Equazioni lineari matriciali
proprietà, metodi numerici ed applicazioni

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Some matrix equations

- Sylvester matrix equation

$$A\mathbf{X} + \mathbf{X}B + D = 0$$

Eigenvalue problems, Control, Model Order Reduction, Assignment problems, Riccati equation

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$$A\mathbf{X} + \mathbf{X}A^\top + D = 0, \qquad D = D^\top$$

Stability analysis in Control and Dynamical systems, Signal processing, eigenvalue computations

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- Algebraic Riccati equation

$$AX + XA^\top - XBB^\top X + D = 0, \qquad D = D^\top$$

Lancaster-Rodman '95, Konstantinov-Gu-Mehrmann-Petkov, '02,

Bini-Iannazzo-Meini '12

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Elliptic PDEs, PDEs with stochastic inputs, bilinear dynamical systems, etc.

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Focus: All or some of the matrices are large (and possibly sparse)

The Lyapunov equation.

$$A\mathbf{X} + \mathbf{X}A^\top + D = 0, \qquad A \text{ stable}$$

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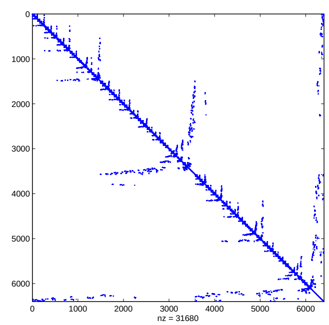
$A =$ 

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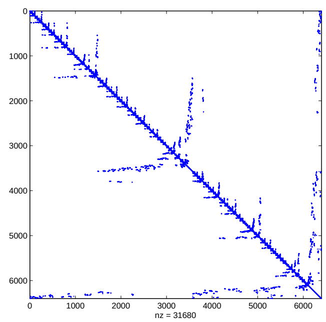
$A =$ 

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Example: For $D = I$ and A symmetric, it holds that $\mathbf{X} = -\frac{1}{2}A^{-1}$

The Lyapunov equation. Some characterizations

$$AX + XA^\top + BB^\top = 0, \qquad A \in \mathbb{R}^{n\times n} \text{ stable}$$

- **The Applied Mathematician perspective**

  $\mathbf{X}$ holds stability information of time-invariant dynamical system:

$$\mathbf{x}'(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{x}(0) = x_0$$

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- **The Analyst perspective**. Closed form solution:

$$X = -\frac{1}{2\pi}\int_{-\infty}^{\infty} (\imath\omega I - A)^{-1} BB^\top (\imath\omega I - A)^{-*} \mathrm{d}\omega = \int_{-\infty}^{0} e^{At} BB^\top e^{At} dt$$

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- **The Algebraist perspective.** Kronecker formulation:

$$(A \otimes I + I \otimes A)\mathbf{x} = b \qquad \mathbf{x} = \mathrm{vec}(\mathbf{X}),\ b = \mathrm{vec}(BB^T)$$

  with $\mathcal{S} := A \otimes I + I \otimes A \in \mathbb{R}^{n^2 \times n^2}$

Linear systems vs linear matrix equations

Large linear systems:

$$\mathcal{S}\mathbf{x} = b,$$

- Krylov subspace methods (CG, MINRES, GMRES, BiCGSTAB, etc.)
- Preconditioners: find P such that

$$\mathcal{S}P^{-1}\widetilde{\mathbf{x}} = b \qquad \mathbf{x} = P^{-1}\widetilde{\mathbf{x}}$$

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Large linear matrix equations:

$$A\mathbf{X} + \mathbf{X}A^\top + BB^\top = 0$$

- No preconditioning - to preserve symmetry
- $\mathbf{X}$ is a large, dense matrix $\Rightarrow$ low rank approximation

$$\mathbf{X} \approx \widetilde{\mathbf{X}} = ZZ^\top, \quad Z\,\text{tall}$$

The Kronecker sum matrix

$$\mathcal{S} := A \otimes I_n + I_n \otimes A,$$

with A symmetric and positive definite, banded with bandwidth b

- Quantum Chemistry and Quantum dynamics
- Signal processing
- Numerical analysis
  - PDE discretizations: e.g., in Finite Differences, Finite Elements, Legendre Spectral Methods, Isogeometric Analysis, ...
- Multivariate Statistics

Sparsity and quasi-sparsity pattern properties of

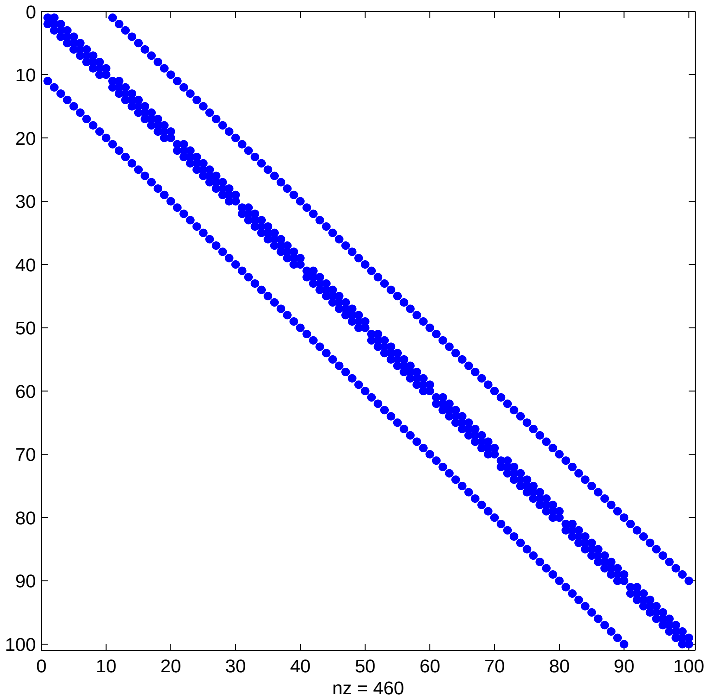
$$f(\mathcal{S})$$

$f \in \{z^{-1}, e^z, z^{\frac{1}{2}}, ...\}$

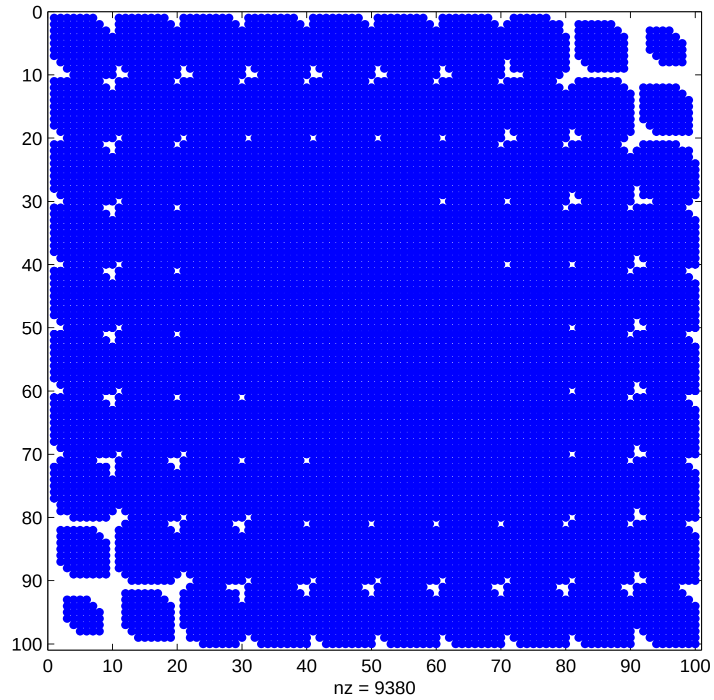
Discretization of 2D Laplace operator on the unit square

$$\mathcal{S} := A \otimes I_n + I_n \otimes A, \qquad A = \text{tridiag}(-1, 2, -1)$$

Sparsity pattern:



