Kronecker sums of matrices
Computation, sparsity properties and applications

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Partially joint work with Michele Benzi, Emory Univ., and also with Claudio Canuto (PoliTo) and Marco Verani (PoliMi)

The Lyapunov operator

Given $M \in \mathbb{R}^{n\times n}$,

$$\mathcal{L} : X \mapsto MX + XM^\top \qquad \text{or} \qquad \ell : x \mapsto (I \otimes M + M \otimes I)x$$

- A structured matrix

- A mathematical tool

In general: $\mathcal{L} : X \mapsto M_1 X + X M_2^\top$, with $M_1 \in \mathbb{R}^{n\times n}, M_2 \in \mathbb{R}^{m\times m}$

(Sylvester operator)

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)

Usual discretization $\Rightarrow$ $\qquad Au = b$ (with $A = T \otimes I + I \otimes T,\ b = \mathrm{vec}(F)$)

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

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

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

h: meshsize

The Poisson equation - matrix formulation

Let $T = \frac{1}{h^2}\mathrm{tridiag}(-1, \underline{2}, -1)$

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

Collecting all nodes together,

$$-u_{xx} \approx TU, \qquad -u_{yy} \approx UT$$

Therefore,

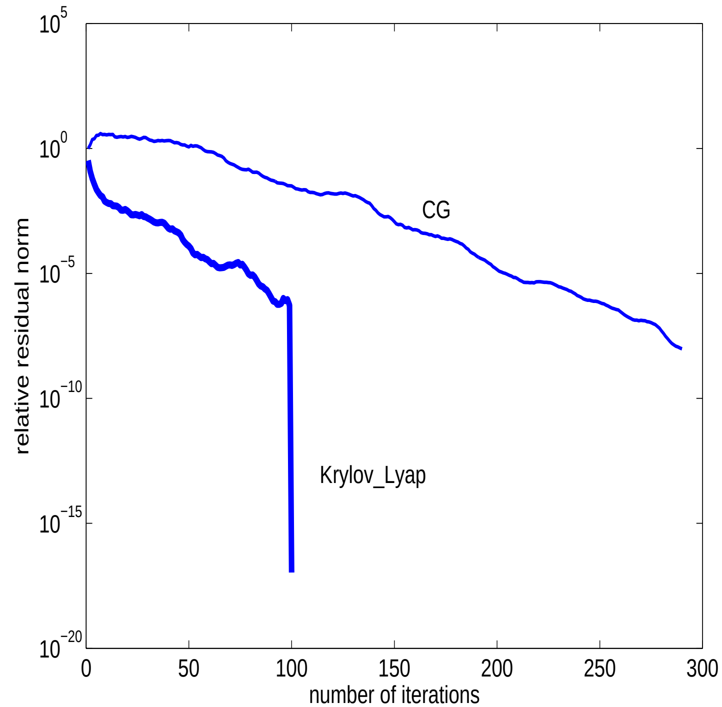
$$-u_{xx} - u_{yy} = f \qquad \Rightarrow \qquad TU + UT = F$$

(here $F_{ij} = f(x_i, y_j)$)

To be compared with $Au = b$

CG for $Ax = b$ vs Iterative solver for $TU + UT = F$

$T \in \mathbb{R}^{n\times n}$, $A \in \mathbb{R}^{n^2\times n^2}$, $\quad n = 100$



For $\texttt{tol} = 10^{-6}$, Elapsed time: CG≈ 0.8, Krylov ≈ 0.4

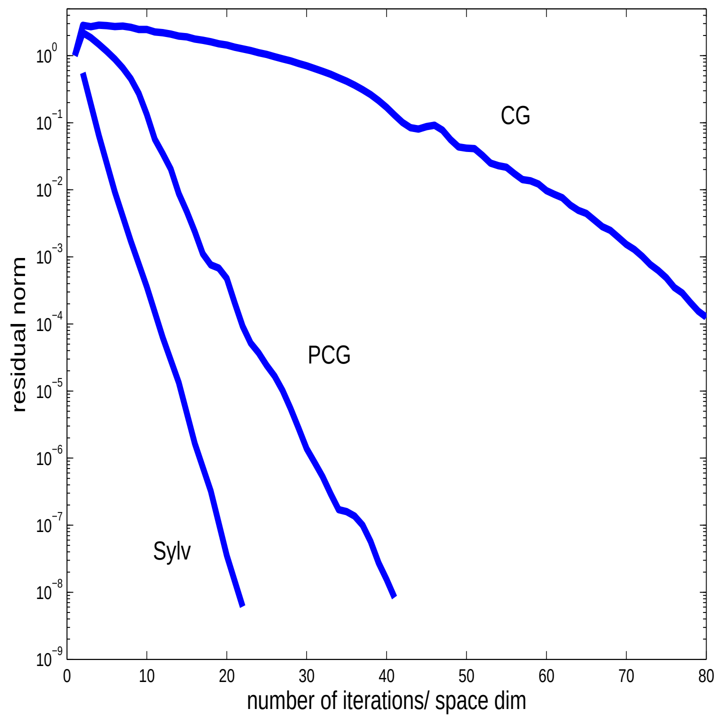
```
>> tic;lyap(T,F);toc
Elapsed time is 0.019335 seconds.
>> tic;A\b;toc
Elapsed time is 0.030765 seconds.
```

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

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

CG for $Ax = b$ vs Iterative solver for $(I \otimes T + T \otimes I)U + UT = F$

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



	CG	PCG	Matrix Eqn solver
Elapsed Time	2.91	0.56	0.08

A 3D convection-diffusion equation

$-\epsilon\Delta u + \mathbf{w}\cdot\nabla u = 1$, in $\Omega = (0,1)^3$, with convection term

$$\mathbf{w} = (x\sin x, y\cos y, e^{z^2-1})$$

Sylvester equation:

$$\left[I \otimes (T_1 + \Phi_1 B_1) + (T_2 + \Psi_2 B_2)^T \otimes I\right] U + U\ (T_3 + B_3 \Upsilon_3) = \mathbf{1}\mathbf{1}^T$$

ϵ	n_x	FGMRES+AGMG CPU time (# its)	GMRES+MI20 CPU time (# its)	Sylv Solver CPU time (# its)
0.0050	100	8.0207 (15)	9.7207 (7)	0.5677 (22)
0.0010	100	7.6815 (14)	9.4935 (7)	0.5446 (22)
0.0005	100	7.3914 (14)	9.6274 (7)	0.5927 (24)

D.Palitta & V.Simoncini (tr 2014)

... A classical approach

Matrix formulation is not new...

- Bickley & McNamee, 1960: Early literature on difference equations
- Wachspress, 1963: Model problem for ADI algorithm
- Ellner & Wachspress (1980's): interplay between the matrix and vector formulations (via preconditioning)

The stiffness matrix

$$S_g := M_1 \otimes I_n + I_n \otimes M_2$$

with $M_1 \neq M_2$, banded, with not necessarily the same dimensions

- Finite differences: M_j second order operator in one space dimension

  $\Rightarrow$ e.g., S_g: 2D Laplace operator in $[a, b]^2$

  $\Rightarrow$ e.g., S_g: 2D conv-diff operator with separable coeff.

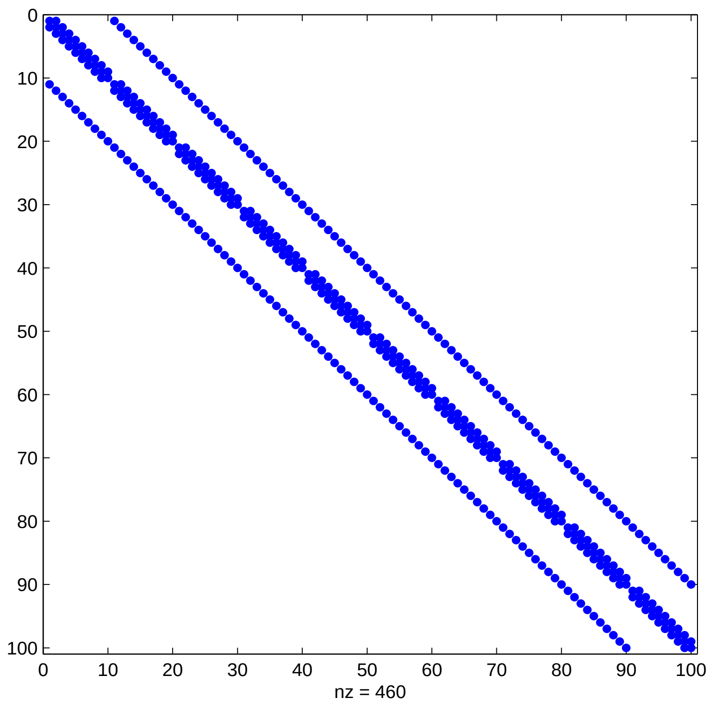
- Legendre Spectral methods: $M_1 = M_2$ spd, nonconstant diag.

