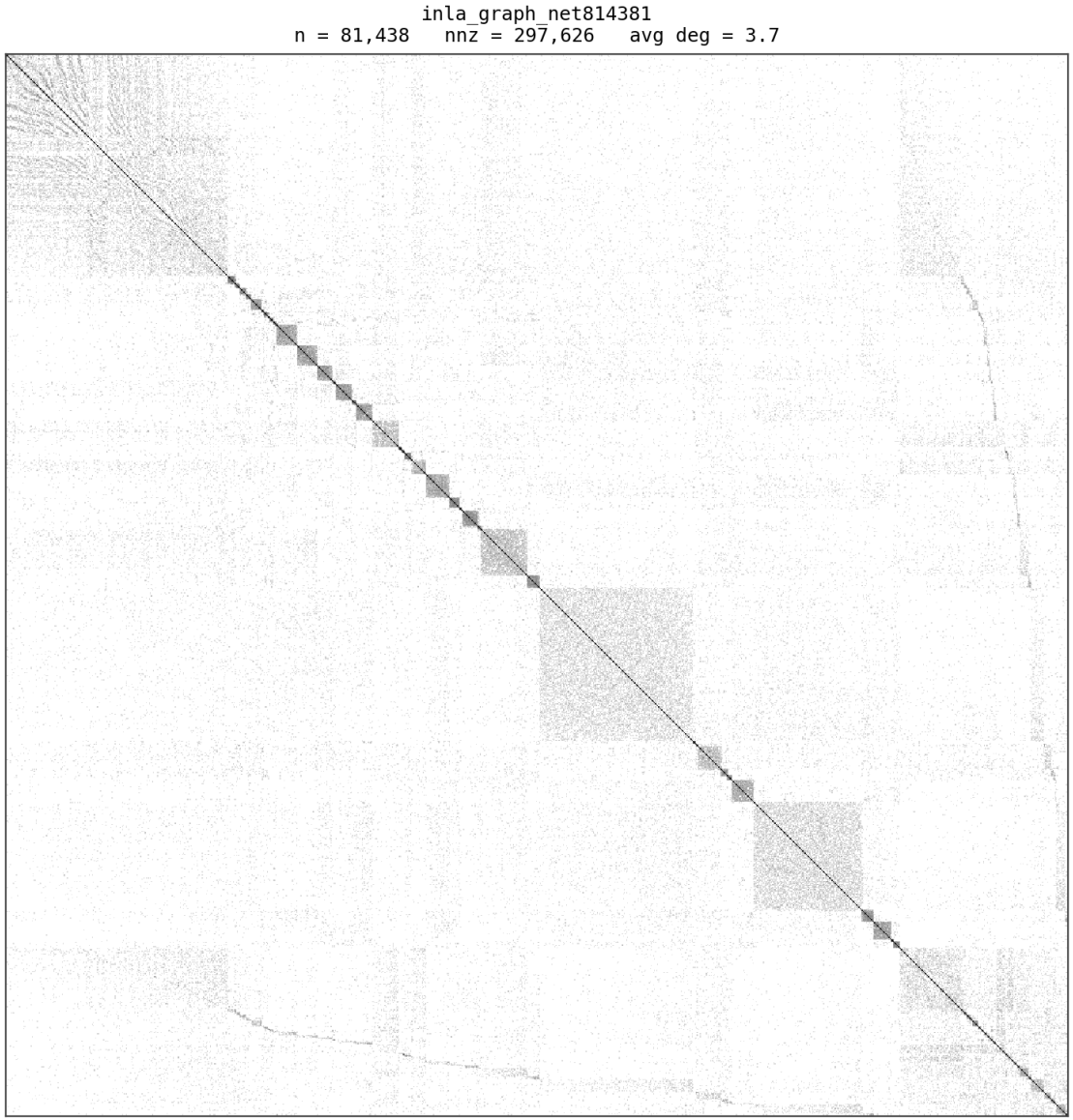

