Approximations of Matrices and Tensors

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Overview

- Statement of the problem
- Matrix SVD
- Best rank k-approximation
- CUR approximation
- Extension to 3-tensors I–III
- Simulations
- Conclusions

Statement of the problem

Data is presented in terms of a matrix

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{bmatrix}.$$

Examples

1. digital picture: 512×512 matrix of pixels,
2. DNA-microarrays: $60,000 \times 30$
   (rows are genes and columns are experiments),
3. web pages activities:
   $a_{i,j}$-the number of times webpage j was accessed from web page i.

or a tensor

Objective: condense data and store it effectively.

Least squares & best rank k-matrix approximation

Least Squares: given $\mathbf{a}_1, \ldots, \mathbf{a}_n \in \mathbb{R}^m$ find the best approximations $\mathbf{b}_1, \ldots, \mathbf{b}_m \in \mathbb{R}^m$ lying in the subspace spanned by $\mathbf{f}_1, \ldots, \mathbf{f}_k \in \mathbb{R}^m$
History Gauss (1794) 1809, Legendre 1805, Adrain 1808

SOL: $A = [\mathbf{a}_1 \ \ldots \ \mathbf{a}_m] = [a_{ij}], B = [\mathbf{b}_1 \ \ldots \ \mathbf{b}_n] \in \mathbb{R}^{m\times n}$,
$\|A - B\|_F^2 := \sum_{i,j} |a_{ij} - b_{ij}|^2, \ F = [\mathbf{f}_1 \ \ldots \ \mathbf{f}_k] \in \mathbb{R}^{m\times k}, X \in \mathbb{R}^{k\times n}$
$\min_{X\in\mathbb{R}^{k\times n}} \|A - FX\|_F^2$ achieved for $X^\star = F^\dagger A$, $B^\star = FF^\dagger A$
$F^\dagger$-Moore-Penrose inverse 1920, 1955

Singular Value Decomposition:
In LS find the best r-dimensional subspace
$\min_{X\in\mathbb{R}^{r\times n}, F\in\mathbb{R}^{m\times r}} \|A - FX\|_F^2$ achieved for $A_r := F^\star X^\star$
History Beltrami 1873, C. Jordan 1874, Sylvester 1889, E. Schmidt 1907, H. Weyl 1912

Singular Value Decomposition - SVD

$A = U\Sigma V^\top$

$$\Sigma = \mathrm{diag}(\sigma_1, \dots, \sigma_{\min(m,n)}) := \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \sigma_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \in \mathbb{R}^{m\times n}$$

$\sigma_1 \ge \dots \ge \sigma_r > 0 = \sigma_i, i > r = \mathrm{rank}\, A$
$U = [\mathbf{u}_1 \dots \mathbf{u}_m] \in \mathbb{O}(m), \quad V = [\mathbf{v}_1 \dots \mathbf{v}_n] \in \mathbb{O}(n)$

$a^\dagger = a^{-1}$ if $a \neq 0$, $a^\dagger = 0$ if $a = 0$

$A^\dagger := V\,\mathrm{diag}(\sigma_1^\dagger, \dots, \sigma_{\min(m,n)}^\dagger)U^\top$

Best rank k-approximation

For $k \le r = \mathrm{rank}\, A$: $\Sigma_k = \mathrm{diag}(\sigma_1, \ldots, \sigma_k) \in \mathbb{R}^{k \times k}$,
$U_k = [\mathbf{u}_1 \ldots \mathbf{u}_k] \in \mathbb{R}^{m \times k}$, $V_k = [\mathbf{v}_1 \ldots \mathbf{v}_k] \in \mathbb{R}^{n \times k}$
$A_k := U_k \Sigma_k V_k^\top$ is the best rank k approximation in Frobenius and operator norm of A

$$\min_{B \in \mathcal{R}(m,n,k)} ||A - B||_F = ||A - A_k||_F.$$

Reduced SVD $A = U_r \Sigma_r V_r^\top$ where $(r \ge)\ \nu$ numerical rank of A if

$$\frac{\sum_{i \ge \nu+1} \sigma_i^2}{\sum_{i \ge 1} \sigma_i^2} \approx 0, (0.01).$$

A_ν is a noise reduction of A. Noise reduction has many applications in image processing, DNA-Microarrays analysis, data compression.
Full SVD: $O(mn \min(m,n))$, k- SVD: $O(kmn)$.