- ...

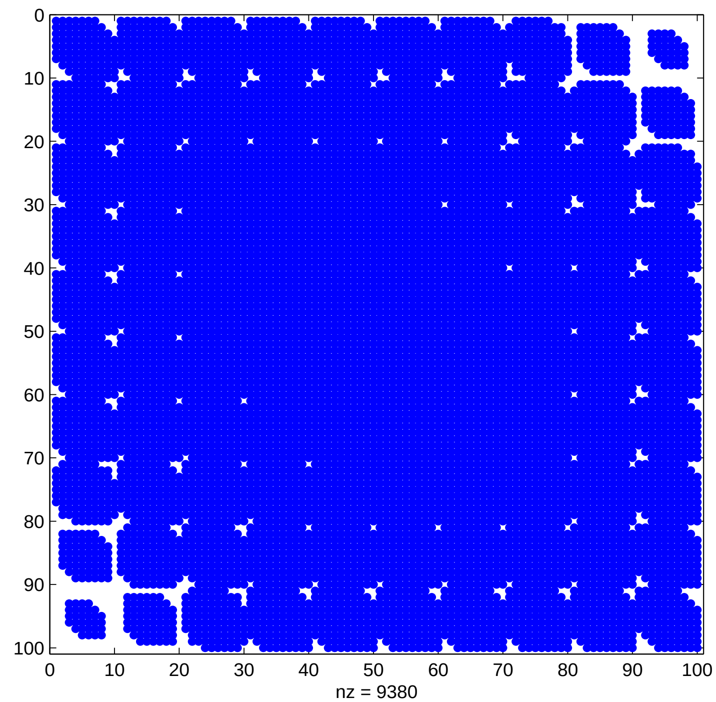
The inverse of the 2D Laplace matrix on the unit square

$$S := M \otimes I_n + I_n \otimes M, \qquad M = \mathrm{tridiag}(-1, 2, -1)$$

Sparsity pattern:



Matrix S

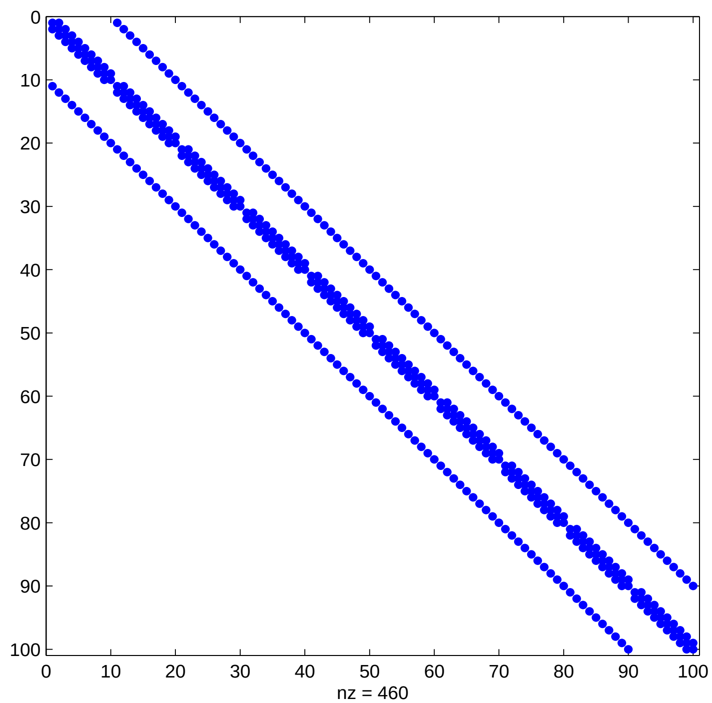


S^{-1}

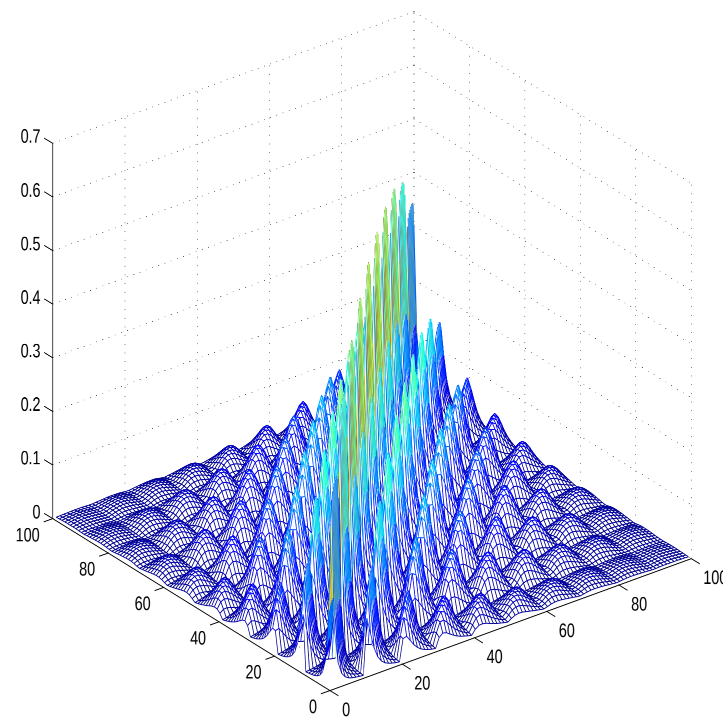
The inverse of the 2D Laplace matrix on the unit square

$$S := M \otimes I_n + I_n \otimes M, \qquad M = \mathrm{tridiag}(-1, 2, -1)$$

Sparsity pattern:



S



$|(S^{-1})_{ij}|$

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

The classical bound (Demko, Moss & Smith):

If S spd is banded with bandwidth b, then

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

where

κ: condition number of S

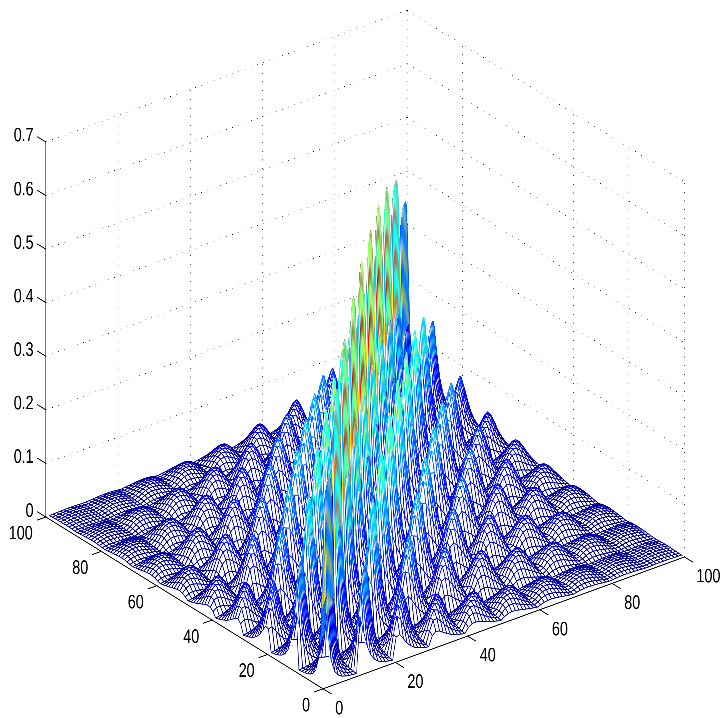
$q := \dfrac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \; < 1$

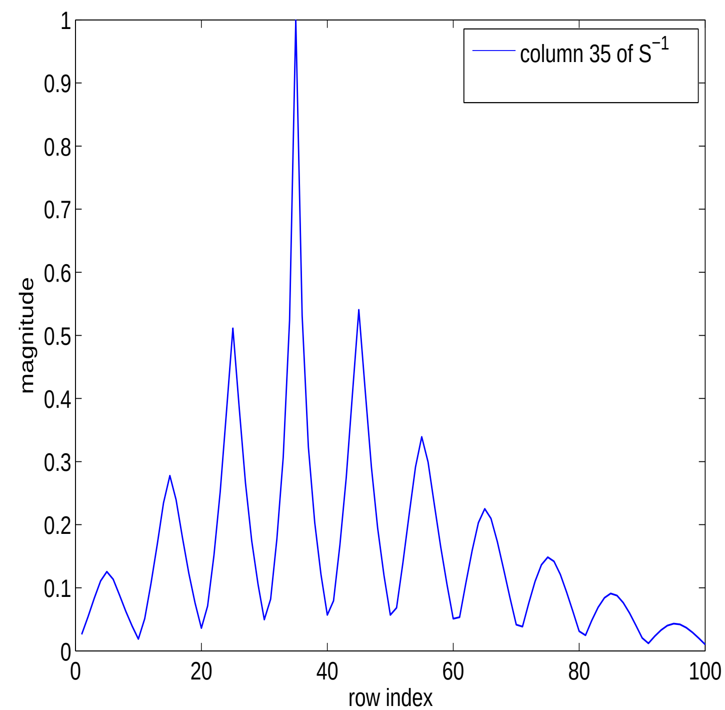
$\gamma := \max\{\lambda_{\min}(S)^{-1}, \frac{(1+\sqrt{\kappa})^2}{2\lambda_{\max}(S)}\}$

($\lambda_{\min}(\cdot), \lambda_{\max}(\cdot)$ smallest and largest eigenvalues of the given symmetric matrix)

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

The true decay





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

Where do the repeated peaks come from?

