Optimizing the Frobenius norm under structural constraints.

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Abstract

TODO: Rewrite this to be more general The approximation of a general matrix $\mathbf{M}$ by a circulant matrix $\mathbf{C}$ is explored. Using the discrete Fourier transform matrix $\mathbf{F}$, the circulant with eigenvalues given by the diagonals of $\mathbf{FMF}^*$ is shown to be equivalent to the nearest circulant in the Frobenius norm, $\mathbf{C}_M$. An intuitive interpretation of this matrix in terms of means and variances of its values is presented.

1 Introduction

TODO: Preamble, justification

Circulant matrices are matrices of the form

$$\mathbf{C} = \begin{bmatrix} c_0 & c_1 & c_2 & \dots & c_{n-2} & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \dots & c_{n-3} & c_{n-2} \\ c_{n-2} & c_{n-1} & c_0 & \dots & c_{n-4} & c_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c_2 & c_3 & c_4 & \dots & c_0 & c_1 \\ c_1 & c_2 & c_3 & \dots & c_{n-1} & c_0 \end{bmatrix} \tag{1}$$

with $c_0, c_1, \ldots, c_{n-1} \in \mathbb{C}$. They see widespread use in signal processing, computation, and physical modelling as matrices with known eigensystems [1, 2]. For $\mathbf{C}$ as in Equation 5, the ordered eigenvalues for $k = 0, 1, \ldots, n-1$ are given by

$$\lambda_k = c_0 + \sum_{l=1}^{n-1} c_l \omega^{lk} \tag{2}$$

and the corresponding k^{th} eigenvector is given by

$$\mathbf{x}_k = \begin{bmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \vdots \\ \omega^{(M-1)k} \end{bmatrix} \tag{3}$$

where $\omega = \exp(\frac{2\pi i}{n})$ is the complex n^{th} root of unity and $i = \sqrt{-1}$.

Much of the utility of circulant matrices arises from this eigensystem. The $n \times n$ matrix of eigenvectors of $\mathbf{C}$ scaled to be unitary,

$$\mathbf{F} = \frac{1}{\sqrt{n}}[\mathbf{x}_0|\mathbf{x}_1|\mathbf{x}_2|\ldots|\mathbf{x}_{n-1}] = \mathbf{F}^{\mathsf{T}}, \tag{4}$$

is simply the discrete Fourier transform (DFT). Circulant matrices therefore have a deep relationship with real and complex analysis [3].

Suppose we would like to take advantage of this depth of theory and practice to approximate the $n \times n$ matrix

$$\mathbf{M} = \begin{bmatrix} m_{11} & m_{12} & \ldots & m_{1n} \\ m_{21} & m_{22} & \ldots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{n1} & m_{n2} & \ldots & m_{nn} \end{bmatrix} \tag{5}$$

by some circulant matrix. This note outlines some results.

2 Approximating M using F

Consider the simple approximation algorithm:

1. construct the diagonal matrix $\mathbf{D}$ where $d_{jj} = (\mathbf{FMF}^*)_{jj}$ and $\mathbf{F}^*$ is the complex conjugate of $\mathbf{F}$,

2. compute $\mathbf{C}_D = \mathbf{F}^*\mathbf{DF}$.

As $\mathbf{D}$ is diagonal and $\mathbf{F}$ is the matrix of eigenvectors for any circulant matrix, $\mathbf{C}_D$ is a circulant matrix with eigenvalues given by d_{jj}. To determine the elements $(\mathbf{C}_D)_{ij}$ in terms of ω, $\mathbf{x}$, and $\mathbf{M}$, first note

$$d_{jj} = \frac{1}{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\omega^{(k-l)(j-1)}m_{lk}. \tag{6}$$

Analogously, taking $\mathbf{F}^*\mathbf{DF}$ gives an i, j element

$$\begin{aligned}(\mathbf{C}_D)_{ij} &= \mathbf{F}^*\mathbf{DF} \\ &= \frac{1}{n^2}\sum_{l=1}^{n}\sum_{k=1}^{n} m_{lk}\mathbf{x}^*_{k-l}\mathbf{x}_{i-j} \\ &= \frac{1}{n}\sum_{l=1}^{n}\sum_{k=1}^{n} m_{lk}\delta_{(i-j) \bmod n,(k-l) \bmod n} \end{aligned} \tag{7}$$

where δ_{ij} is the Kronecker delta defined by

$$\delta_{ij} = \begin{cases} 0 \text{ if } i \neq j \\ 1 \text{ if } i = j. \end{cases} \tag{8}$$

Equation 7 indicates that $\mathbf{C}_D$ is generated by replacing the values of M along each circulant diagonal by the corresponding diagonal mean. Expressed as in Equation 1, $\mathbf{C}_D$ is the circulant matrix with

$$c_k = \frac{1}{n}\sum_{\{i,j|(i-j) \bmod n=k\}} m_{ij} := \overline{m}_k \tag{9}$$

Remarkably, though this was not the original motivation, $\mathbf{C}_D$ is also optimal in the sense of [1]: it minimizes the Frobenius norm.

