

Compression, inversion and sparse approximate PCA of dense kernel matrices in near linear computational complexity

Florian Schäfer

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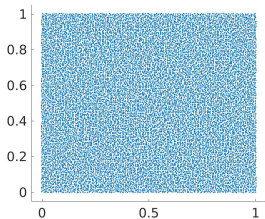
<http://arxiv.org/abs/1706.02205>

Outline

- 1 A numerical experiment
- 2 Disintegration of measure and Gaussian elimination
- 3 Near-linear complexity algorithms using the theory of Gamblets
- 4 Further numerical results

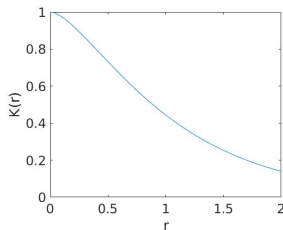
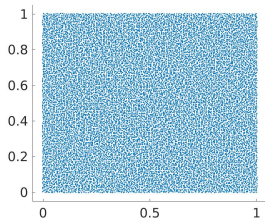
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- $\{x_i\}_{i \in I} \subset [0, 1]^2$, with $\#I = N = 16641$



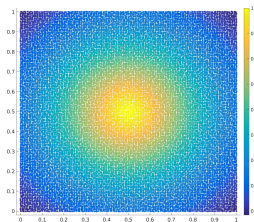
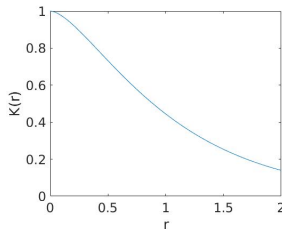
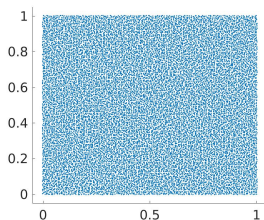
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- $\Gamma_{i,j} := K(\|x_i - x_j\|)$.



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- We need to apply the Matrix and its inverse, and compute its determinant.
- Γ is dense, and hence has N^2 storage cost. Direct inversion via Gaussian elimination has $\mathcal{O}(N^3)$ complexity in time.

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- We provide a simple algorithm, with rigorous error bounds and near-linear complexity.

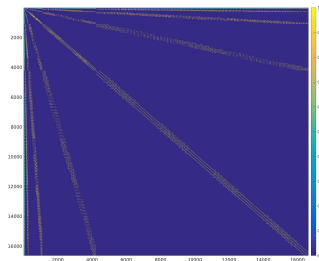
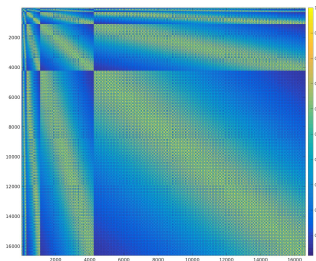
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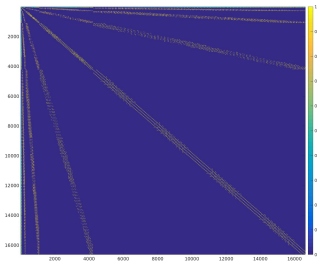
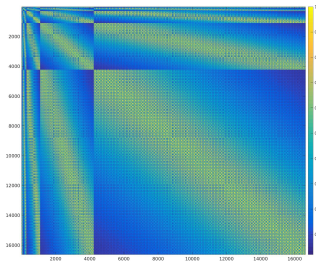


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- $\#S_2 = 5528749 = 0.0189N^2$. We have thrown away all but 2 percent of the entries, without even touching them!

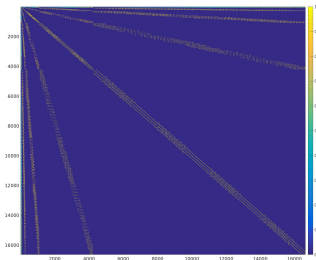
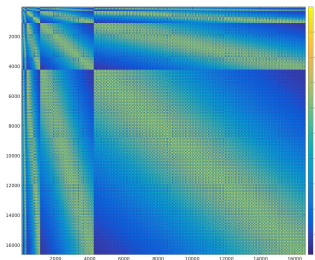


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- We will see later: S_2 does not depend on the entries of Γ .