Matrix $\mathcal{S}$



$\mathcal{S}^{-1}$

Discretization of 2D Laplace operator on the unit square

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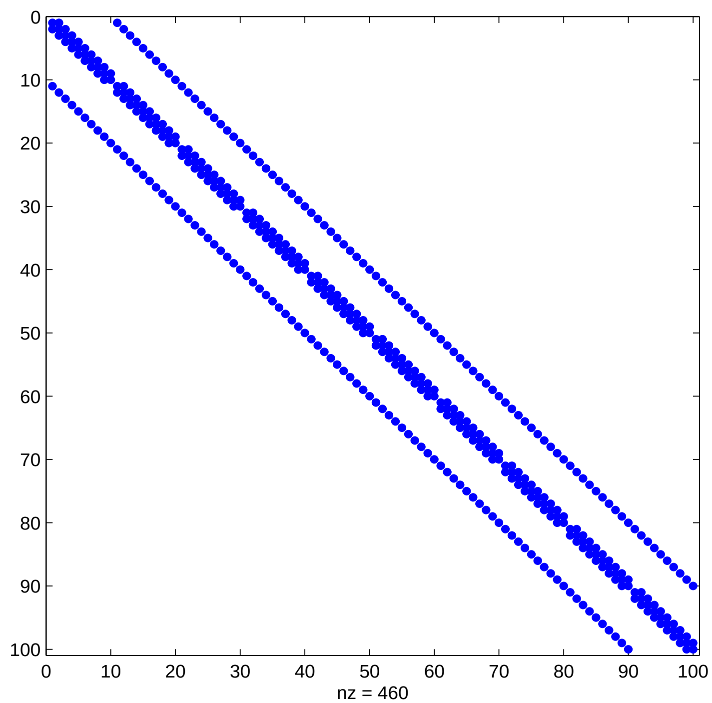
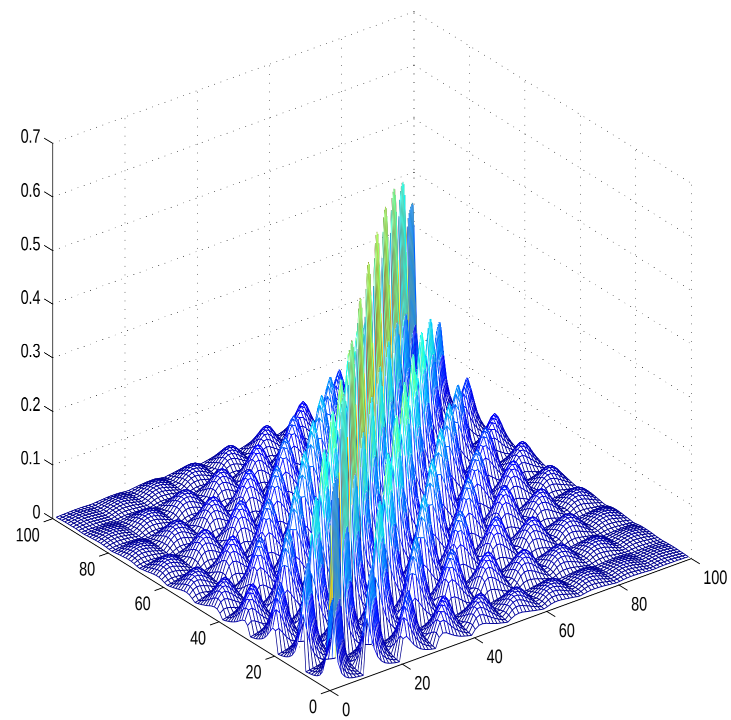
Sparsity pattern:





Matrix $\mathcal{S}$ $\qquad\qquad$ $|(\mathcal{S}^{-1})_{ij}|$

The exponential decay of the entries of $\mathcal{S}^{-1}$

The classical bound (Demko, Moss & Smith):

If $\mathcal{S}$ spd is banded with bandwidth b, then

$$|(\mathcal{S}^{-1})_{ij}| \le \gamma q^{\frac{|i-j|}{b}}$$

where

$\kappa = \lambda_{\max}(\mathcal{S})/\lambda_{\min}(\mathcal{S})$ (cond. number of $\mathcal{S}$)

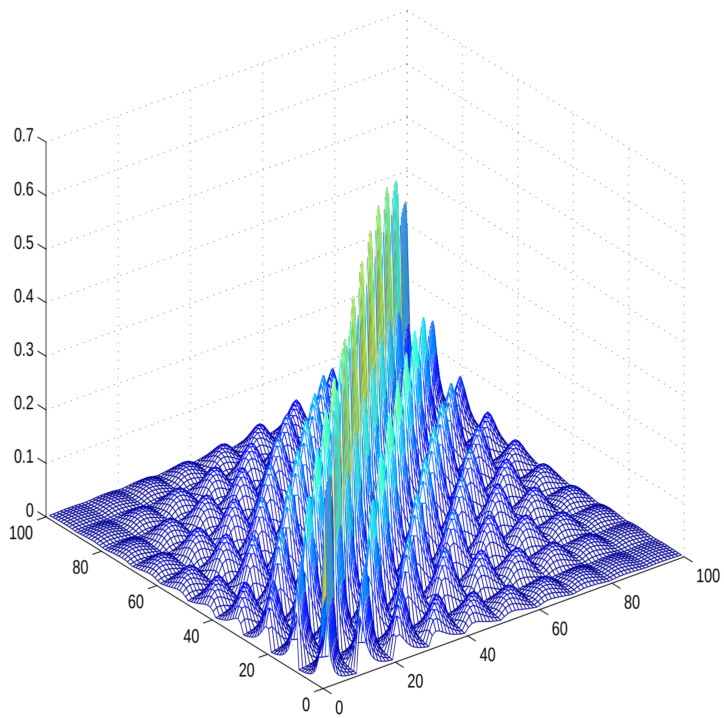
$$q := \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} < 1$$

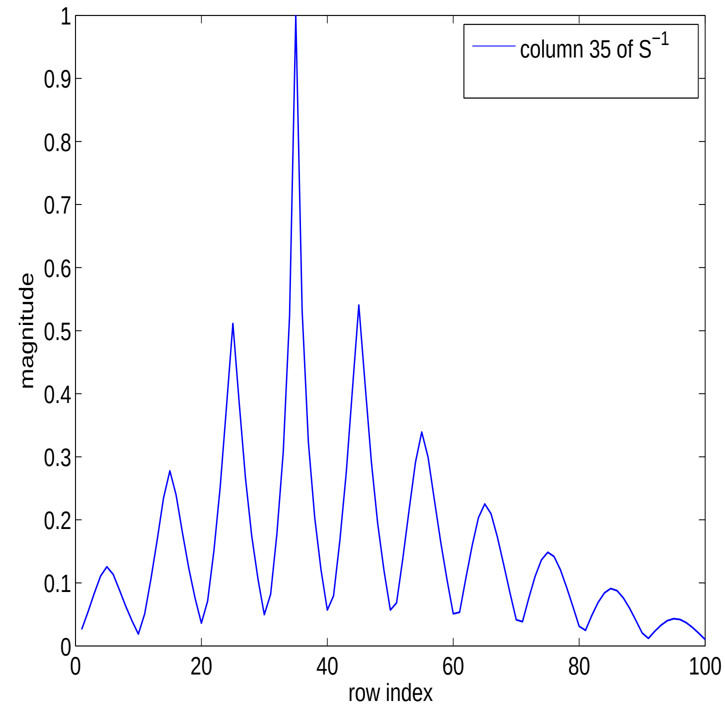
$\gamma := \max\{\lambda_{\min}(\mathcal{S})^{-1}, \hat{\gamma}\}$, and $\hat{\gamma} = \dfrac{(1+\sqrt{\kappa})^2}{2\lambda_{\max}(\mathcal{S})}$

($\lambda_{\min}(\mathcal{S}), \lambda_{\max}(\mathcal{S})$ smallest and largest eigenvalues of $\mathcal{S}$)

Many contributions: Bebendorf, Hackbusch, Benzi, Boito, Razouk, Golub, Tuma, Concus, Meurant, Mastronardi, Ng, Tyrtyshnikov, Nabben, ...