SVD algorithms

I. Kogbetliantz 1955, (modified Jacobi): $B_k = U_k B_{k-1} V_k^\top$
two dimensional SVD reduction operations reducing norm off-diagonal elements

II. QR algorithm (1961) U_k, V_k obtained by G-S on $B_{k-1}, B_{k-1}^\top$

III. Lanczo's algo $B_0 = UAV^\top$ bidiagonal

a. Golub-Kahan-Reinsch 1970- implicit QR to tridiagonal $B_k^\top B$
b. LAPACK improvement

Allows finding A_k cost $O(kmn)$
Approximation to smallest singular values and vectors

Big matrices

Dimensions of A big $m, n \geq 10^6$

Find a good algorithm by reading l rows or columns of A at random and update the approximations.

Friedland-Kaveh-Niknejad-Zare [2] proposed randomized k-rank approximation by reading l rows or columns of A at random and updating the approximations.

The main feature of this algorithm is that each update is a better rank k-approximation.

Each iteration: $||A - B_{t-1}||_F \geq ||A - B_t||_F$.
Complexity $O(kmn)$.

CUR approximation-I

From $A \in \mathbb{R}^{m\times n}$ choose submatrices consisting of p-columns $C \in \mathbb{R}^{m\times p}$ and q rows $R \in \mathbb{R}^{q\times n}$

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \dots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \dots & a_{3,n} \\ a_{4,1} & a_{4,2} & a_{4,3} & \dots & a_{4,n} \\ \vdots & \vdots & \vdots & \vdots & \\ a_{m-1,1} & a_{m-1,2} & a_{m-1,3} & \dots & a_{m-1,n} \\ a_{m,1} & a_{m,2} & a_{m,3} & \dots & a_{m,n} \end{bmatrix},$$

R - red - blue, C - red - magenta.

Approximate A using C, R.

CUR approximation-II

$\langle m \rangle := \{1, \ldots, m\}$
$A = [a_{ij}] \in \mathbb{R}^{m \times n}, \ \|A\|_{\infty,e} := \max_{i \in \langle m \rangle, j \in \langle n \rangle} |a_{ij}|$
$I = \{1 \le \alpha_1 < \ldots < \alpha_q \le m\}$
$J = \{1 < \beta_1 < \ldots < \beta_p \le n\}$
$A_{IJ} := [a_{ij}]_{i \in I, j \in J}$,
$R = A_{I\langle n \rangle} = [a_{\alpha_k j}], k = 1, \ldots, q, \quad j = 1, \ldots, n$
$C = A_{\langle m \rangle J} = [a_{i\beta_l}], i = 1, \ldots, m, \quad l = 1, \ldots, p.$
The set entries of A read
$\mathcal{S} := \langle m \rangle \times \langle n \rangle \backslash ((\langle m \rangle \backslash I) \times (\langle n \rangle \backslash J))$,
$\#\mathcal{S} = mp + qn - pq$
Goal: approximate A by CUR
for appropriately chosen C, R and $U \in \mathbb{R}^{p \times q}$.

CUR-approximation III

Introduced by Goreinov, Tyrtyshnikov and Zmarashkin [7, 8]
Suppose that $A, F \in \mathbb{R}^{m\times n}$ and $\mathrm{rank}\,(A-F) \le p$.
Then there exists p rows and columns of A:
$R \in \mathbb{R}^{p\times n}, C \in \mathbb{R}^{m\times p}$
and $U \in \mathbb{R}^{p\times p}$ such that
$||A - CUR||_2 \le ||F||_2(1 + 2\sqrt{pn} + 2\sqrt{pm})$
Good choice of C, R, U: Goreinov and Tyrtyshnikov [6]:
$\mu_p := \max_{I\subset\langle m\rangle, J\subset\langle n\rangle, \#I=\#J=p} |\det A_{IJ}| > 0$
Suppose that
$|\det A_{IJ}| \ge \delta\mu_p, \delta \in (0,1], I \subset \langle m\rangle, J \subset \langle n\rangle, \#I = \#J = p$.
Then $||A - CA_{IJ}^{-1}R||_{\infty,e} \le \frac{p+1}{\delta}\sigma_{p+1}(A)$