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

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

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Let

$X_t \in \mathbb{R}^{n \times n}$ be such that $x_t = \mathrm{vec}(X_t)$

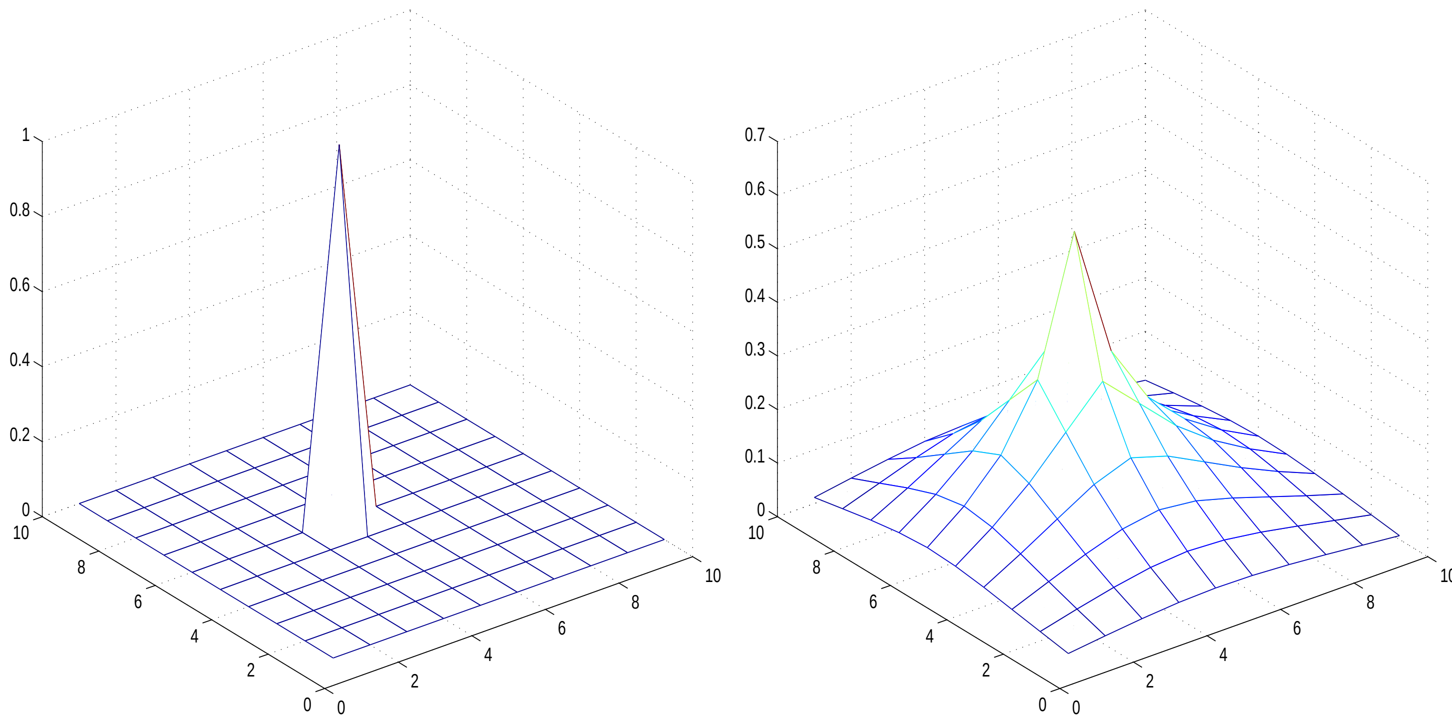
$E_t \in \mathbb{R}^{n \times n}$ be such that $e_t = \mathrm{vec}(E_t)$

Then

$$S x_t = e_t \qquad \Leftrightarrow \qquad M X_t + X_t M = E_t$$

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

$$t = 35, \qquad Sx_t = e_t \qquad \Leftrightarrow \qquad MX_t + X_tM = E_t$$



matrix E_t and matrix X_t

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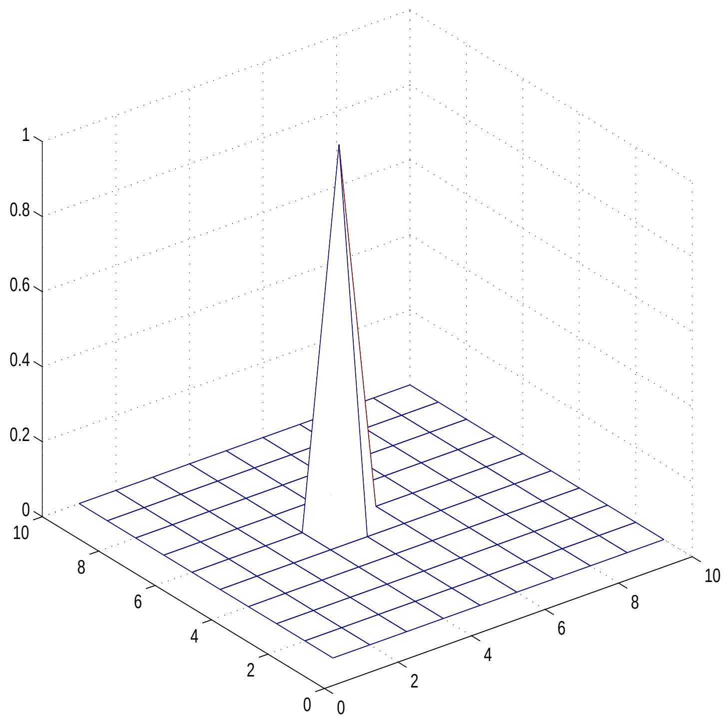
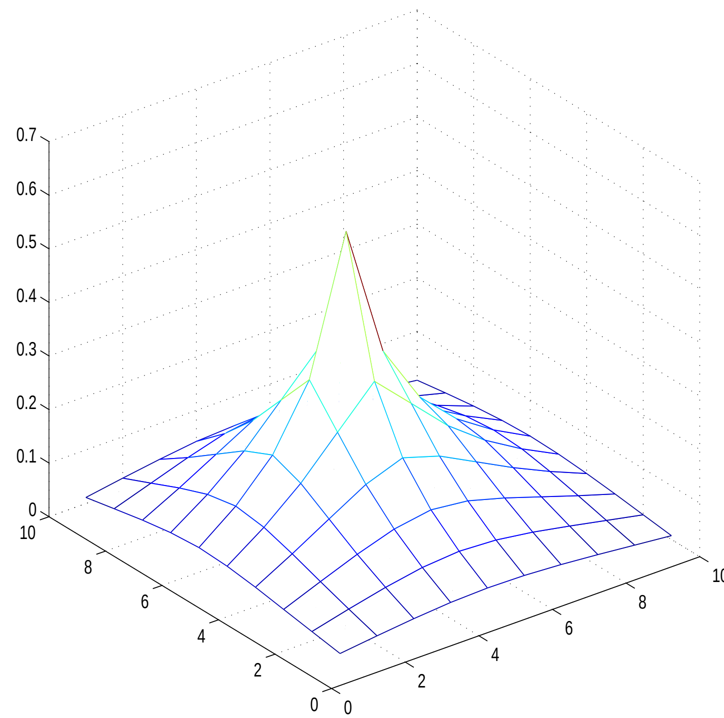
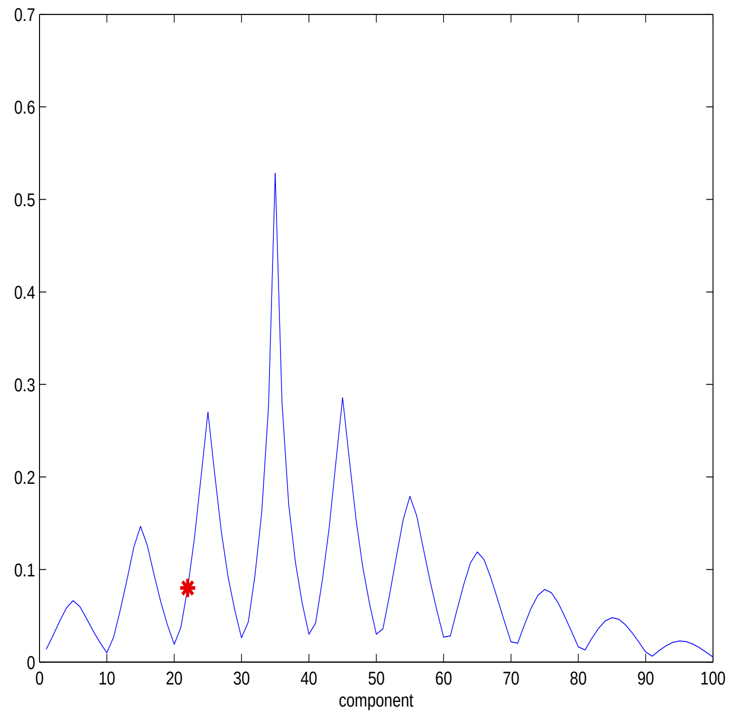