The actual decay





... a very peculiar pattern $\Rightarrow$ much higher sparsity

Where do the repeated peaks come from?

For $\mathcal{S} = A \otimes I_n + I_n \otimes A \in \mathbb{R}^{n^2 \times n^2}$:

$$x_t := (\mathcal{S}^{-1})_{:,t} = \mathcal{S}^{-1} e_t \qquad \Leftrightarrow \qquad \text{Solve : } \mathcal{S}\mathbf{x}_t = e_t$$

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Let

$\mathbf{X}_t \in \mathbb{R}^{n \times n}$ be such that $\mathbf{x}_t = \text{vec}(\mathbf{X}_t)$

$E_t \in \mathbb{R}^{n \times n}$ be such that $e_t = \text{vec}(E_t)$

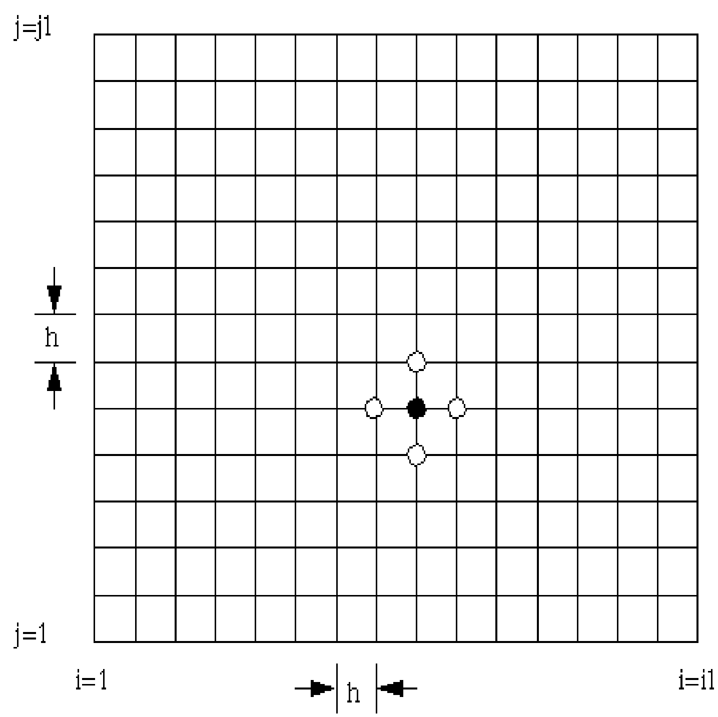
Then

$$\mathcal{S}\mathbf{x}_t = e_t \qquad \Leftrightarrow \qquad A\mathbf{X}_t + \mathbf{X}_t A = E_t$$

The Poisson equation - revisited

$$-u_{xx} - u_{yy} = f, \quad \text{in} \quad \Omega = (0,1)^2$$

+ Dirichlet b.c. (zero b.c. for simplicity)



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FD Discretization: $U_{i,j} \approx u_{x_i,y_j}$, with (x_i, y_j) interior nodes, so that

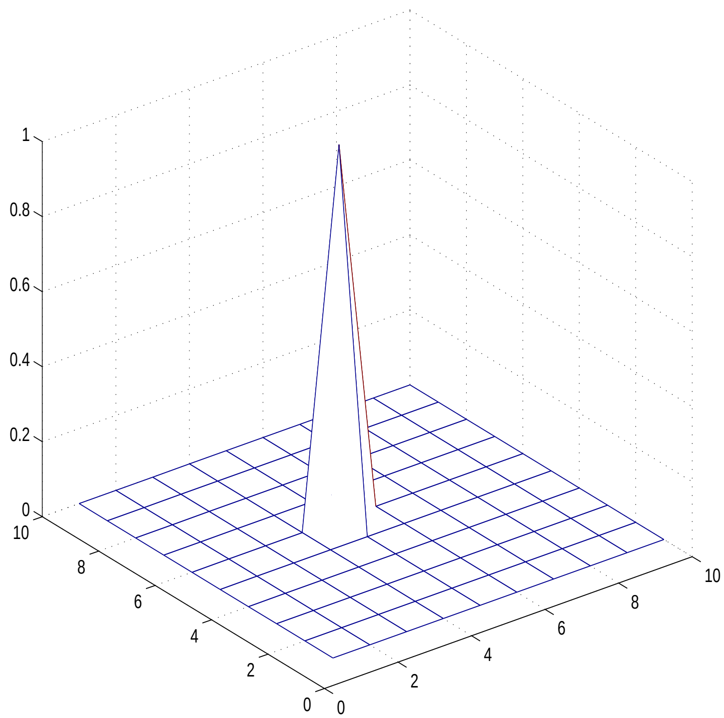
$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} = \frac{1}{h^2}[1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix}$$

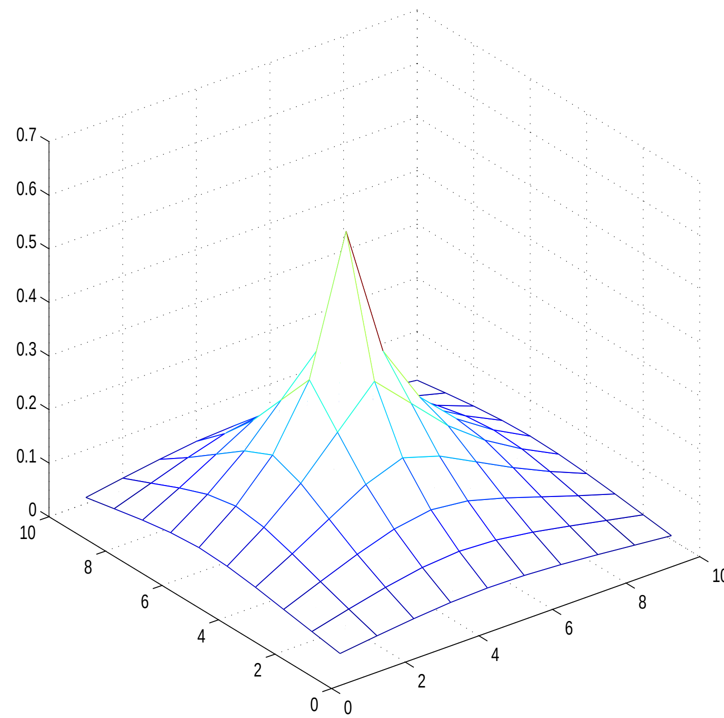
$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = \frac{1}{h^2}[U_{i,j-1}, \, U_{i,j}, \, U_{i,j+1}] \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

$$A\mathbf{U} + \mathbf{U}A = F, \qquad F_{ij} = f(x_i, y_j)$$

For $\mathcal{S}$ the 2D Laplace operator, $t = 1, \ldots, n^2$

$$t = 35, \qquad \mathcal{S}\mathbf{x}_t = e_t \qquad \Leftrightarrow \qquad A\mathbf{X}_t + \mathbf{X}_t A = E_t$$