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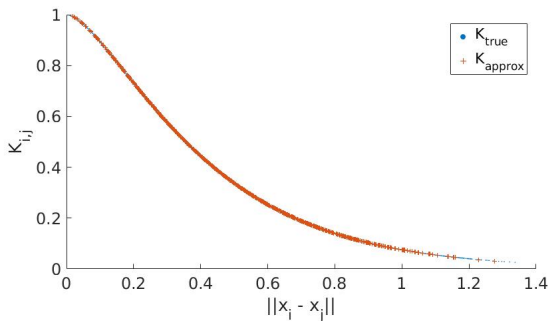
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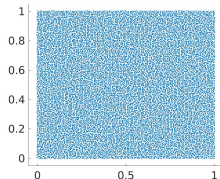
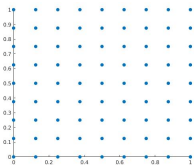
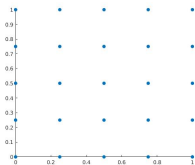
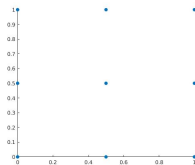
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- Decompose $\{x_i\}_{i \in I}$ into a nested hierarchy as:

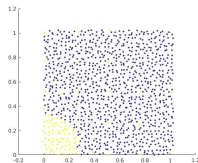
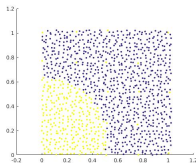
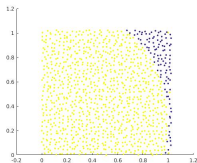
$$\{x_i\}_{i \in I^{(1)}} \subset \{x_i\}_{i \in I^{(2)}} \subset \{x_i\}_{i \in I^{(3)}} \subset \cdots \subset \{x_i\}_{i \in I^{(q)}} = \{x_i\}_{i \in I} \quad (1.1)$$



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- We define $J^{(k)} := I^{(k)} \setminus I^{(k-1)}$ and define the sparsity pattern:

$$S_2 := \left\{ (i, j) \in I \times I \mid i \in J^{(k)}, j \in J^{(l)}, \text{dist}(x_i, x_j) \leq 2 * 2^{-\min(k, l)} \right\}.$$

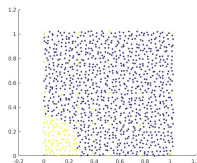
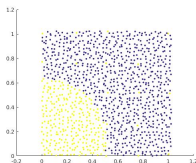
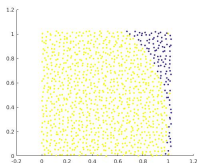


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- We order the elements of I from coarse to fine, that is from $J^{(1)}$ to $J^{(q)}$.



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- Allows for sampling of $X \sim N(0, \Gamma)$ in near-linear time.

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- show that even though the Matérn family is not covered rigorously by our theoretical results, we get good approximation results, in particular in the interior of the domain.
- show that as a byproduct of our algorithm we obtain a sparse approximate PCA with near optimal approximation property.

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- Choose Y , such that Y and $\mathbb{E}[f(X)|Y]$ can be sampled cheaply.

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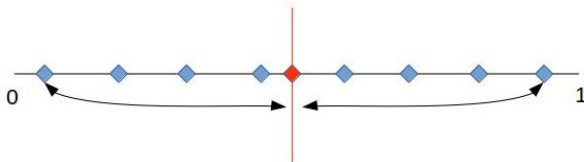
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- When using Cholesky decomposition, this yields a factor 4 improvement of computational speed.

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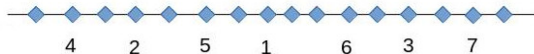
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- (Block-)Cholesky decomposition is computationally equivalent to the disintegration of Gaussian measures.
- Follows immediately from well known formulas, but rarely used in the literature. One Example: Bickson (2008).