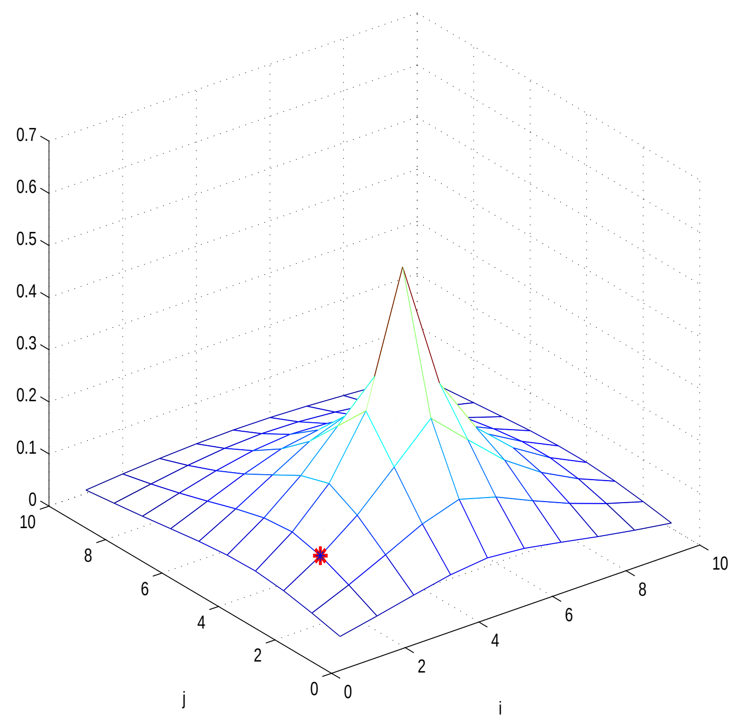


matrix E_t and matrix X_t

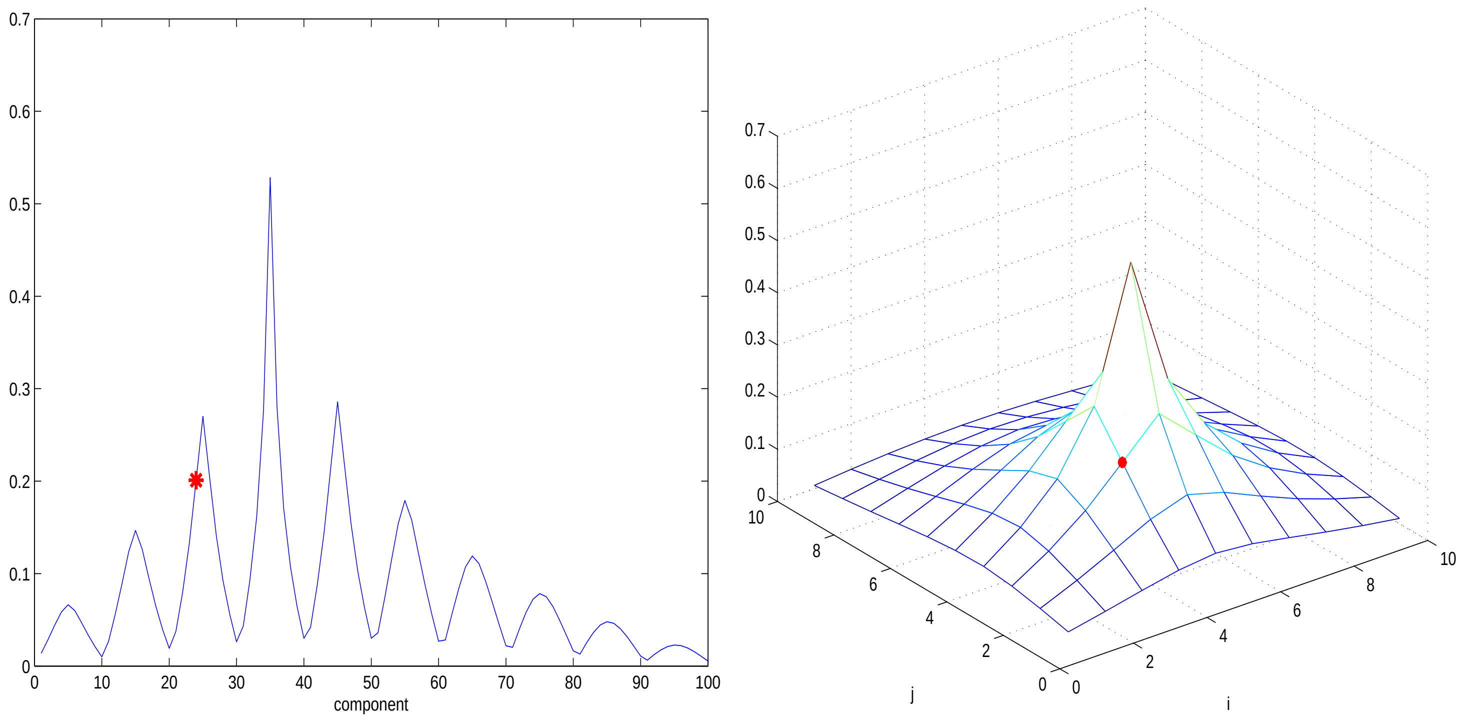
E_t has only one nonzero element

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





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



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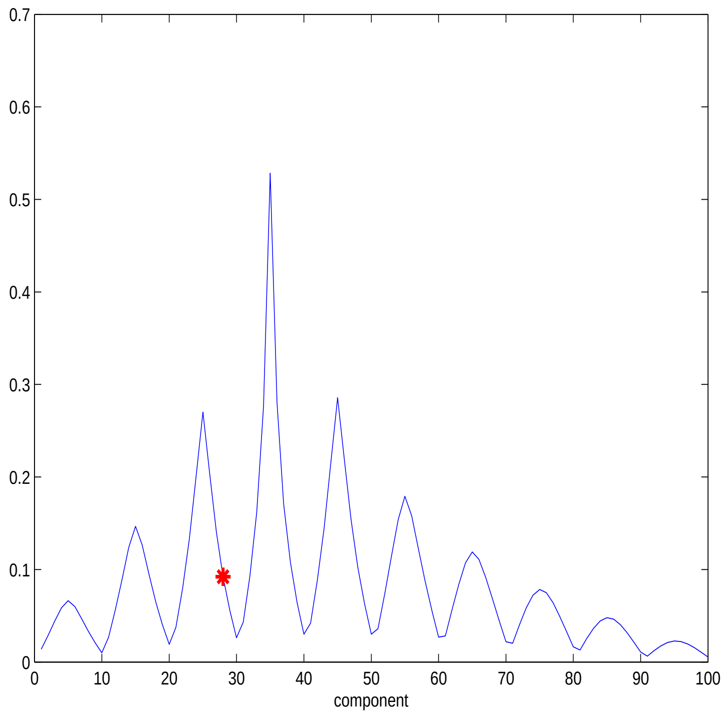