matrix E_t and matrix $\mathbf{X}_t$

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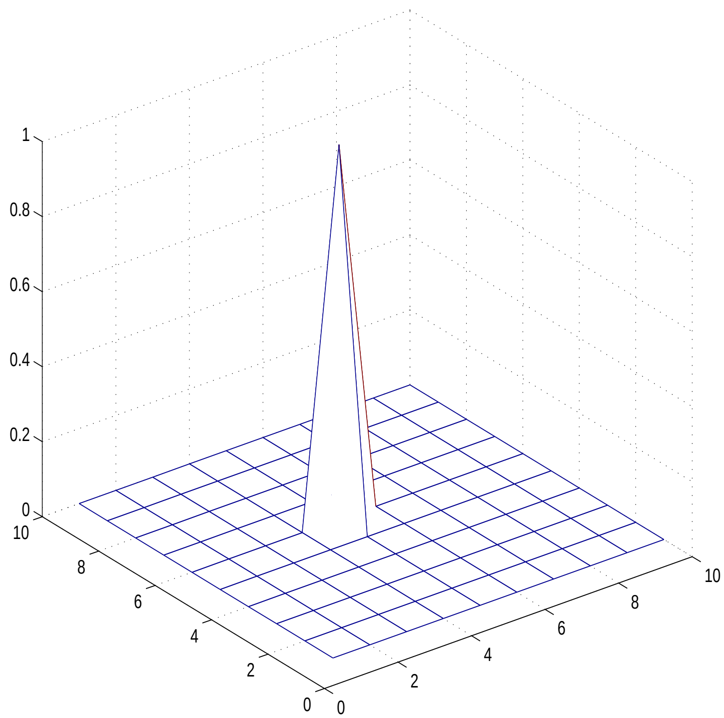
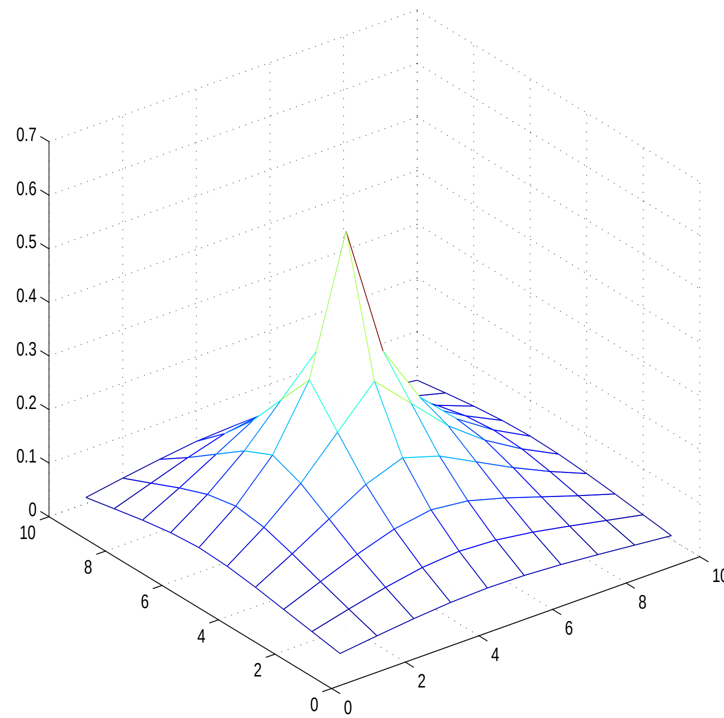
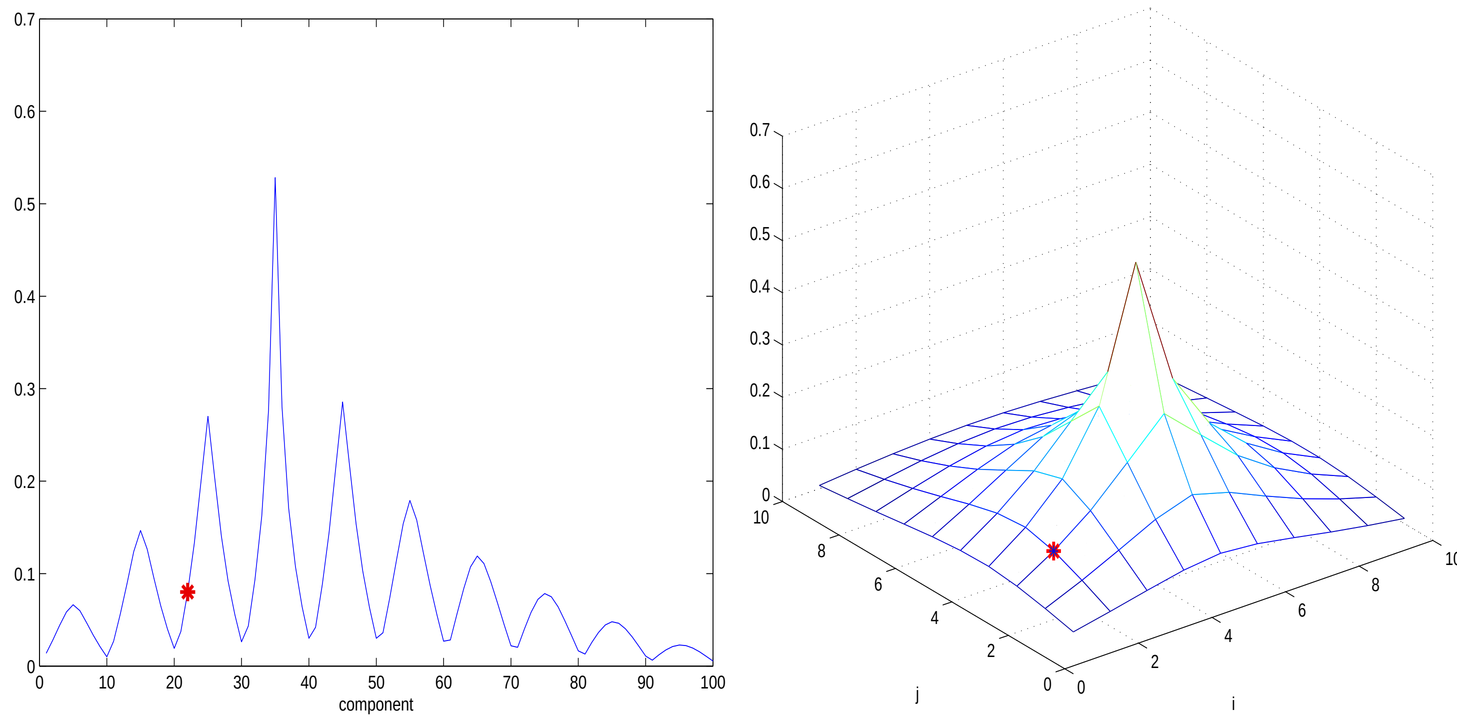