CUR-approximations: IV

Random A approximation algorithm:
Read at random q rows and p columns of A: $R \in \mathbb{R}^{q\times n}$, $C \in \mathbb{R}^{m\times p}$
A low rank approximation $B = CUR$,
for a properly chosen $U \in \mathbb{R}^{p\times q}$.
U_{opt}, corresponding to $F := CU_{\mathrm{opt}}R$ and an optimal k-rank approximation B of F, if needed by updating the approximations.
Complexity $O(k^2 \max(m,n))$.
$U_{\mathrm{opt}} \in \arg\min_{U\in\mathbb{R}^{p\times q}} \sum_{(i,j)\in\mathcal{S}}(a_{i,j} - (CUR)_{i,j})^2$
Average error
$\mathrm{Error}_{\mathrm{av}}(B) = \left(\frac{1}{\#\mathcal{S}} \sum_{(i,j)\in\mathcal{S}}(a_{i,j} - b_{,ij})^2\right)^{\frac{1}{2}}$.

CUR-approximations: V

Given A the best choice of U is
$U_b \in \arg\min_{U\in\mathbb{R}^{p\times q}} ||A - CUR||_F$
$U_b = C^\dagger A R^\dagger$
Complexity: $O(pqmn)$.
In [3] we characterize for $r \le \min(p, q)$
$U_{b,r} \in \arg\min_{U\in\mathcal{C}_r(p,q)} ||A - CUR||_F$
Least squares solution
$U_{\mathrm{opt}} \in \arg\min_{U\in\mathbb{R}^{p\times q}} \sum_{(i,j)\in\mathcal{S}} (a_{i,j} - (CUR)_{i,j})^2$
Example:

Cameraman: $n = m = 256$, $p = q = 80$.
Number of variables: $pq = 6400$.
Number of equations: $2 \times 256 \times 80 - 6400 = 34,560$.

Problems with executing least squares with Matlab:
very long time of execution time and poor precision.

Nonnegative CUR-approximation

$A \geq 0$: entries of A are nonnegative

$$U_{\mathrm{opt}} \in \arg \min_{U \in \mathbb{R}^{p \times q}} \sum_{(i,j) \in \mathcal{S}} (a_{i,j} - (CUR)_{i,j})^2,$$

subject to constrains: $(CUR)_{i,j} \geq 0, \ (i,j) \in \mathcal{S}$.

Or

$$U_b \in \arg \min_{U \in \mathbb{R}^{p \times q}} ||A - CUR||_F,$$

subject to constrains: $(CUR) \geq 0$.

Minimization of strictly convex quadratic function in a convex polytope.

Algorithm for $\tilde{U}_{\mathrm{opt}}$

Thm $U_{\mathrm{opt}} = A^{\dagger}_{I,J}$.
Suppose that $\#I = \#J = p$ and $A_{I,J}$ is invertible. Then $U_{\mathrm{opt}} = A^{-1}_{I,J}$ is the exact solution of the least square problem

$$(CUR)_{I,\langle n\rangle} = A_{I,\langle n\rangle}, \ (CUR)_{\langle m\rangle,J} = A_{\langle m\rangle,J},$$

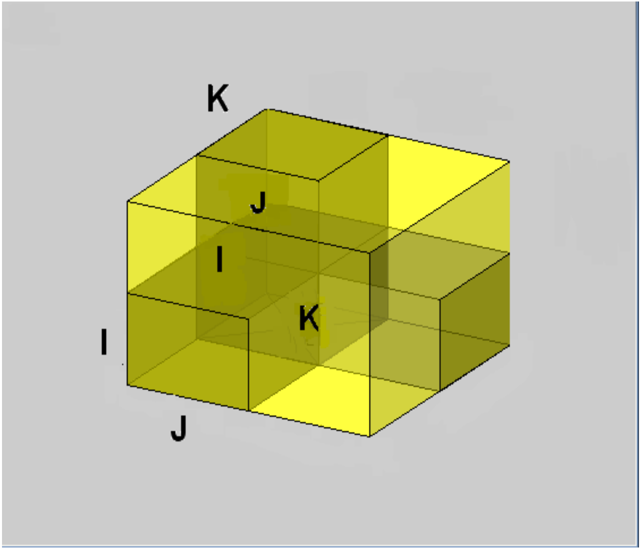
back to Goreinov-Tyrtyshnykov.
Instead of finding $A_{I,J}$ with maximum determinant we try several $I \subset \langle m\rangle, J \subset \langle n\rangle, \#I = \#J = p$, from which we chose the best I, J:

- $A_{I,J}$ has maximal numerical rank r_p,
- $\prod_{i=1}^{r_p} \sigma_i(A_{I,J})$ is maximal.

$$\tilde{U}_{\mathrm{opt}} := A^{\dagger}_{I,J,r_p}$$

A_{I,J,r_p} is the best rank r_p approximation of A_{IJ}.
A is approximated by $C\tilde{U}_{\mathrm{opt}}R$.