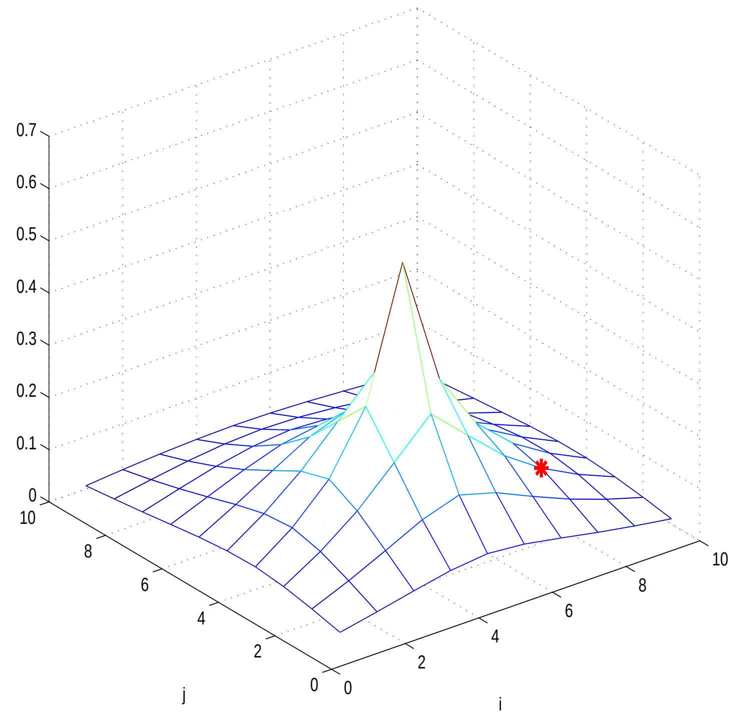

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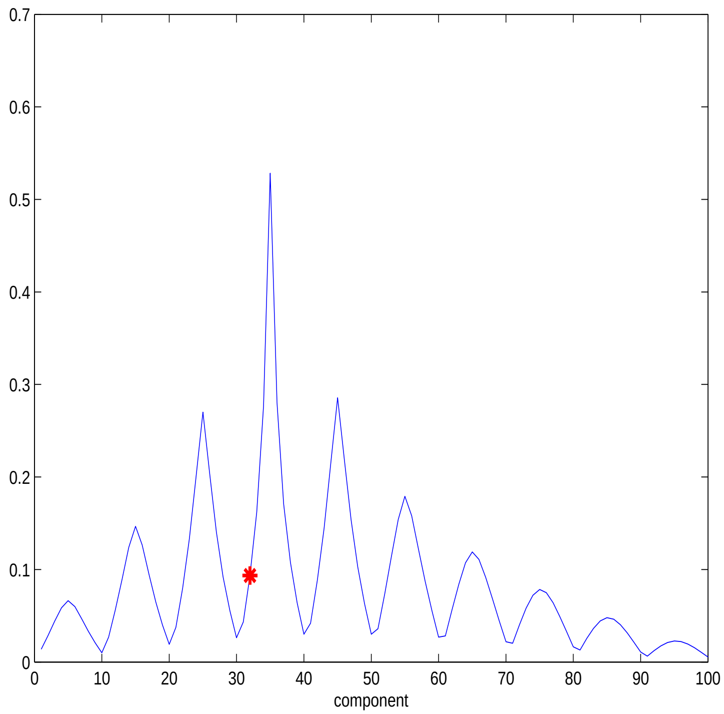

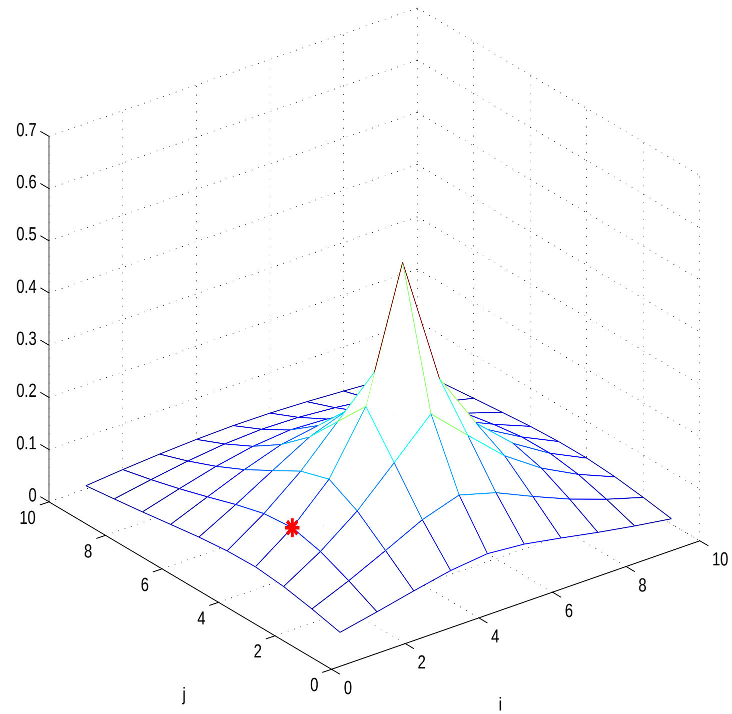

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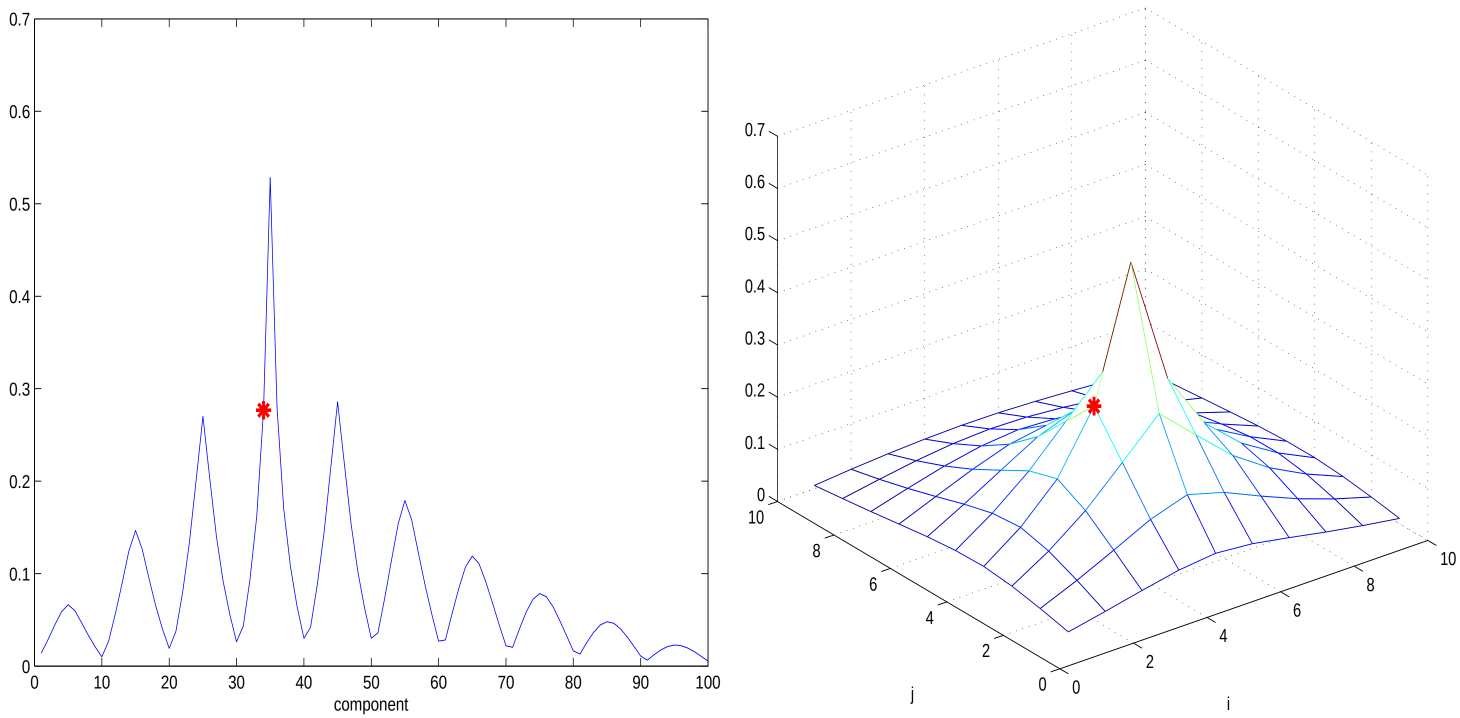