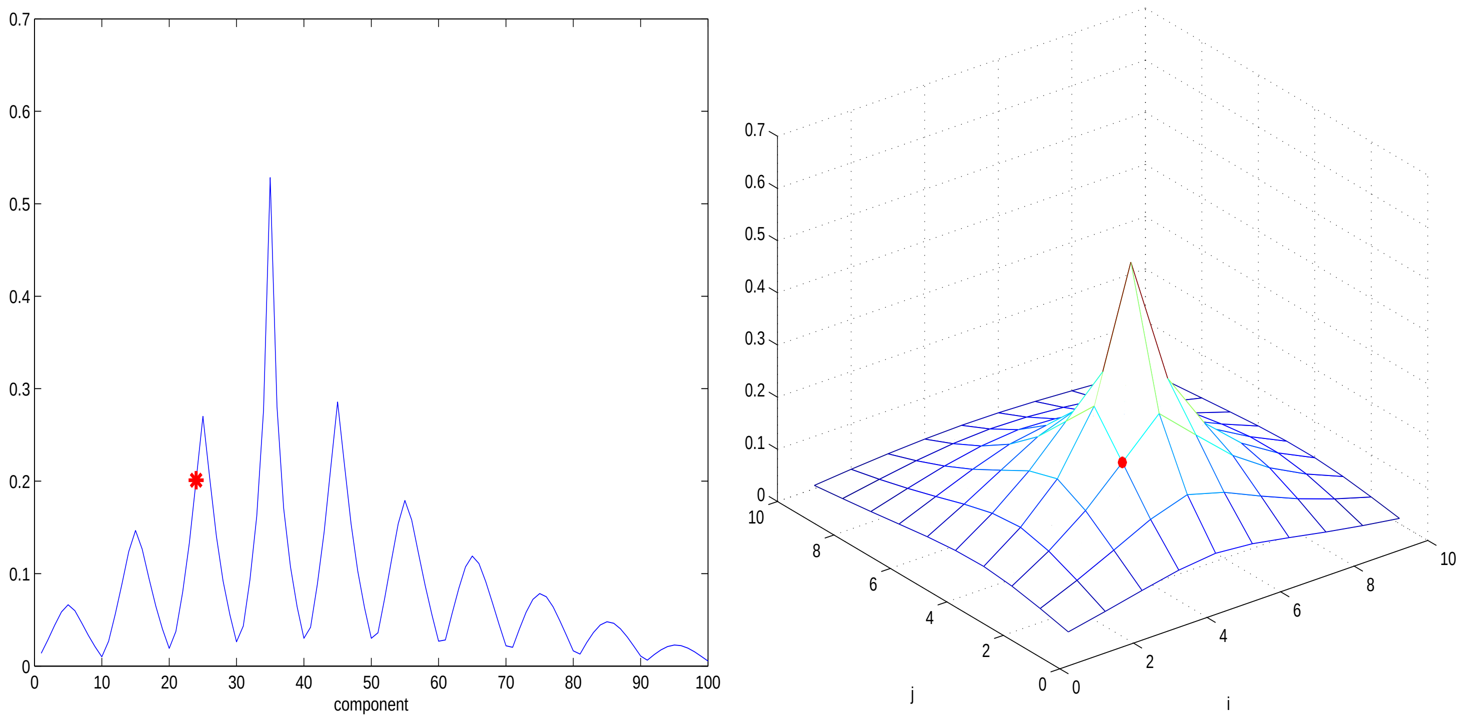
matrix E_t and matrix $\mathbf{X}_t$

E_t has only one nonzero element

Lexicographic order: $(E_t)_{ij}$, $j = \lfloor (t-1)/n \rfloor + 1$, $i = tn\lfloor (t-1)/n \rfloor$



Left: Row of $\mathcal{S}^{-1}$ Right: same row on the grid



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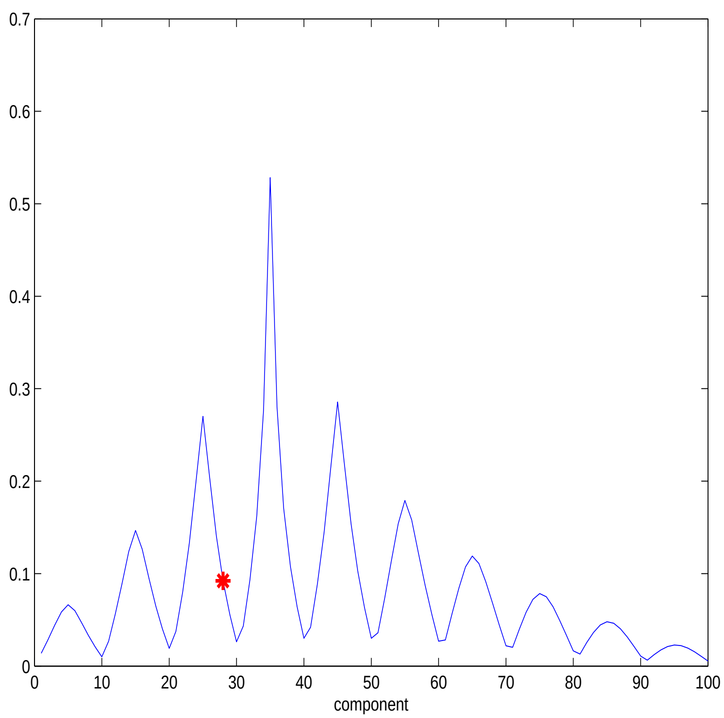

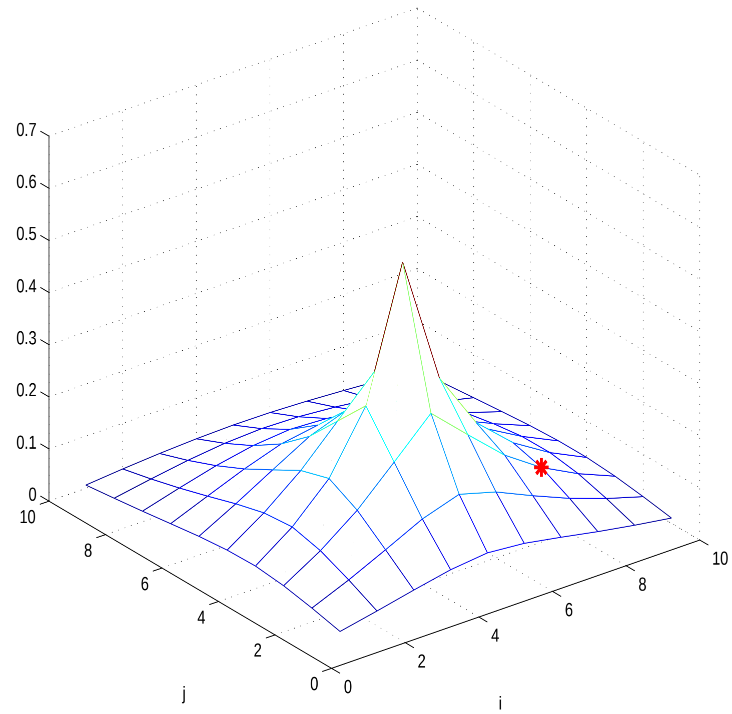

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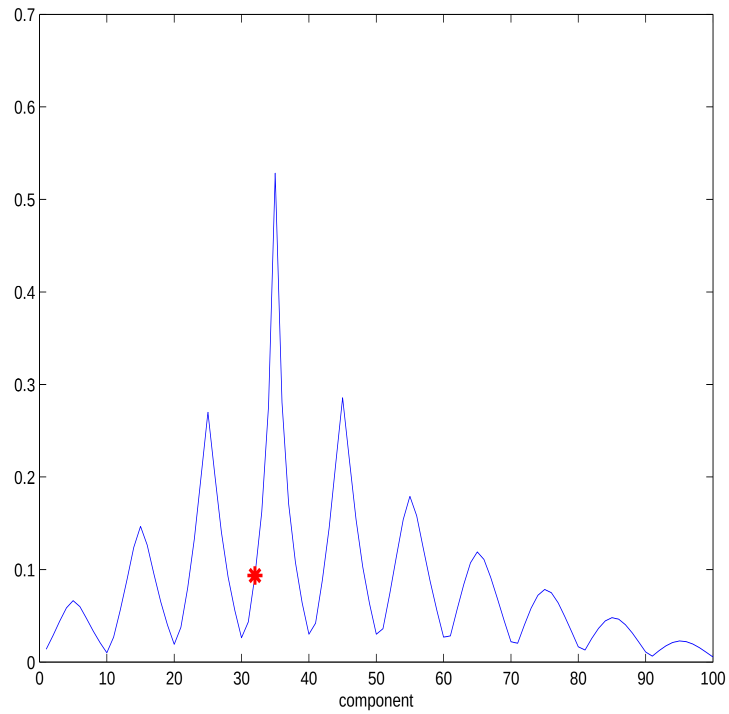