Theorem 1 ($\mathbf{C}_D$ is Frobenius optimal)**.** $\mathbf{C}_D$ *minimizes* $||\mathbf{C} - \mathbf{M}||_F$ *for circulant* $\mathbf{C}$*, where* $||\mathbf{A}||_F$ *is the Frobenius norm of* $\mathbf{A}$*.*

Proof. We can write $||\mathbf{C}-\mathbf{M}||_F$ as

$$\sqrt{\operatorname{trace}\left((\mathbf{C}-\mathbf{M})^*(\mathbf{C}-\mathbf{M})\right)}. \tag{10}$$

Any $\mathbf{C}$ which minimizes Equation 10 will also minimize $||\mathbf{C}-\mathbf{M}||_F^2$. Therefore we seek to minimize

$$\operatorname{trace}\left((\mathbf{C}-\mathbf{M})^*(\mathbf{C}-\mathbf{M})\right) = \operatorname{trace}\mathbf{M}^*\mathbf{M} - \operatorname{trace}\mathbf{M}^*\mathbf{C} - \operatorname{trace}\mathbf{C}^*\mathbf{M} + \operatorname{trace}\mathbf{C}^*\mathbf{C}. \tag{11}$$

$\mathbf{M}^*\mathbf{M}$ is constant in $\mathbf{C}$, so this term can be ignored in the optimization. The latter three terms can be considered individually to express them as terms of the c_i. $\operatorname{trace}\mathbf{C}^*\mathbf{C}$ is the simplest, as

$$\operatorname{trace}\mathbf{C}^*\mathbf{C} = n\sum_{i=0}^{n-1} c_i^* c_i. \tag{12}$$

The negative terms can be expressed

$$\begin{aligned}
\operatorname{trace}\mathbf{M}^*\mathbf{C} &= \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ji}^* c_{(i-j) \bmod n} \\
&= \sum_{i=0}^{n-1} c_i \left(\sum_{j=1}^{n-i} m_{j,j+i}^* + \sum_{j=1}^{i} m_{n-i+j,j}^*\right) \\
&= n\sum_{i=0}^{n-1} c_i \overline{m}_i^*
\end{aligned} \tag{13}$$

and

$$\operatorname{trace}\mathbf{C}^*\mathbf{M} = n\sum_{i=0}^{n-1} c_i^* \overline{m}_i. \tag{14}$$

So we seek to minimize

$$\begin{aligned}
F(\mathbf{c}) &= n\sum_{i=0}^{n-1} c_i^* c_i - n\sum_{i=0}^{n-1} c_i^* \overline{m}_i - n\sum_{i=0}^{n-1} c_i \overline{m}_i^* \\
&= n\left(\langle \mathbf{c}, \mathbf{c}\rangle - \langle \overline{\mathbf{m}}, \mathbf{c}\rangle - \langle \mathbf{c}, \overline{\mathbf{m}}\rangle\right)
\end{aligned} \tag{15}$$

where $\langle \mathbf{x}, \mathbf{y}\rangle \geq 0$ is the Hermitian inner product of $\mathbf{x}, \mathbf{y} \in \mathbb{C}$, $\mathbf{c} = (c_0, c_1, \ldots, c_{n-1})^\mathsf{T}$ is the first row of $\mathbf{C}$, and $\overline{\mathbf{m}} = (\overline{m}_0, \overline{m}_1, \ldots, \overline{m}_{n-1})^\mathsf{T}$ is the vector of diagonal means of $\mathbf{M}$.

$\langle \overline{\mathbf{m}}, \mathbf{c} \rangle$ and $\langle \mathbf{c}, \overline{\mathbf{m}} \rangle$ are maximized when $\mathbf{c} = t\overline{\mathbf{m}}$ for $t \in \mathbb{R}$ and $\langle \mathbf{c}, \mathbf{c} \rangle$ simply gives the squared magnitude of $\mathbf{c}$. Therefore, the minimizer of Equation 15 must be $\mathbf{c} = t\overline{\mathbf{m}}$ for some $t \in \mathbb{R}$. Substituting this into Equation 15:

$$\begin{aligned} F(t\overline{\mathbf{m}}) &= n\left(t^2\langle \overline{\mathbf{m}}, \overline{\mathbf{m}} \rangle - t\langle \overline{\mathbf{m}}, \overline{\mathbf{m}} \rangle - t\langle \overline{\mathbf{m}}, \overline{\mathbf{m}} \rangle\right) \\ &= n||\overline{\mathbf{m}}||^2(t^2 - 2t), \end{aligned} \tag{16}$$

which has a minimum of $-n||\overline{\mathbf{m}}||^2$ when $t = 1$. Therefore, $\mathbf{c} = \overline{\mathbf{m}}$ minimizes $F(\mathbf{c})$ and so the optimal circulant matrix $\mathbf{C}$ to approximate $\mathbf{M}$ in the Frobenius norm satisfies Equation 9. □