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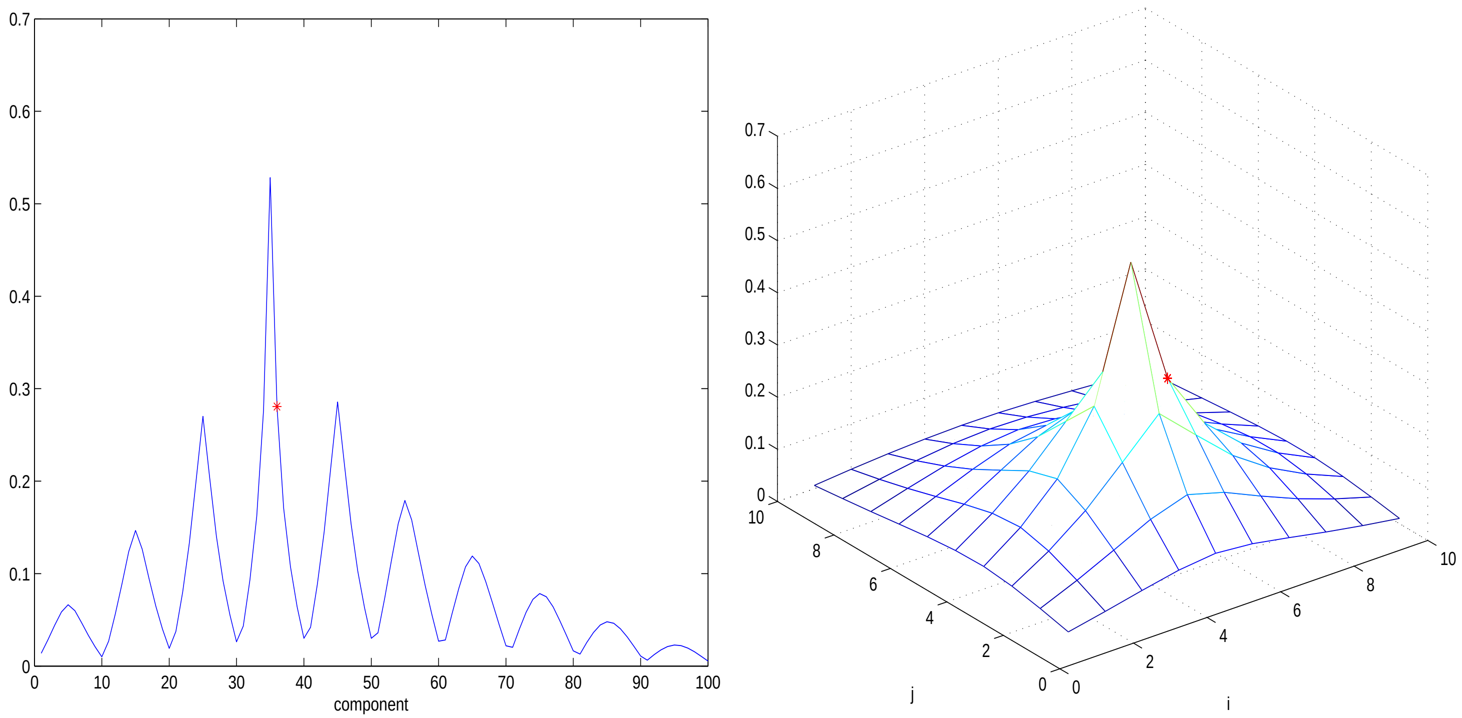

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Resolving the entry indexing using $MX_t + X_tM = E_t$

$$(S^{-1})_{k,t} = (S^{-1})_{\ell+n(m-1),t} = e_\ell^\top X_t e_m, \quad \ell, m \in \{1, \ldots, n\}$$

$\Rightarrow$ All the elements of the t-th column, $(S^{-1})_{:,t}$, are obtained by varying $m, \ell \in \{1, \ldots, n\}$

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$\Rightarrow$ All the elements of the t-th column, $(S^{-1})_{:,t}$, are obtained by varying $m, \ell \in \{1, \ldots, n\}$

From the Lyapunov equation theory,

$$X_t = \frac{1}{2\pi}\int_{-\infty}^{\infty} (\imath\omega I + M)^{-1} E_t (\imath\omega I + M)^{-*} \mathrm{d}\omega$$

with $E_t = e_i e_j^\top$, $j = \lfloor (t-1)/n \rfloor + 1$, $i = t - n\lfloor (t-1)/n \rfloor$

Therefore,

$$e_\ell^\top \mathcal{X}_t e_m = \frac{1}{2\pi}\int_{-\infty}^{\infty} e_\ell^\top (\imath\omega I + M)^{-1} e_i e_j^\top (\imath\omega I + M)^{-*} e_m \mathrm{d}\omega$$

Qualitative bounds

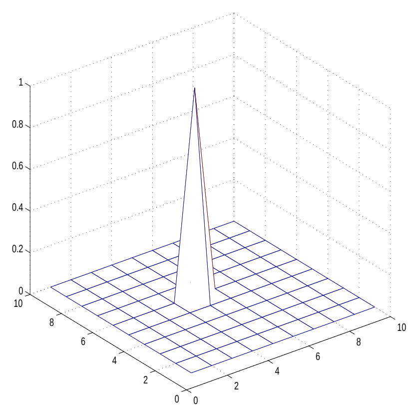
Let $\kappa = \lambda_{\max}/\lambda_{\min} = \mathrm{cond}(M)$

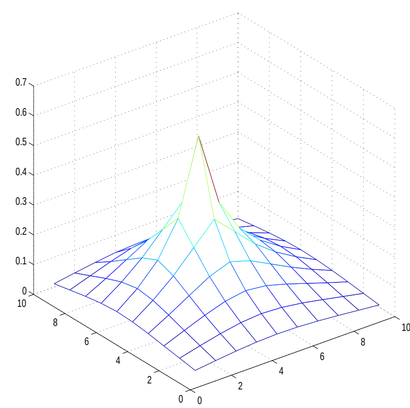
i)Assume $\ell, i, m, j \; : \; \ell \neq i$, $m \neq j$. $\mathfrak{n}_2 := |\ell - i| + |m - j| - 2 > 0$

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

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

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

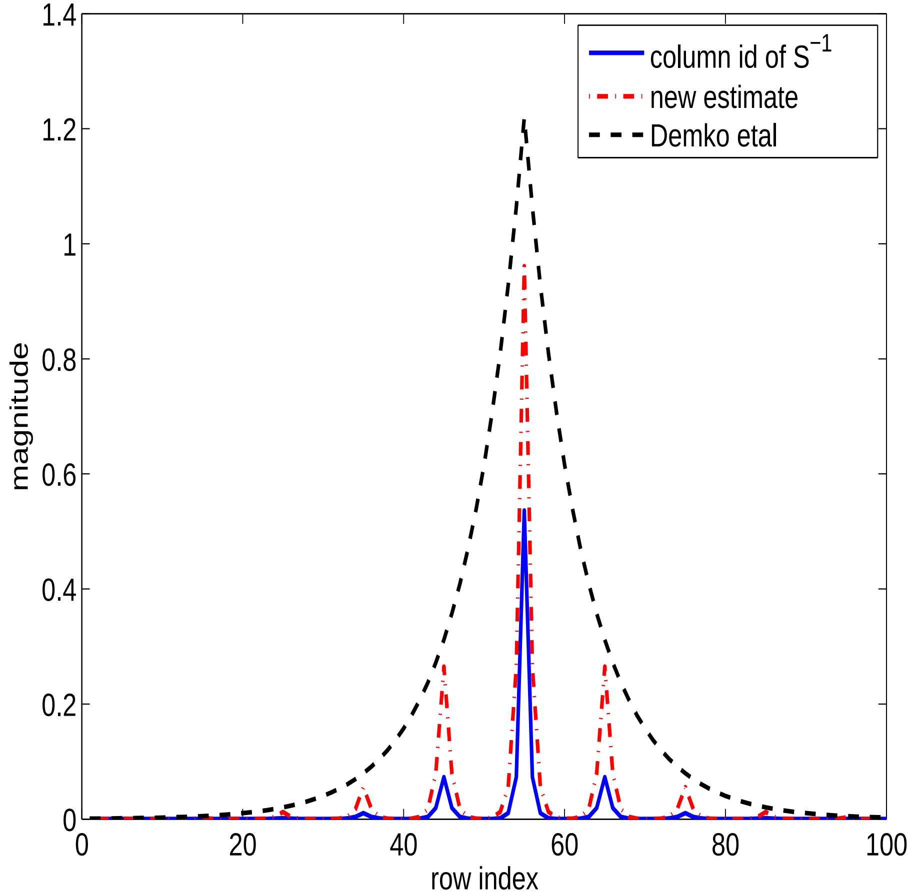




(i, j) and (ℓ, m)