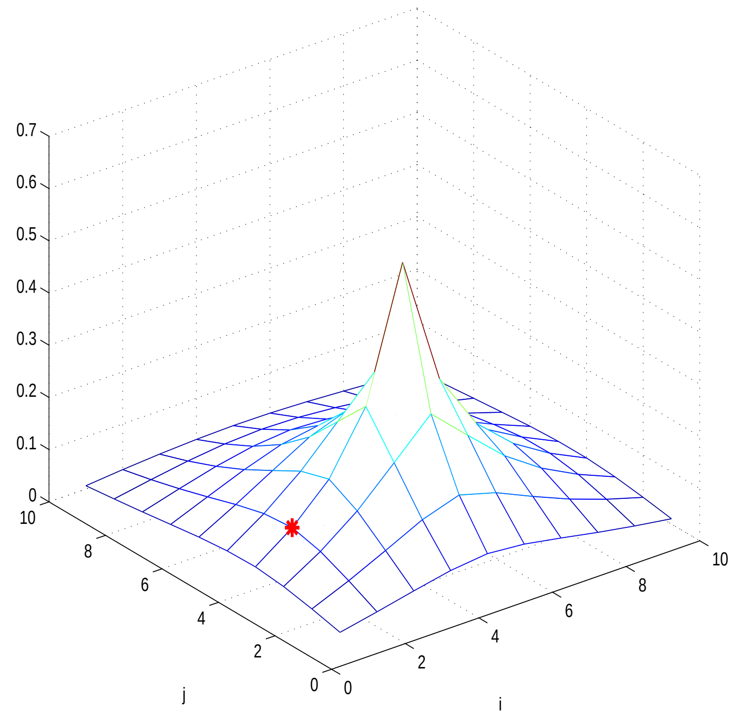

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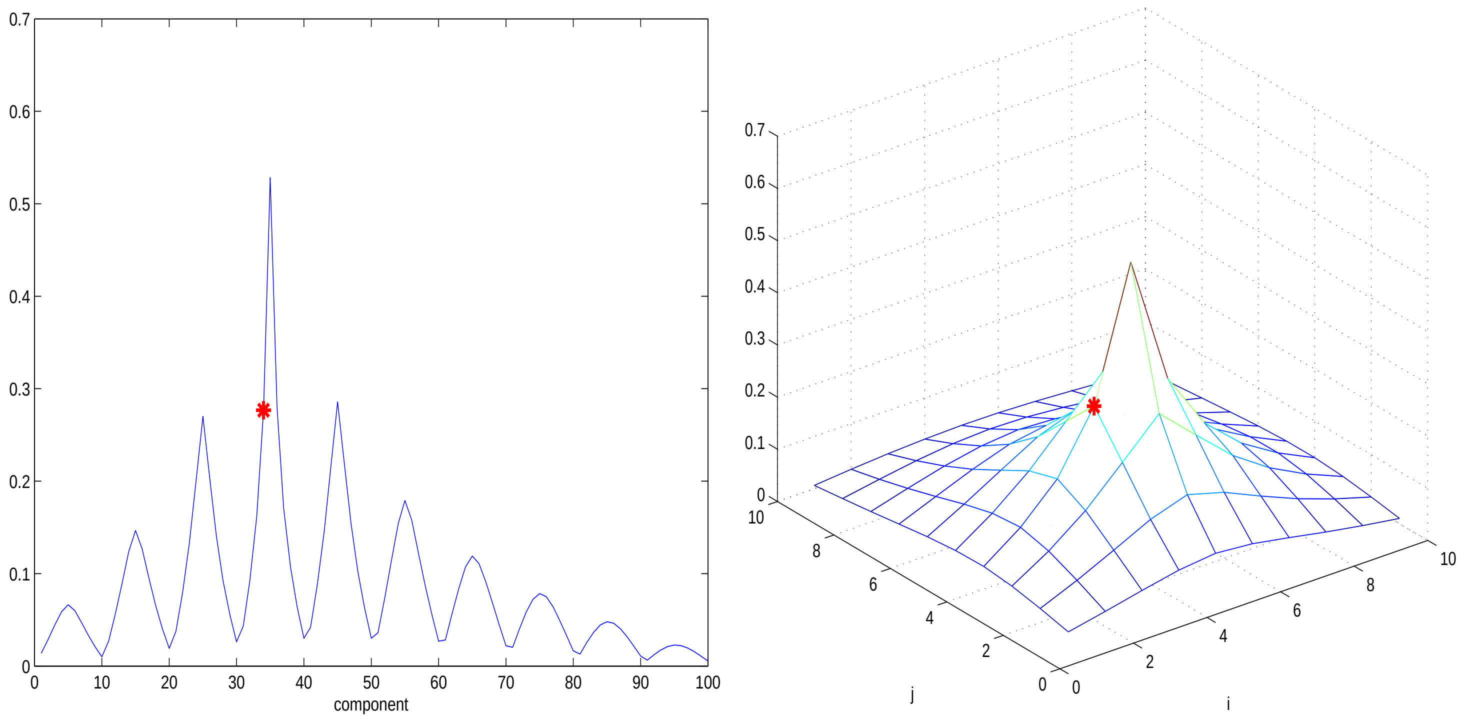

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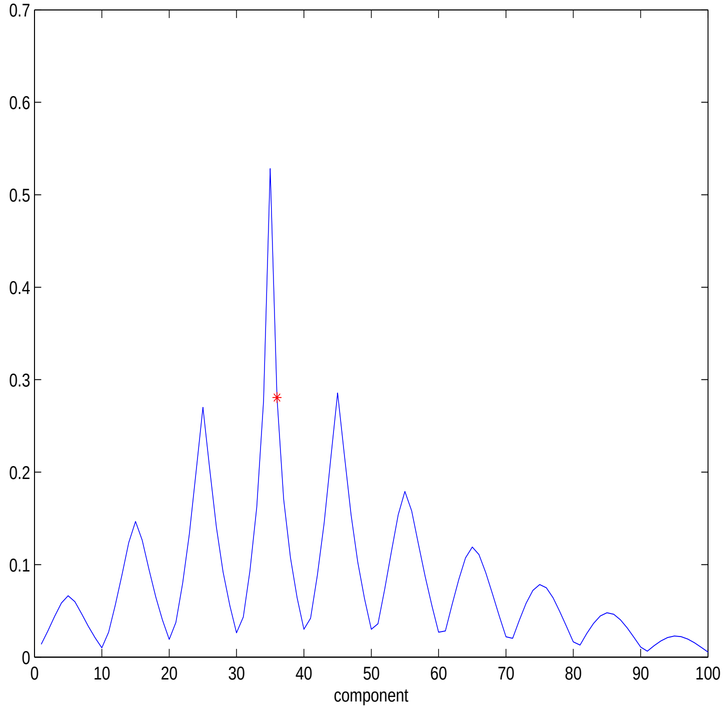

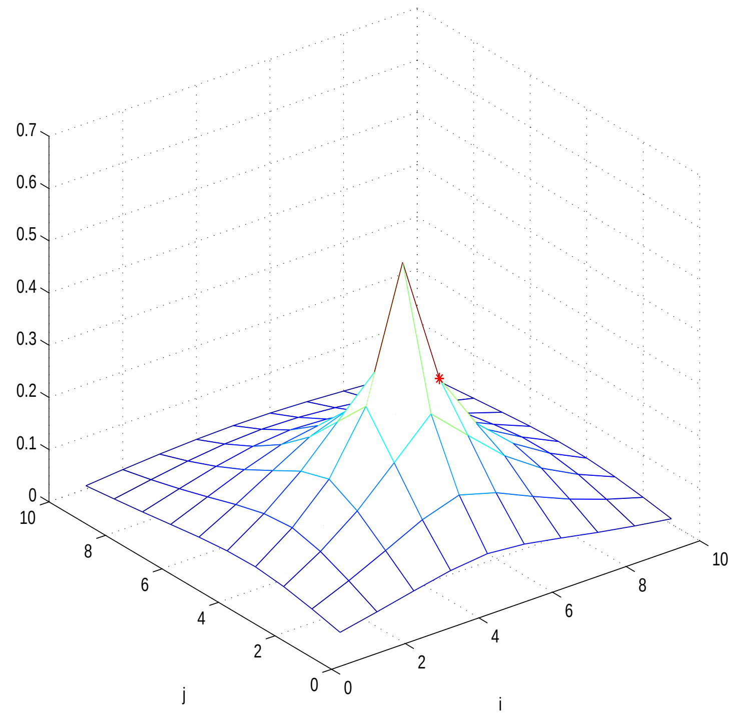

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Qualitative bounds (more general than for the Laplacian!)