Extension to tensors: I



Extensions to 3-tensors: II

$\mathcal{A} = [a_{i,j,k}] \in \mathbb{R}^{m\times n\times \ell}$ - 3-tensor
given $I \subset \langle m\rangle, J \subset \langle n\rangle, K \subset \langle \ell\rangle$ define
$R := \alpha_{\langle m\rangle,J,K} = [a_{i,j,k}]_{\langle m\rangle,J,K} \in \mathbb{R}^{m\times(\#J\cdot\#K)}$,
$C := \alpha_{I,\langle n\rangle,K} \in \mathbb{R}^{\langle n\rangle\times(\#I\cdot\#K)}$,
$D := \alpha_{I,J,\langle \ell\rangle} \in \mathbb{R}^{l\times(\#I\cdot\#J)}$
Problem: Find 3-tensor $\mathcal{U} =\in \mathbb{R}^{(\#J\cdot\#K)\times(\#I\cdot\#K)\times(\#I\cdot\#J)}$
such that $\mathcal{A}$ is approximated by the Tucker tensor
$\mathcal{V} = \mathcal{U} \times_1 C \times_2 R \times_3 D$
where $\mathcal{U}$ is the least squares solution

$$\mathcal{U}_{\rm opt} \in \arg\min_{\mathcal{U}\in\mathbb{R}^{\text{three tensor}}} \sum_{(i,j,k)\in\mathcal{S}} \left(a_{i,j,k} - (\mathcal{U} \times_1 C \times_2 R \times_3 D)_{i,j,k}\right)^2$$

$\mathcal{S} = (\langle m\rangle \times J \times K) \cup (I \times \langle n\rangle \times K) \cup (I \times J \times \langle \ell\rangle)$

Extension to 3-tensors: III

For $\#I = \#J = p,\ \#K = p^2,\ I \subset \langle m \rangle, J \subset \langle n \rangle, K \subset \langle \ell \rangle$
generically there is an exact solution to $\mathcal{U}_{\mathrm{opt}} \in \mathbb{R}^{p^3 \times p^3 \times p^2}$
obtained by unfolding in third direction:
View $\mathcal{A}$ as $A \in \mathbb{R}^{(mn) \times \ell}$ by identifying
$\langle m \rangle \times \langle n \rangle \equiv \langle mn \rangle,\ I_1 = I \times J,\ J_1 = K$ and apply CUR again.

More generally, given $\#I = p,\ \#J = q,\ \#K = r$.
For $L = I \times J$ approximate $\mathcal{A}$ by $\mathcal{A}_{\langle m \rangle, \langle n \rangle, K} E^{\dagger}_{L,K} \mathcal{A}_{I,J,\langle \ell \rangle}$
Then for each $k \in K$ approximate each matrix $\mathcal{A}_{\langle m \rangle, \langle n \rangle, \{k\}}$ by
$\mathcal{A}_{\langle m \rangle, J, \{k\}} E^{\dagger}_{I,J,\{k\}} \mathcal{A}_{I, \langle n \rangle, \{k\}}$

Symmetric situation for 4-tensors $\mathcal{A} \in \mathbb{R}^{m \times n \times l \times q}$.