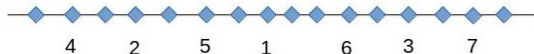
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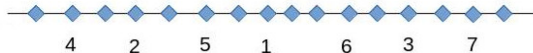
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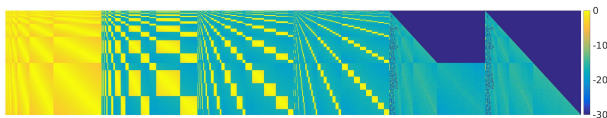
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- Lets start computing the Cholesky decomposition
- We observe a *fade-out* of entries!

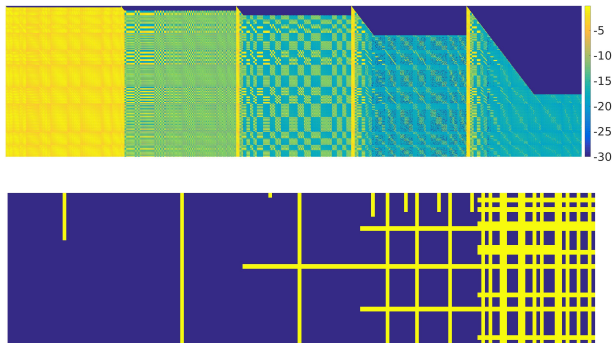


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- In 2d, use quadsection:



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- Bisective/Quadsective ordering is the reverse of nested dissection.
- Indeed, for P the order-reversing permutation matrix, we have:

$$\begin{aligned}(\Theta)^{-1} &= (LL^T)^{-1} = L^{-T}L^{-1} \\ \implies P(\Theta)^{-1}P &= PL^{-T}PPL^{-1}P = (PL^{-T}P)(PL^{-T}P)^T,\end{aligned}$$

- But we have $L^{-1} = L^T(\Theta)^{-1}$.
- For a sparse elimination ordering of Θ , the reverse ordering leads to sparse factorisation of $(\Theta)^{-1}$

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- Remaining problems with our approach:
- Nested dissection does not lead to near-linear complexity algorithms
- Precision matrix will not be exactly sparse. How is it localised?
- The answer can be found in the recent literature on numerical homogenisation:

Sparse factorisation of dense matrices using gamblets

- “Gamblet” bases have been introduced as part of the game theoretical approach to numerical PDE (Owhadi (2017), Owhadi and Scovel (2017)).

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- Assume our covariance matrix is

$$\Theta_{i,j} = \int_{[0,1]^2} \phi_i^{(q)}(x) G(x,y) \phi_j^{(q)}(y) \, dx \, dy$$

For $\phi_i^{(q)} := \mathbb{1}_{[(i-1)h^q, ih^q]}$ and G the Green's function of a second order elliptic PDE.

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- Corresponds to $X_i(\omega) = \int_0^1 \phi_i^{(q)}(x) u(x, \omega) dx$, with $u(\omega)$ solution to elliptic SPDE with Gaussian forcing.

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- For $\phi_i^{(k)} := \mathbb{1}_{[(i-1)h^k, ih^k]}$, Owhadi and Scovel (2017) shows:
- $\psi_i^{(k)} := \mathbb{E} \left[u \mid \int_0^1 u(x) \phi_j^{(k)}(x) dx = \delta_{i,j} \right]$ is exponentially localised, on a scale of h^k :

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- Main idea: Estimate on exponential decay of a conditional expectation implies exponential decay of a Cholesky factors.

Sparse factorisation of dense matrices using gamblets

- Transform to multiresolution basis to obtain block matrix:

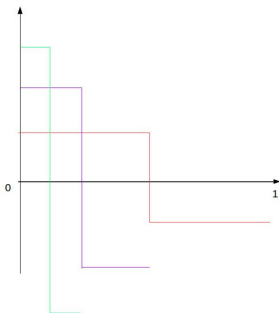
$$(\Gamma_{k,l})_{i,j} = \int_{[0,1]^2} \phi_i^{(k),\chi}(x) G(x,y) \phi_j^{(l),\chi}(y) \, dx \, dy$$

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- Where the $\{\phi_j^{(k),\chi}\}_{j \in J^{(k)}}$ are chosen as Haar basis functions.