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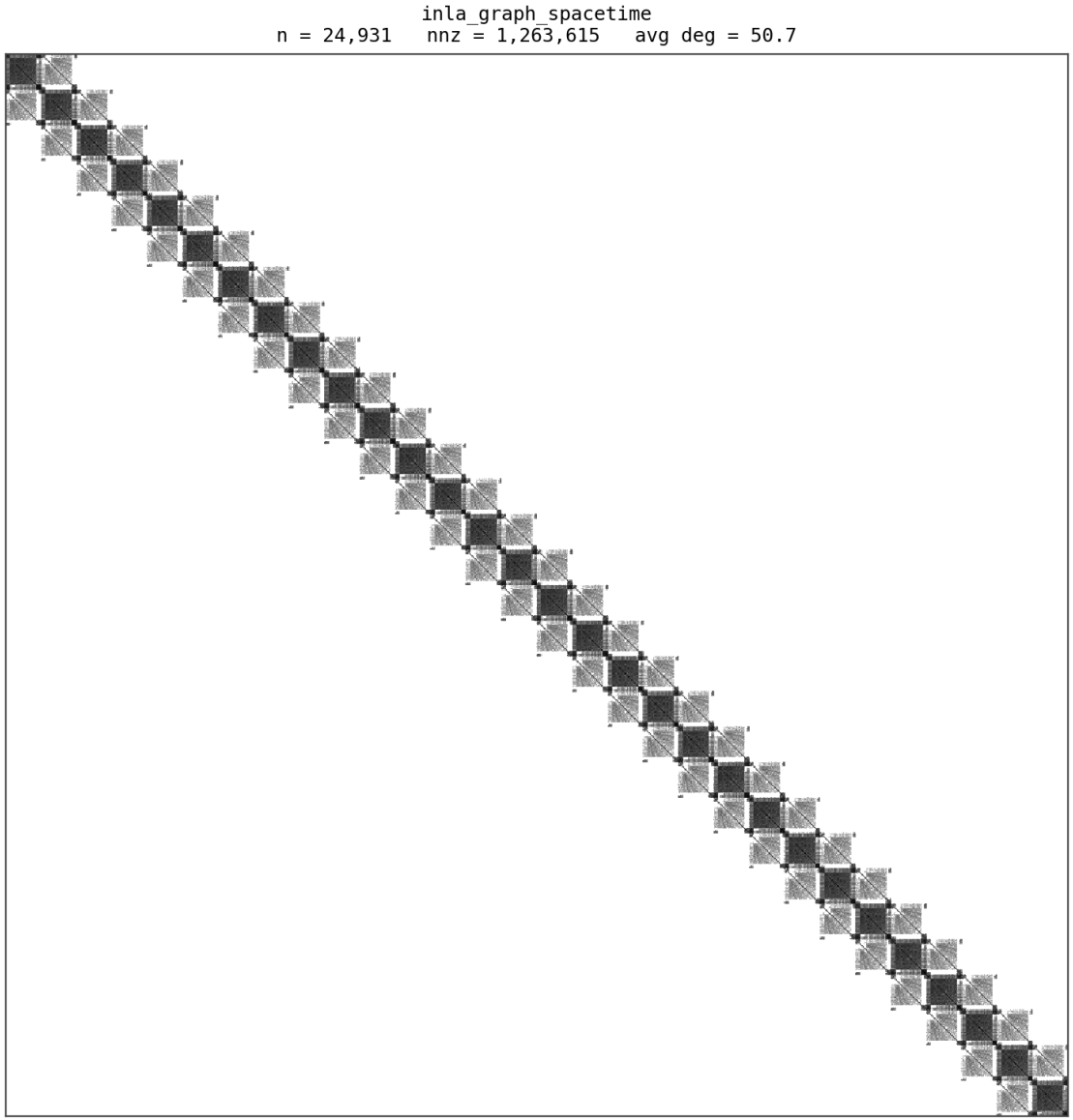