Other methods of approximation of tensors

I. HOSVD: Unfolding $\mathcal{A} \in \mathbb{R}^{m\times n\times l}$
in each direction + SVD yields orthonormal bases
$[\mathbf{u}_1 \dots \mathbf{u}_m], [\mathbf{v}_1, \dots, \mathbf{v}_n], [\mathbf{w}_1 \dots \mathbf{w}_l]$ of $\mathbb{R}^m, \mathbb{R}^n, \mathbb{R}^l$
$\mathcal{A}$ represented by $\mathcal{S} = [s_{i,j,k}]$ not diagonal but some good properties
II. Best (r_1, r_2, r_3) $(\le (m, n, l))$ approximation
$\min_{\mathbf{U}\in \mathrm{Gr}(r_1,\mathbb{R}^m),\mathbf{V}\in \mathrm{Gr}(r_2,\mathbb{R}^n),\mathbf{W}\in \mathrm{Gr}(r_3,\mathbb{R}^l)} \|\mathcal{A} - P_{\mathbf{U}\otimes\mathbf{V}\otimes\mathbf{W}}(\mathcal{A})\| =$
$\max_{\mathbf{U}\in \mathrm{Gr}(r_1,\mathbb{R}^m),\mathbf{V}\in \mathrm{Gr}(r_2,\mathbb{R}^n),\mathbf{W}\in \mathrm{Gr}(r_3,\mathbb{R}^l)} \|P_{\mathbf{U}\otimes\mathbf{V}\otimes\mathbf{W}}(\mathcal{A})\|$
Using unfolding + SVD gives iteration algorithm for U_k, V_k, W_k updating one subspace each step ASVD
$(1, 1, 1)$ EXM: $\max_{\|\mathbf{u}\|=\|\mathbf{v}\|=\|\mathbf{w}\|=1} \sum_{i,j,k} a_{i,j,k} u_i v_j w_k$
Critical point: $\mathcal{A} \times \mathbf{v} \otimes \mathbf{w} = \sigma\mathbf{u}, \mathcal{A} \times \mathbf{u} \otimes \mathbf{w} = \sigma\mathbf{v}, \mathcal{A} \times \mathbf{u} \otimes \mathbf{v} = \sigma\mathbf{w}$
Power iterations: $\mathcal{A} \times \mathbf{v}_k \otimes \mathbf{w}_k = \alpha_k \mathbf{u}_{k+1}, \mathcal{A} \times \mathbf{u}_{k+1} \otimes \mathbf{w}_k = \beta_k \mathbf{v}_{k+1}, \mathcal{A} \times \mathbf{u}_{k+1} \otimes \mathbf{v}_{k+1} = \gamma_k \mathbf{w}_{k+1}$
Modified Jacobi
Modified QR algorithm

Simulations: Tire I

Figure: Tire image compression (a) original, (b) SVD approximation, (c) CLS approximation, $t_{\max} = 100$.

Figure 1 portrays the original image of the Tire picture from the Image Processing Toolbox of MATLAB, given by a matrix $A \in \mathbb{R}^{205 \times 232}$ of rank 205, the image compression given by the SVD (using the MATLAB function `svds`) of rank 30 and the image compression given by $B_b = CU_bR$.

Simulations: Tire II

The corresponding image compressions given by the approximations B_{opt_1}, B_{opt_2} and $\tilde{B}_{opt}$ are displayed respectively in Figure 2. Here, $t_{\max} = 100$ and $p = q = 30$. Note that the number of trials $t_{\max}$ is set to the large value of 100 for all simulations in order to be able to compare results for different (small and large) matrices.

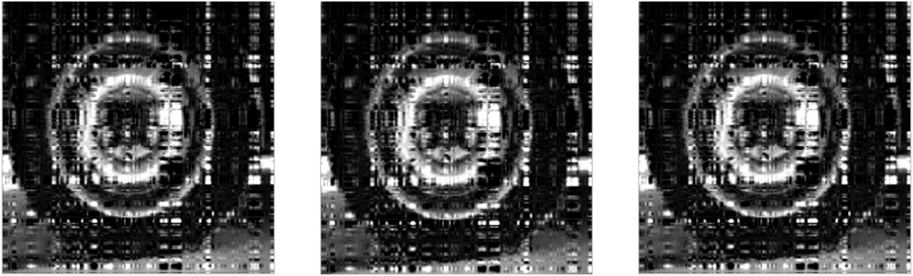


Figure: Tire image compression with (a) B_{opt_1}, (b) B_{opt_2}, (c) $\tilde{B}_{opt}$, $t_{\max} = 100$.