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- Furthermore, the stiffness matrices decay exponentially on each level:

$$B_{i,j}^{(k)} := \int_0^1 \chi_i^{(k)}(x) G^{-1} \chi_j^{(k)}(x) dx \leq \exp(-\gamma \|x_i - x_j\|)$$

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- Finally, we have for a constant κ :

$$\text{cond} \left(B^{(k)} \right) \leq \kappa, \forall k$$

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$$\Gamma_{22} - \Gamma_{21}\Gamma_{11}^{-1}\Gamma_{12} = \text{Cov} \left[\int u\phi^{(2),\chi} \mathrm{d}x \middle| \int u\phi^{(1),\chi} \mathrm{d}x \right] = \left(B^{(2)}\right)^{-1}$$

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- $\left(\Gamma_{21}\Gamma_{11}^{-1}\right)_{i,j} = \int \phi_i^{(2),x} \chi_j^{(1)} dx \leq C \exp\left(-\frac{\gamma}{h} \left\|x_i^{(2)} - x_j^{(1)}\right\|\right)$

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Sparse factorisation of dense matrices using gamblets

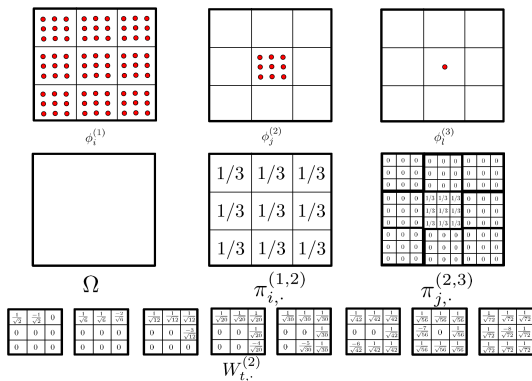
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- These factors can be approximated in time complexity by (block-)Cholesky decomposition in computational complexity of $\mathcal{O}\left(N \log^2(N) \left(\log(1/\epsilon) + \log^2(N)\right)^{4d+1}\right)$ in time and $\mathcal{O}(N \log(N) \log^d(N \frac{1}{\epsilon}))$ in space for an approximation error of ϵ .

Sparse factorisation of dense matrices using gamblets

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Sparse factorisation of dense matrices using gamblets

- How about $\phi_i^{(q)} = \delta_{x_i^{(q)}}$, i.e. pointwise sampling?
- In Owhadi and Scovel (2017), analogue results for pointwise samples are obtained using averaging:



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- Factorisation can be done in $\mathcal{O}(N \text{poly}(\rho \log(N)))$, error decays exponentially with ρ .

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- The multiresolution basis, in order to satisfy the conditions of the proof of bounded condition numbers given in Owhadi and Scovel (2017) needs to satisfy the vanishing moment condition:

$$\int_{\tau_i^{(k)}} p \phi_i^{(k), \chi} dx = 0, \forall p \in \mathcal{P}_{s-1}(\tau_i^{(k)}),$$

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- Therefore, the multiresolution basis depends on the operator.
- Also, averaging over large regions required for coarse basis functions. Leads to $\mathcal{O}(N^2)$ complexity of basis transform.

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- Conditions in Owhadi and Scovel (2017) are (roughly speaking):

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Sparse factorisation of dense matrices using gamblets

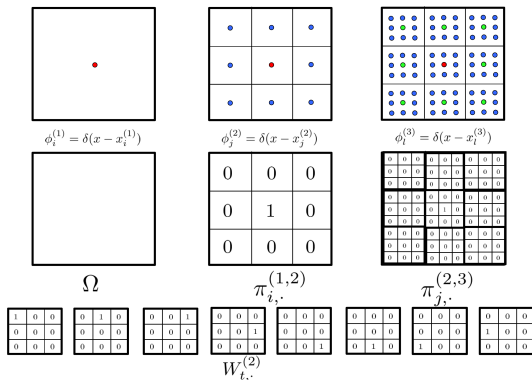
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- The gamblets find the optimal orthogonalisation themselves!

Sparse factorisation of dense matrices using gamblets

- We can use subsampling as an aggregation scheme!



Sparse factorisation of dense matrices using gamblets

- Our algorithm now consists of three steps:
 - 1 Reorder the variables hierarchically
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- At this point, for theoretical guarantees we need to replace step three with an incomplete Block factorisation. All numerical evidence indicates that this is not necessary.