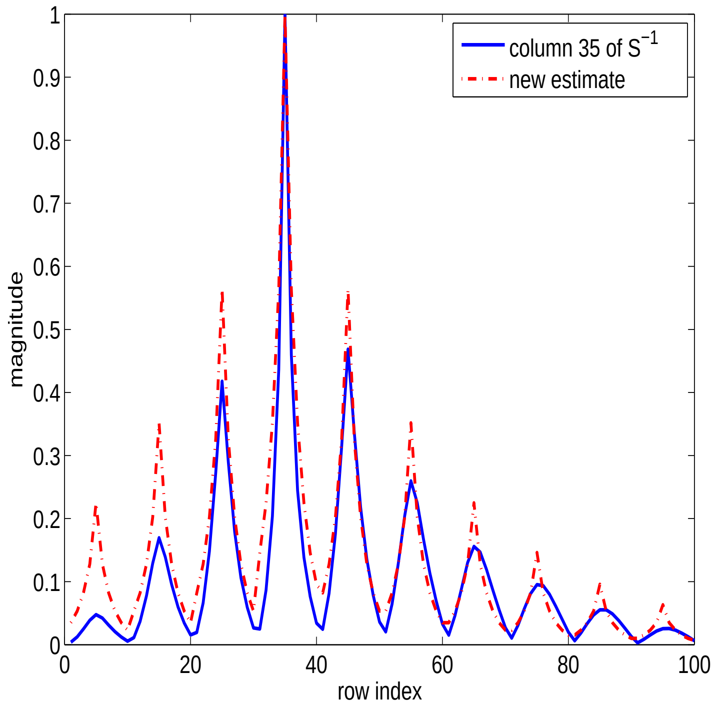
Examples. Symmetric positive definite matrix

$$M = \mathrm{tridiag}(-0.5, \underline{2}, -0.5) \in \mathbb{R}^{10\times 10}$$



Examples. Legendre stiffness matrix (scaled to have peak equal to 1)

$$M = \text{tridiag}(\delta_k, \underline{\gamma_k}, \delta_k)$$



$$\gamma_k = \frac{2}{(4k-3)(4k+1)}$$

$$k = 1, \ldots, n, \quad \text{and}$$

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

$$k = 1, \ldots, n-1$$

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 $h \leq h_0$, $x, y \in R_h$,

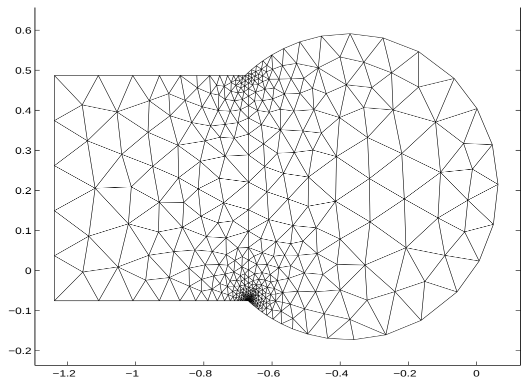
$$G_h(x,y) \leq \begin{cases} C \log \frac{C}{|x-y|+h} & \text{if } d = 2 \\ \frac{C}{(|x-y|+h)^{d-2}} & \text{if } d \geq 3 \end{cases}$$

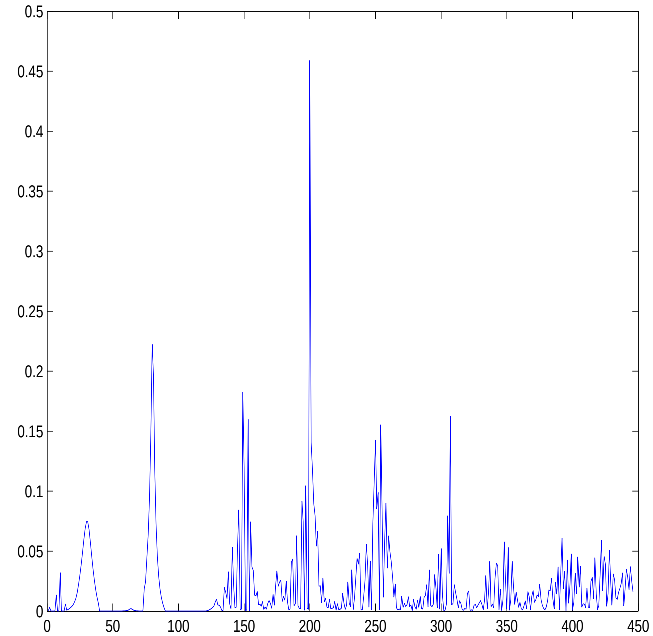
(Bramble & Thomee, '69)

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

Generalizations. Next step.

A: Negative Laplacian matrix





Left: Discretization of the domain

Right: entries of column 200 of A^{-1} for that domain

An application. I

Adaptive Legendre-Galerkin discretizations for PDEs:

H_0^1 Tensorized Babuska-Shen basis in $\Omega = (0,1) \times (0,1)$:

$$\eta_{\mathbf{k}}(x_1, x_2) = \eta_{k_1}(x_1)\eta_{k_2}(x_2), \quad k_1, k_2 \geq 2, \quad \mathbf{k} = (k_1, k_2)$$

$\{\eta_{k_i}\}$: k_i-order Legendre polyn (1D BS basis)

Stiffness matrix:

$$(\eta_{\mathbf{k}}, \eta_{\mathbf{m}})_{H_0^1(\Omega)} = (\eta_{k_1}, \eta_{m_1})_{H_0^1(I)}(\eta_{k_2}, \eta_{m_2})_{L^2(I)} + (\eta_{k_1}, \eta_{m_1})_{L^2(I)}(\eta_{k_2}, \eta_{m_2})_{H_0^1(I)}$$

Kronecker structure: $S_\eta^p = M_p \otimes I_p + I_p \otimes M_p$ (max p polyn degree)

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Kronecker structure: $S_\eta^p = M_p \otimes I_p + I_p \otimes M_p$ (max p polyn degree)

Note: If higher order polynomial used, then S_η^p simply expands (augmented M_p)

An application. II

Adaptive Legendre-Galerkin discretizations for PDEs:

- Inner product:

$$v = \sum \hat{v}_{\mathbf{k}} \eta_{\mathbf{k}}, \qquad \|v\|^2_{H^1_0} = \hat{v}^T S_\eta \hat{v}$$

An application. II

Adaptive Legendre-Galerkin discretizations for PDEs:

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- (Full!) Orthonormalization: $\{\Phi_{\mathbf{k}}\}$ orth basis,

$$v = \sum \tilde{v}_{\mathbf{k}} \Phi_{\mathbf{k}}, \qquad \|v\|^2_{H^1_0} = \tilde{v}^T G^T S_\eta (G\tilde{v}) = \tilde{v}^T \tilde{v}$$

with $G = L^{-1}$ where $S_\eta = LL^T$

An application. II

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  with $G = L^{-1}$ where $S_\eta = LL^T$

- (Cheap!) Quasi-orthonormalization: $\{\Psi_{\mathbf{k}}\}$ quasi-orth basis,

$$v = \sum \check{v}_{\mathbf{k}} \Psi_{\mathbf{k}}, \qquad \|v\|^2_{H^1_0} = \tilde{v}^T \check{G}^T S_\eta (\check{G}\tilde{v}) \approx \tilde{v}^T D \tilde{v}$$

  $\check{G}$ very sparse version of G, $\quad D$ diagonal

An application. II

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  $\check{G}$ very sparse version of G, D diagonal

Q: Does such a $\check{G}$ exist? ...Yes! Because of sparsity of S_η^{-1}

More applications. Using sparsity in solution strategies

$$MX + XM = BB^T$$

$M = \mathrm{tridiag}(-1, 4, -1) \in \mathbb{R}^{n\times n}$, $n = 100$ and $B = [e_{50}, \ldots, e_{60}]$