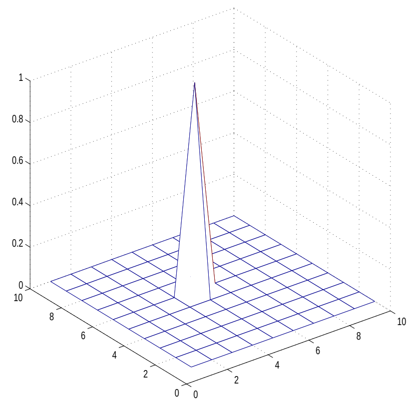
Let $\kappa = \lambda_{\max}/\lambda_{\min} = \mathrm{cond}(A)$

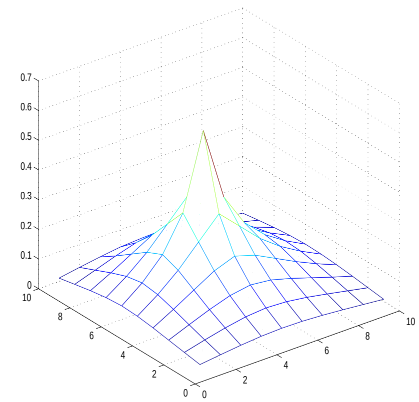
i)Assume $\ell, i, m, j \ : \ \ell \neq i,\ m \neq j.$ $\mathfrak{n}_2 := |\ell - i| + |m - j| - 2 > 0$

$$|(\mathcal{S}^{-1})_{k,t}| \leq \frac{\sqrt{\kappa^2+1}}{2\lambda_{\min}} \frac{1}{\sqrt{\mathfrak{n}_2}}.$$

ii)Assume $\ell, i, m, j \ : \ \ell = i$ or $m = j.$ $\mathfrak{n}_1 := |\ell - i| + |m - j| - 1 > 0$

$$|(\mathcal{S}^{-1})_{k,t}| \leq \frac{\kappa\sqrt{\kappa^2+1}}{2} \frac{1}{\sqrt{\mathfrak{n}_1}}.$$

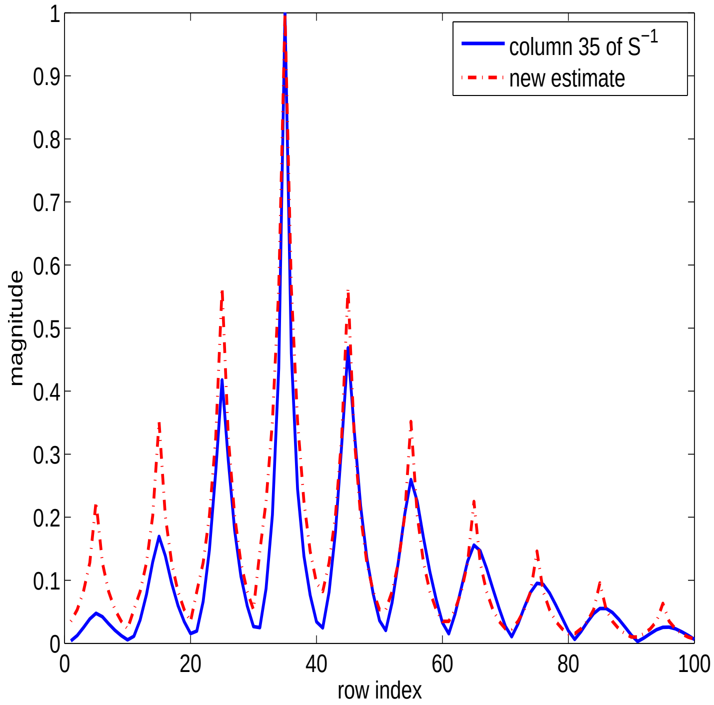




(i, j) and (ℓ, m)

Example. Legendre stiffness matrix (scaled to have unit peak)

$$A = \mathrm{tridiag}(\delta_k, \underline{\gamma_k}, \delta_k)$$



$$\gamma_k = \frac{2}{(4k-3)(4k+1)} \quad k = 1, \ldots, n, \quad \text{and}$$

$$\delta_k = \frac{-1}{(4k+1)\sqrt{(4k-1)(4k+3)}} \quad k = 1, \ldots, n-1$$

Canuto, Simoncini, Verani 2014

Connections to point-wise estimates for discrete Laplacian

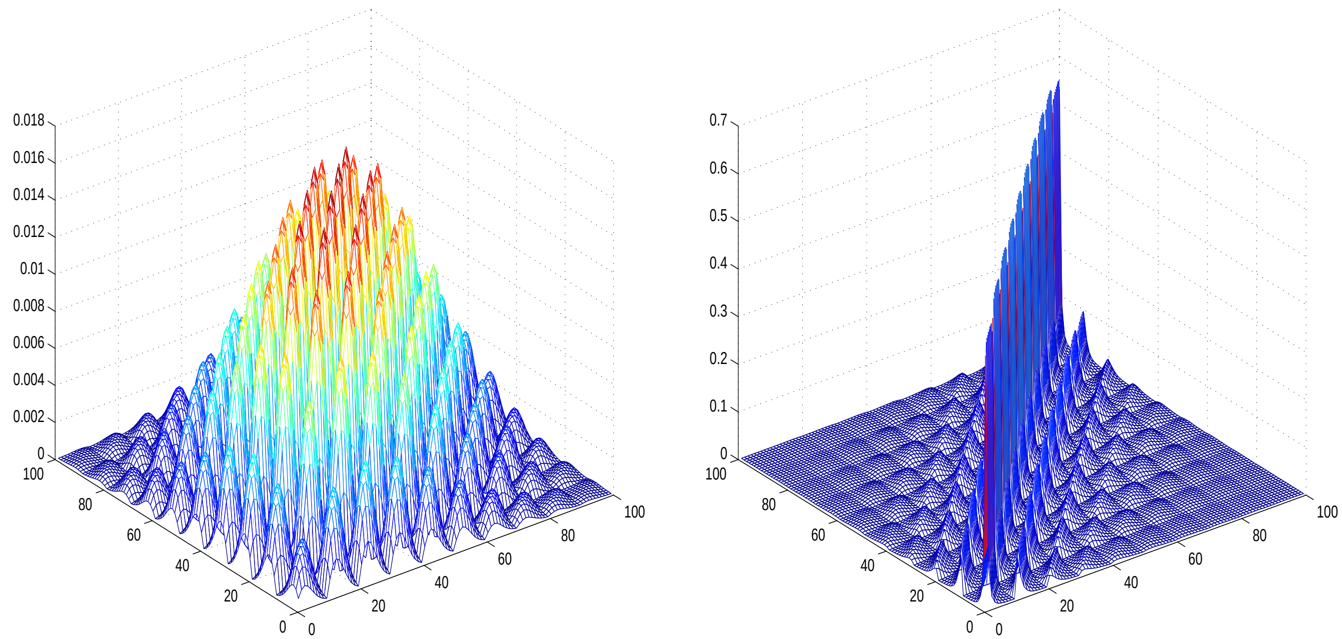
For the discrete Green function G_h on the discrete d-dimensional grid R_h, there exist constants h_0 and C such that for $h \leq h_0$, $x, y \in R_h$,

$$G_h(x,y) \leq \begin{cases} C \log \frac{C}{|x-y|+h} & \text{if } d = 2 \\ \frac{C}{(|x-y|+h)^{d-2}} & \text{if } d \geq 3 \end{cases}$$

(Bramble & Thomee, '69)

Our estimate: entries depend on inverse square root of the distance!