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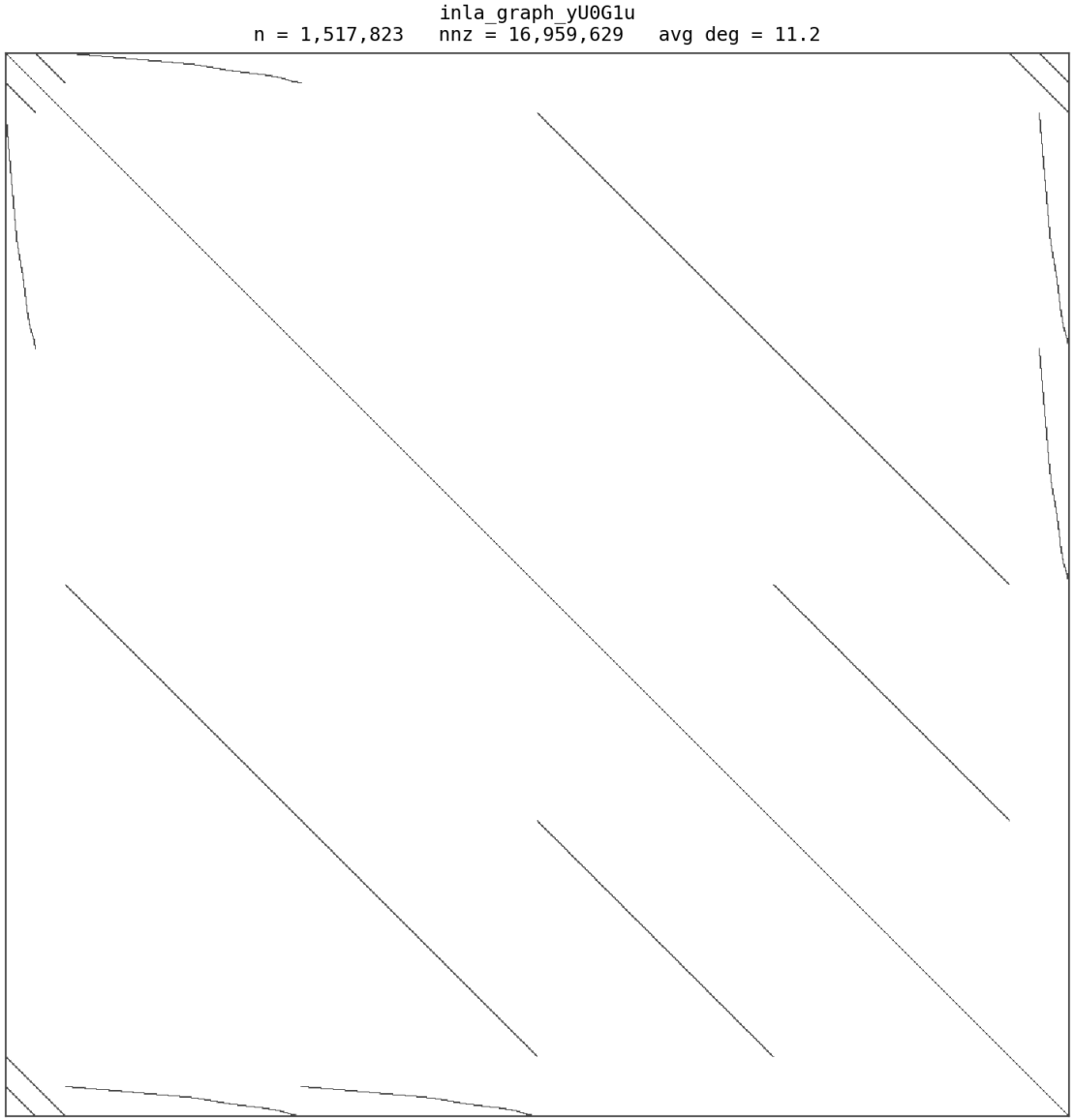

Bayesian Inference: simple ideas

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- Laplace approximations
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Computational issues

Numerical methods for sparse matrices

- Factorise $\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^T$
- Partial inverse $\boldsymbol{Q}^{-1}$ for all $i \sim j$ or $i = j$.
- Determinant $\log |\boldsymbol{Q}|$
- Solve $\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{b}$ and $\boldsymbol{Q}\boldsymbol{X} = \boldsymbol{B}$

```
for (i = 0; i < dimensionSize; i++) {
    for (j = 0; j <= i; j++) {
        float sum = 0;
        for (k = 0; k < j; k++)
            sum += L[i][k] * L[j][k];

        if (i == j)
            L[i][j] = sqrt(A[i][i] - sum);
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Most important ingredient to scalable inference, is to handle sparse matrices well!

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            sum += L[i][k] * L[j][k];

        if (i == j)
            L[i][j] = sqrt(A[i][i] - sum);
        else
            L[i][j] = (1.0 / L[j][j] * (A[i][j] - sum));
    }
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```

Most important ingredient to scalable inference, is to handle sparse matrices well!

Computational issues

Numerical methods for sparse matrices

- Factorise $\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^T$
- Partial inverse $\boldsymbol{Q}^{-1}$ for all $i \sim j$ or $i = j$.
- Determinant $\log |\boldsymbol{Q}|$
- Solve $\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{b}$ and $\boldsymbol{Q}\boldsymbol{X} = \boldsymbol{B}$

```
for (i = 0; i < dimensionSize; i++) {
    for (j = 0; j <= i; j++) {
        float sum = 0;
        for (k = 0; k < j; k++)
            sum += L[i][k] * L[j][k];

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```

Most important ingredient to scalable inference, is to handle sparse matrices well!