More applications. Using sparsity in solution strategies

$$MX + XM = BB^T$$

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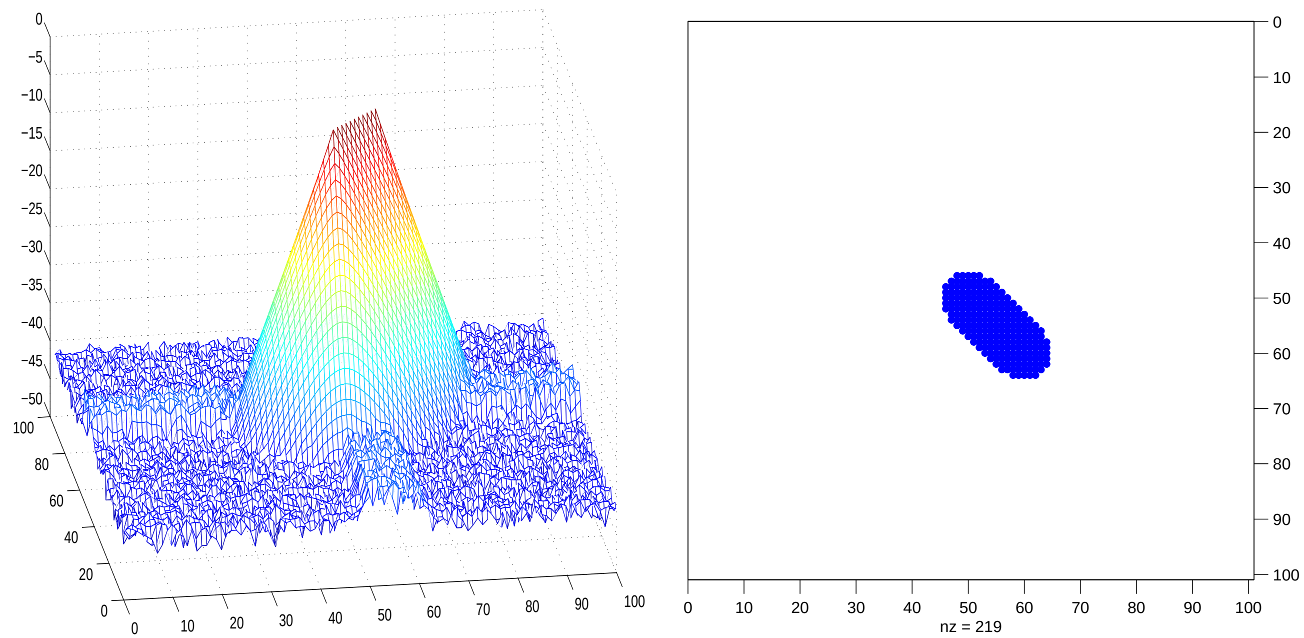
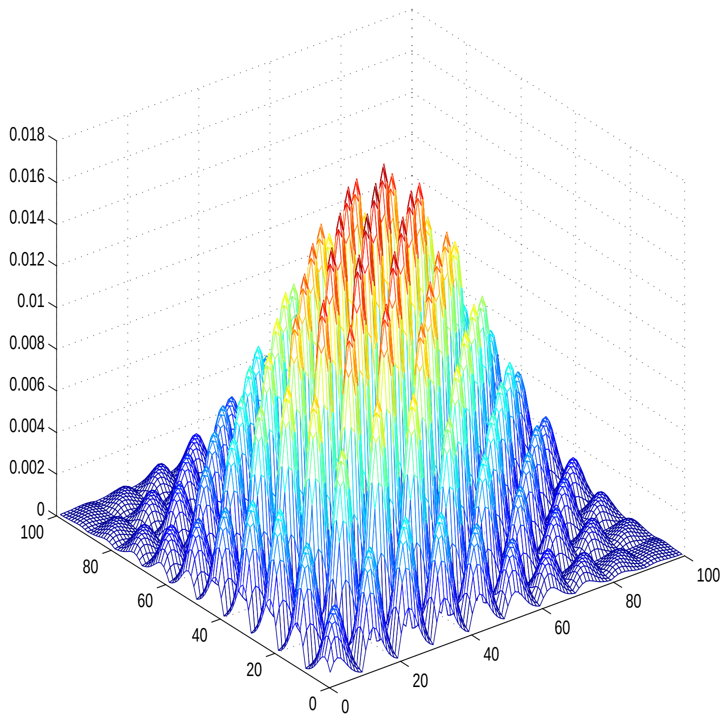


Left: pattern of X with log scale, $\texttt{nnz}(X) = 9724$

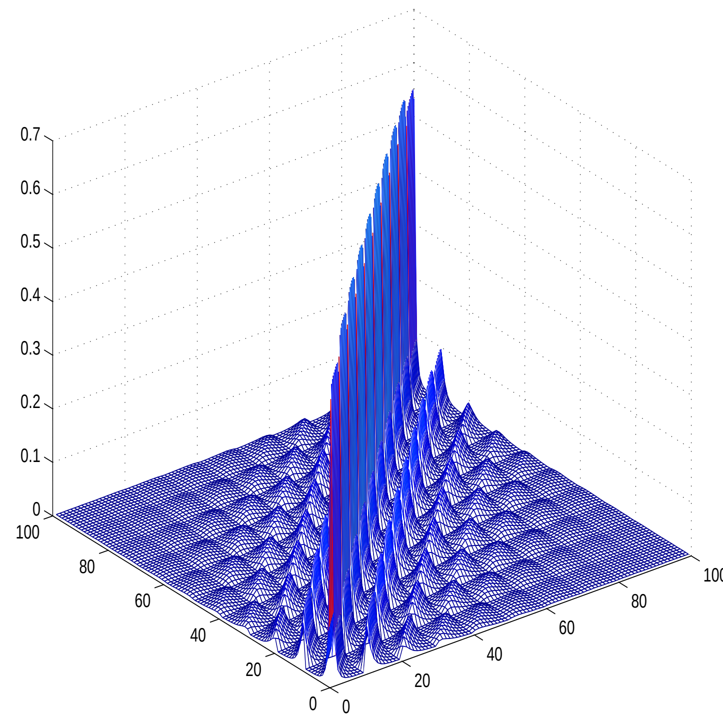
Right: Sparsity pattern of truncated ver. of X: all entries below 10^{-5} are omitted

More applications. Decay of functions of Kronecker sum matrices

$A = M \otimes I + I \otimes M$ (discretization of negative Laplacian)



$|e^{-5A}|_{ij}$



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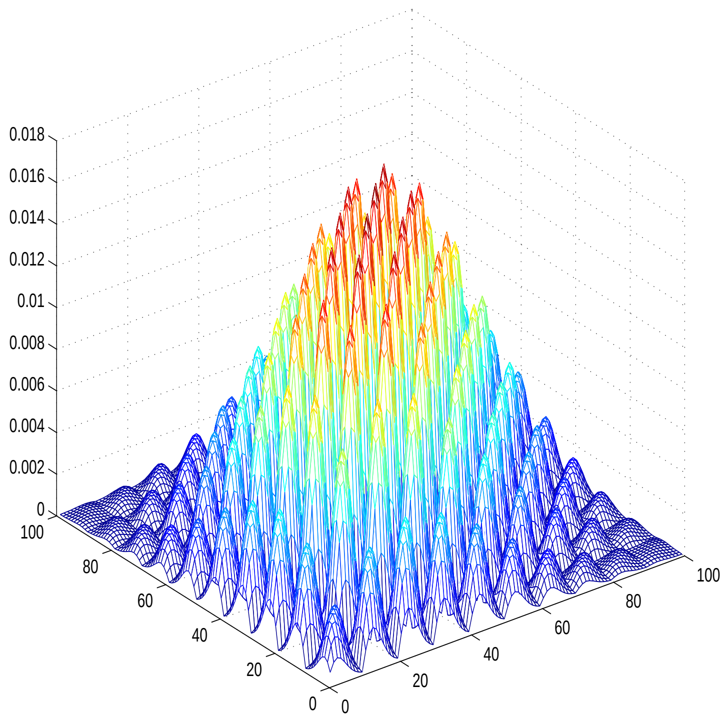

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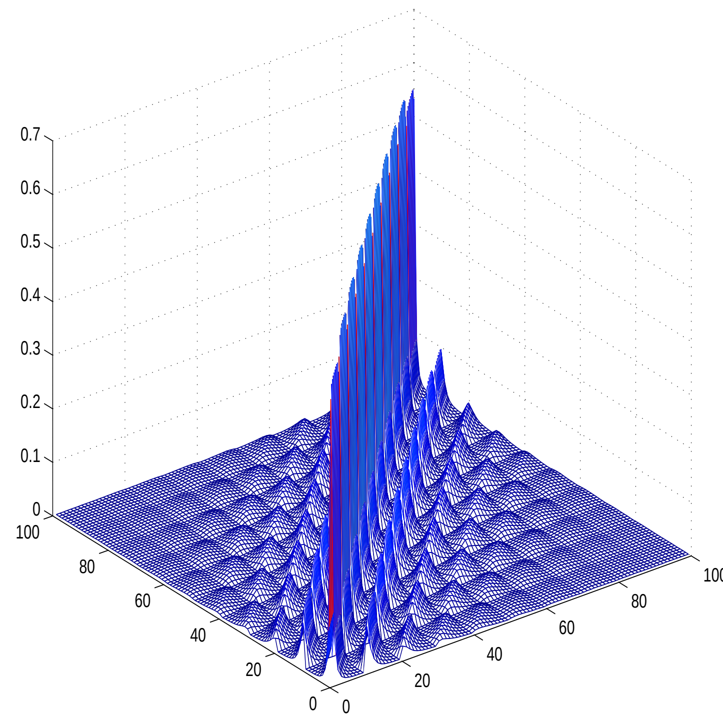

$|A^{-\frac{1}{2}}|_{ij}$

In addition: drastically lower computational costs for $f(A)v$

Conclusions and further work ahead

- The Lyapunov operator has a very rich structure
- Appropriate computational devices
- Powerful mathematical tool
- Structure recurrent in many application problems...
- ... Generalize to more hidden structures

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