Typical decay plot for $f(\mathcal{S})$, with $\mathcal{S}$ Laplace operator as before



$f(\mathcal{S}) = e^{-5\mathcal{S}}$ $\qquad\qquad$ $f(\mathcal{S}) = \mathcal{S}^{-\frac{1}{2}}$

(Bounds for Laplace or Stieltjes functions)

In general, $\mathcal{S} = A_1 \oplus A_2 := A_1 \otimes I + I \otimes A_2$, $\ A_1, A_2$ banded spd

Benzi, Simoncini 2015

Generalizations

- Three-dimensional case
- (banded) Non-symmetric matrices
- “Quasi” Kronecker structure
- Numerical solution of PDEs on structured grids

$-\Delta u = 1, \quad \Omega = (0,1)^3 \quad \Rightarrow \quad \mathcal{S} = (A \otimes I \otimes I + I \otimes A \otimes I + I \otimes I \otimes A)$

CG for $\mathcal{S}x = b$ vs Iterative solver for $(I \otimes A + A \otimes I)\mathbf{U} + \mathbf{U}A = F$

$A \in \mathbb{R}^{n \times n}$, $\mathcal{S} \in \mathbb{R}^{n^3 \times n^3}$, $\qquad n = 50$

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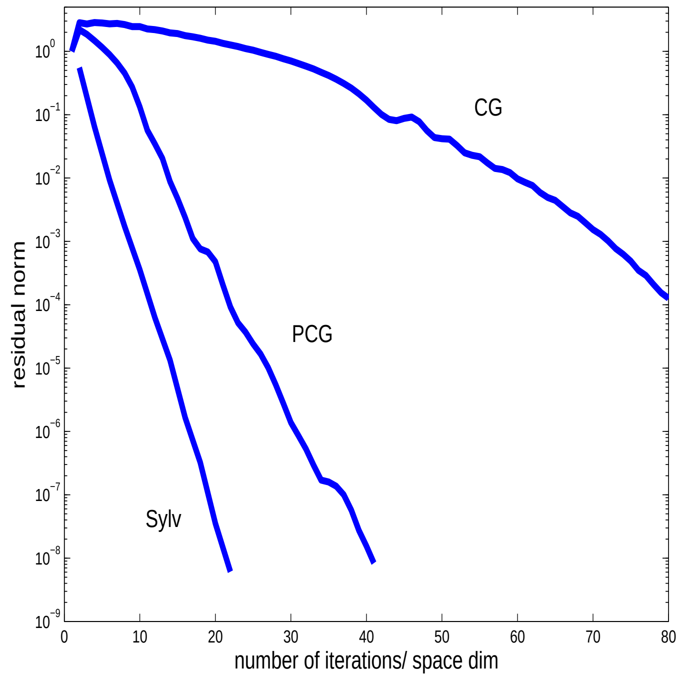
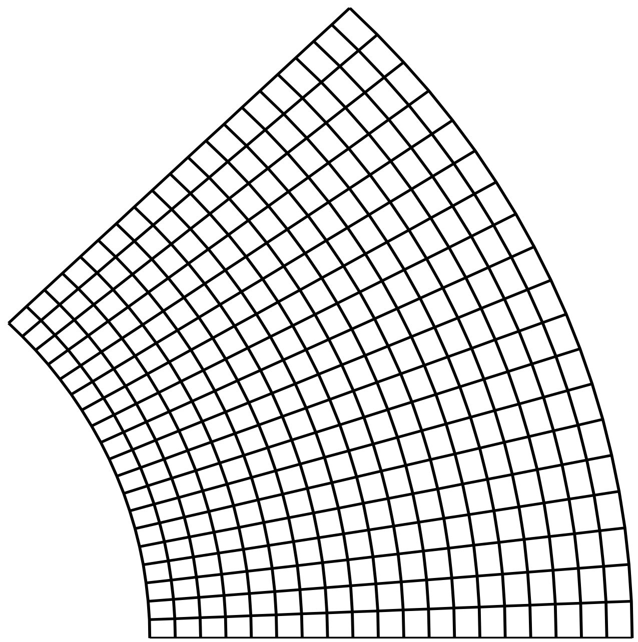


	CG	PCG	Matrix Eqn solver
Comput. Time	2.91	0.56	0.08

Generalizations. Solutions to PDEs

$$-u_{xx} - u_{yy} = f, \qquad (x, y) \in \Omega$$



In polar coordinates (r, θ): $\qquad -u_{rr} - \frac{1}{r} u_r - u_{\theta\theta} = \widetilde{f}$

$\Rightarrow \qquad A_1 \mathbf{X} + \mathbf{X} A_2 = F$

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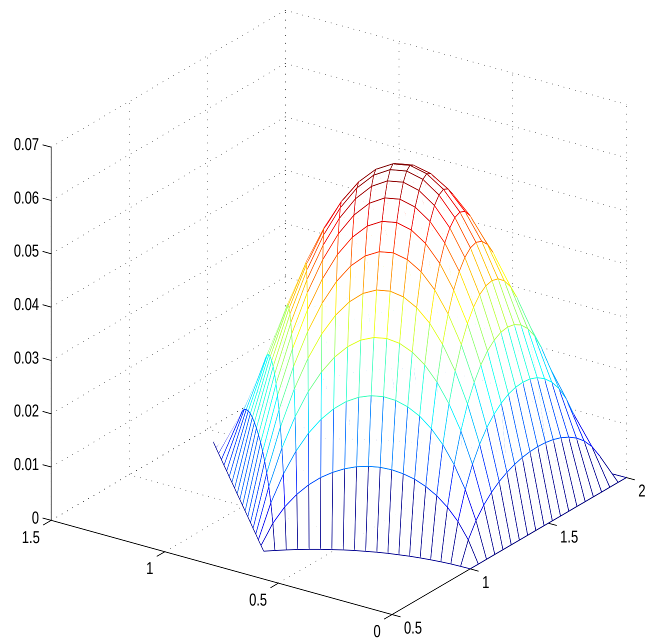

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Structured grids

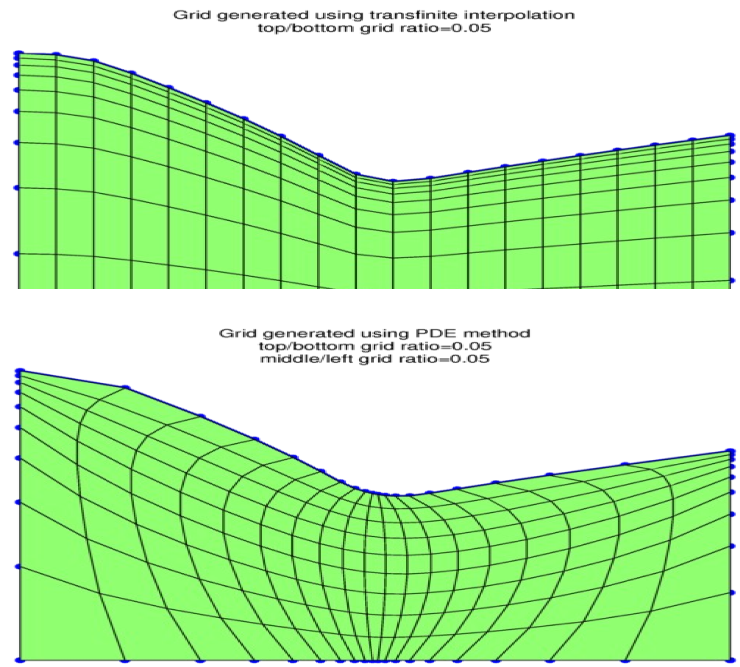
Applications

- Computational Aero- and Fluid-Dynamics
- Seminconductor devices
- Object modelling
- Parallel computation
- ...

Classical strategies (building blocks)

- Conformal mappings (Boundary-fitted curvilinear coord.)
- Algebraic grid generators (Transfinite interpolation)
- Elliptic, hyperbolic grids with controls
- Variational methods
- ...

Grid generation. An example



(grids from `http://www.math.fsu.edu/ okhanmoh/research.html`)

Conclusions

- Matrix equations have very broad applicability

  (structure recurrent in many application problems...)

- Recent appropriate computational devices

- Important tool for matrix sparsity analysis

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