Not that much around...

- HPC community like “dense” more than “sparse”
- **R-INLA** uses TAUCS (outdated $>$ 20 years ago)
- CHOLMOD (what is used in R, MATLAB, does not scale well in parallel and do not handle inverse)
- PARDISO (good, not open-source and is now commercial, so...)
- etc...
- With the right person around, we can “just write our own”, right?

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Cholesky factorisation

```
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    }
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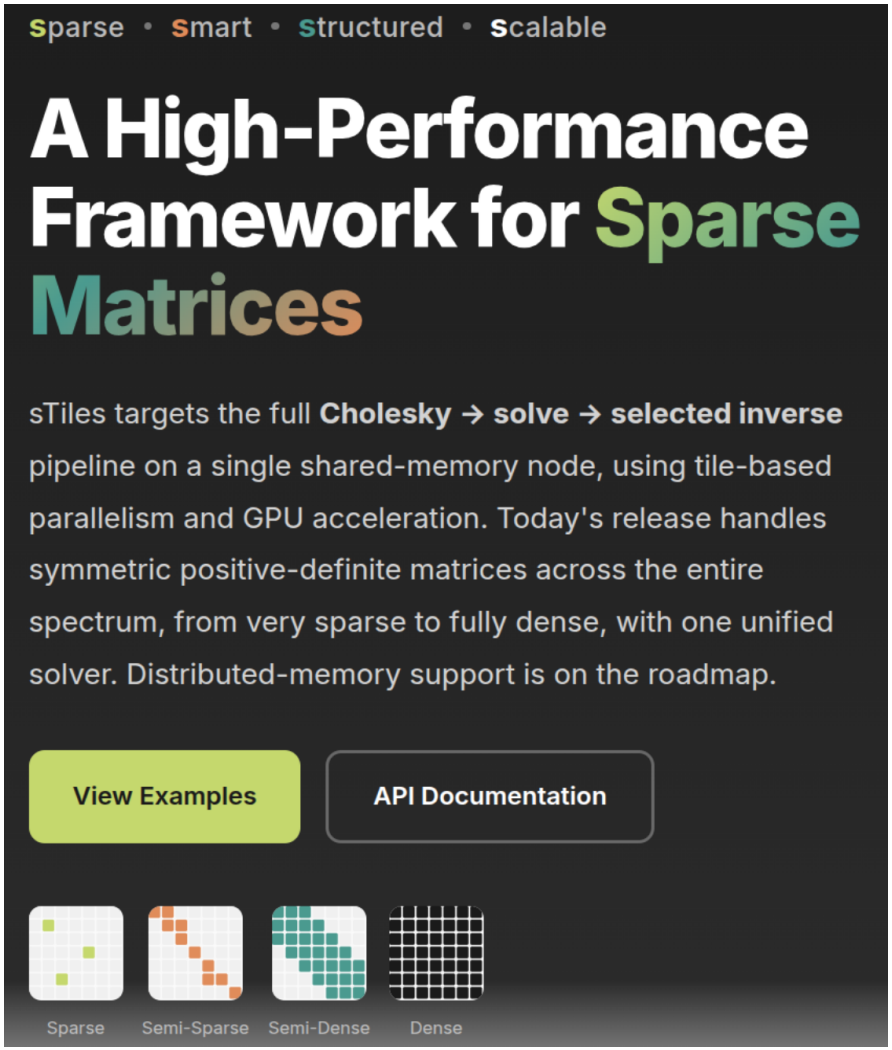
3 years later...



sTiles

3 years later...

- We're getting there
- Announced in Glasgow'25 in May
- ...the we found some new problematic cases
- that took another year to fix
- Written for modern CPU and will have GPU acceleration (for hard cases)
- Results are *very* good, with excellent parallel scaling
- Handle hard cases particulary well
- Open source when done
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Thank you · شكرا

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Science and Technology