Simulations: Table 1

In Table 1 we present the S-average and total relative errors of the image data compression. Here, $B_b = CU_bR$, $B_{opt_2} = CU_{opt_2}R$ and $\tilde{B}_{opt} = C\tilde{U}_{opt}R$. Table 1 indicates that the less computationally costly FSVD with B_{opt_1}, B_{opt_2} and $\tilde{B}_{opt}$ obtains a smaller S-average error than the more expensive complete least squares solution CLS and the SVD. On the other hand, CLS and the SVD yield better results in terms of the total relative error. However, it should be noted that CLS is very costly and cannot be applied to very large matrices.

	rank	SAE	TRE
B_{svd}	30	0.0072	0.0851
B_b	30	0.0162	0.1920
B_{opt_1}	30	$1.6613 \cdot 10^{-26}$	0.8274
B_{opt_2}	30	$3.2886 \cdot 10^{-29}$	0.8274
$\tilde{B}_{opt}$	30	$1.9317 \cdot 10^{-29}$	0.8274

Table: Comparison of rank, S-average error and total relative error.

Simulations: Cameraman 1

Figure 3 shows the results for the compression of the data for the original image of a camera man from the Image Processing Toolbox of MATLAB. This data is a matrix $A \in \mathbb{R}^{256 \times 256}$ of rank 253 and the resulting image compression of rank 69 is derived using the SVD and the complete least square approximation CLS given by $B_b = CU_bR$.

Figure: Camera man image compression (a) original, (b) SVD approximation, (c) CLS approximation, $t_{\max} = 100$.

Simulations: Cameraman 2

Figure 4 is FSVD approximation $B_{opt_2} = CU_{opt_2}R$ and $\tilde{B}_{opt} = C\tilde{U}_{opt}R$. Here $t_{\max} = 100$ and $p = q = 80$. Table 2 gives S-average and total relative errors.

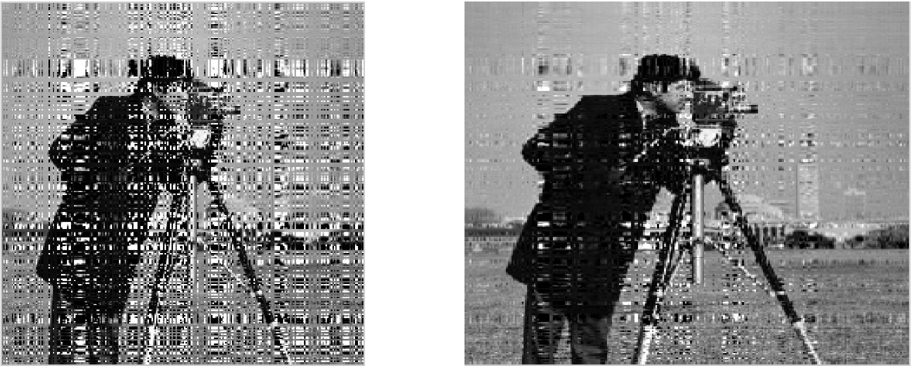


Figure: Camera man image compression. FSVD approximation with (a) $B_{opt_2} = CU_{opt_2}R$, (b) $\tilde{B}_{opt} = C\tilde{U}_{opt}R$. $t_{\max} = 100$.

Simulations: Table 2

	rank	SAE	TRE
B_{svd}	69	0.0020	0.0426
B_b	80	0.0049	0.0954
B_{opt_1}	—	—	—
B_{opt_2}	80	$3.7614 \cdot 10^{-27}$	1.5154
$\tilde{B}_{opt}$	69	$7.0114 \cdot 10^{-4}$	0.2175

Table: Comparison of rank, S-average error and total relative error.

Canal at night 1

Figure: Canal image (a) original, (b) SVD approximation, $t_{\max} = 100$.

Canal at night 2

Figure: Canal image compression (a) CLS approximation, (b) FSVD with $\tilde{B}_{opt}$, $t_{\max} = 100$.

Conclusions

Fast low rank approximation using CUR approximation of A of dimension $m \times n$, $C \in \mathbb{R}^{m \times p}$, $R \in \mathbb{R}^{q \times n}$ are submatrices of A $U \in \mathbb{R}^{p \times q}$ computable by least squares to fit best the entries of C and R.

Advantage: low complexity $O(pq \max(m, n))$.

Disadvantage: problems with computation time and approximation error

Drastic numerical improvement when using $\tilde{U}_{\mathrm{opt}}$.

Least squares can be straightforward generalized to tensors

Many methods of linear algebra can be adopted to tensors

with partial success

and many open problems

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