Two additional results

- As observed in Owhadi 2017, Hou and Zhang 2017, gamblets provide a near-optimal sparse PCA. We obtain a PCA with the same approximation property, by keeping only the first k columns of L .

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- As observed in Owhadi 2017, Hou and Zhang 2017, gamblets provide a near-optimal sparse PCA. We obtain a PCA with the same approximation property, by keeping only the first k columns of L .
- By reversing the elimination ordering, we obtain a near linear complexity Cholesky factorisation of the sparse/exponentially decaying inverse of Θ .

Problems at the boundary

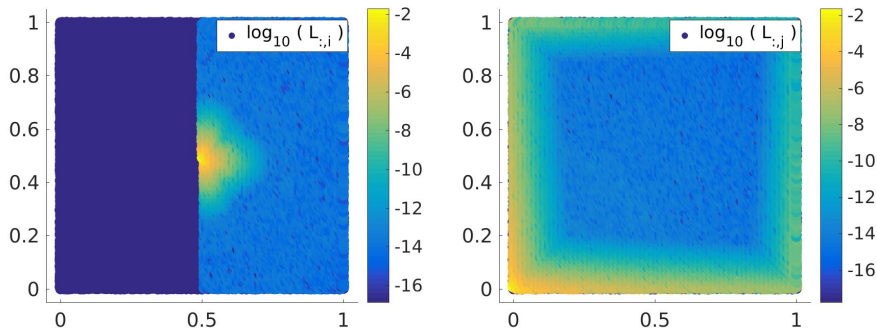
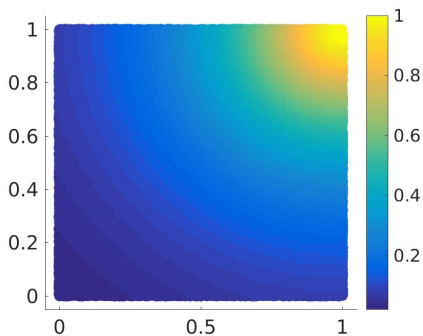
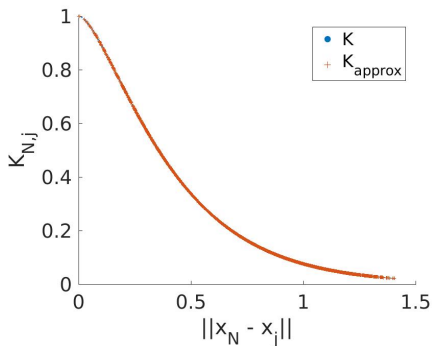
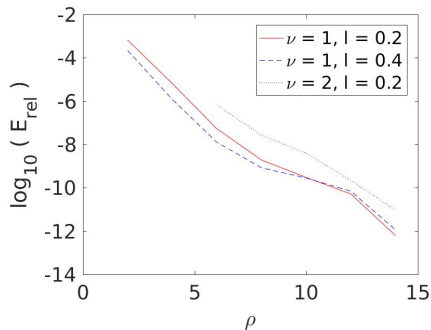
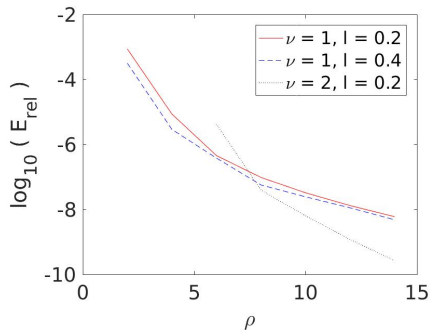


Figure: $\nu = 1, l = 0.4$

Problems at the boundary



Decay of approximation error



Sparse approximate PCA

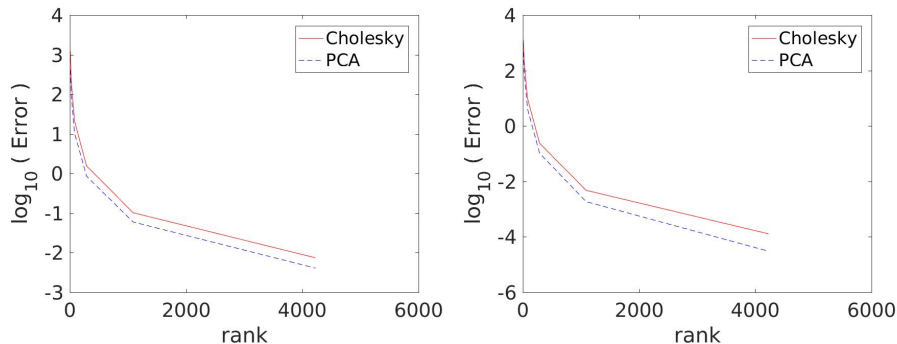
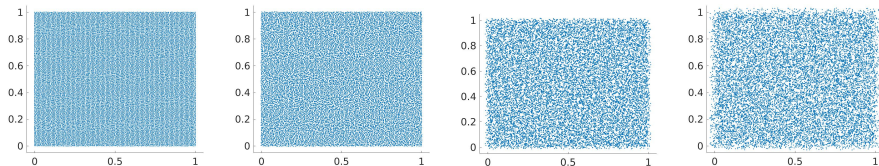


Figure: Near optimal sparse PCA: First panel: $\nu = 1, l = 0.2, \delta_x = 0.2$ and $\rho = 6$. Second panel: $\nu = 2, l = 0.2$ and $\delta_x = 0.2$ and $\rho = 8$.

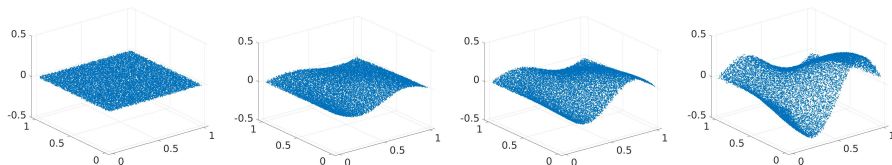
Perturbation of the Mesh



δ_x	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ / \ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}} / \ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
0.2	4.336e-03	1.560e-06	1.669e-02	1.026e-06	2.125e+07	7.675e-02
0.4	4.495e-03	1.617e-06	1.706e-02	1.063e-06	2.128e+07	7.683e-02
2.0	4.551e-03	1.638e-06	1.820e-02	1.077e-06	2.127e+07	7.682e-02
4.0	8.158e-03	2.940e-06	2.976e-02	1.933e-06	2.119e+07	7.652e-02

Table: Compression and accuracy for $q = 7$, $l = 0.2$, $\rho = 5$, $\nu = 1$ and different values of δ_x .

Data on low dimensional manifold



δ_z	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
0.0	5.049e-03	1.560e-06	1.885e-02	1.026e-06	2.126e+07	7.677e-02
0.1	6.341e-02	1.648e-06	1.232e-01	1.077e-06	2.083e+07	7.521e-02
0.2	1.204e-01	1.749e-06	2.203e-01	1.126e-06	1.976e+07	7.137e-02
0.4	1.954e-01	3.550e-06	5.098e-01	2.197e-06	1.722e+07	6.218e-02

Table: Compression and accuracy for $q = 7$, $l = 0.2$, $\rho = 5$, $\nu = 1$, $\delta_x = 2$ and different values of δ_z .

Fractional Operators

ν	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
1.0	1.266e-03	4.556e-07	4.987e-03	2.995e-07	2.776e+07	1.003e-01
1.1	1.813e-03	6.423e-07	6.216e-03	4.190e-07	2.776e+07	1.003e-01
1.3	3.235e-03	1.129e-06	1.039e-02	7.312e-07	2.776e+07	1.003e-01
1.5	5.245e-03	1.811e-06	1.652e-02	1.166e-06	2.776e+07	1.003e-01
1.6	6.800e-03	2.333e-06	2.148e-02	1.498e-06	2.776e+07	1.003e-01
1.8	9.891e-03	3.362e-06	3.088e-02	2.147e-06	2.776e+07	1.003e-01
2.0	1.238e-02	4.180e-06	3.892e-02	2.662e-06	2.776e+07	1.003e-01

Table: Compression and accuracy for $q = 7$, $l = 0.2$, $\rho = 6$, $\delta_x = 0.2$ and different values of ν .