Recognizing that the value of the squared Frobenius norm is

$$||\mathbf{C} - \mathbf{M}||_F^2 = \operatorname{trace} \mathbf{M}^*\mathbf{M} + F(\mathbf{c}) = \sum_{i=1}^{n}\sum_{j=1}^{n} ||m_{ij}||^2 + F(\mathbf{c}),$$

substituting $\mathbf{c} = \overline{\mathbf{m}}$ gives a minimum

$$\begin{aligned} ||\mathbf{C}_D - \mathbf{M}||_F^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} ||m_{ij}||^2 - n||\overline{\mathbf{m}}||^2 \\ &= n\left(\sum_{k=0}^{n-1} \sum_{\{1\le i,j\le n | (i-j) \bmod n = k\}} \frac{||m_{ij}||^2}{n} - \sum_{k=0}^{n-1} ||\overline{m}_k||^2\right) \\ &= n\sum_{k=0}^{n-1} \sigma_k^2 \end{aligned} \tag{17}$$

where σ_k^2 is the variance of values along the k^{th} diagonal of $\mathbf{M}$. Therefore the value of the Frobenius norm $||\mathbf{C}_D - \mathbf{M}||_F$ is given by the total standard deviation of the values of $\mathbf{M}$ from their respective circulant diagonals!

3 General structured matrices

The proof provided for Theorem 1 does not apply to circulant matrices alone, as the grouping of terms in the sums is arbitrary. First, we provide a general definition of a structured matrix.

Definition 1 (Structured matrix)**.** *Suppose we have a matrix* $\mathbf{A}$ *with entries* a_{ij} *following a regular pattern in* i *and* j*, that is*

$$a_{ij} = a_{f(i,j)} \tag{18}$$

where $f : \{0, 1, \ldots, n-1\}^2 \mapsto \{0, 1, 2, \ldots, K\}$ *is the index function defining the membership of the index pair* i, j *to a constant index set indexed by* k*. Then we say that* $\mathbf{A}$ *is* structured*. Additionally define the* k^{th} *index set*

$$\mathcal{A}_k = \{(i, j) | f(i, j) = k\}$$

with cardinality $|A_k| = n_k > 0$*.*

With this definition, we can prove that means following the structured pattern are Frobenius-optimal.

Theorem 2 (Means optimize the structured approximation of $\mathbf{M}$ in the Frobenius norm.)**.** *The optimal structured matrix* $\mathbf{A}$ *for index function* $f(i, j)$ *and index sets* $\mathcal{A}_0, \mathcal{A}_1, \ldots, \mathcal{A}_K$ *to approximate a given matrix* $\mathbf{M}$ *is given by the matrix* $\mathbf{A}_M$ *with*

$$a_{ij} = a_{f(i,j)} = \overline{m}_k \tag{19}$$

where

$$\overline{m}_k := \frac{1}{n_k} \sum_{\mathcal{A}_k} m_{ij}. \tag{20}$$

is the mean of entries of $\mathbf{M}$ *over the corresponding index set. Furthermore,* $||\mathbf{M} - \mathbf{A}_M||_F$ *is given by the total standard deviation of the values of* $\mathbf{M}$ *within each index set from the corresponding mean.*

Proof. Suppose we have a matrix $\mathbf{M}$ and would like to approximate it with a matrix $\mathbf{A}$ structured as in Definition 1 to minimize the squared Frobenius norm of the difference:

$$||\mathbf{M} - \mathbf{A}||_F^2.$$

Taking $\overline{m}_k$ to be the mean of entries in $\mathbf{M}$ for the k^{th} index set as in Equation 20, define the vector of all such means

$$\overline{\mathbf{m}} = (\overline{m}_0, \overline{m}_1, \ldots, \overline{m}_K)^\mathsf{T}.$$

Further, denote the vector of unique a_k as

$$\mathbf{a} = (a_0, a_1, \ldots, a_K)^\mathsf{T}$$

and the diagonal matrix of n_k as

$$\mathbf{N} = \text{diag}(n_0, n_1, \ldots, n_K).$$

Then we can generalize Equation 15 as

$$\begin{aligned} F(\mathbf{a}) &= \mathbf{a}^*\mathbf{N}\mathbf{a} - \overline{\mathbf{m}}^*\mathbf{N}\mathbf{a} - \mathbf{a}^*\mathbf{N}\overline{\mathbf{m}} \\ &= (\mathbf{a} - \overline{\mathbf{m}})^*\mathbf{N}\,(\mathbf{a} - \overline{\mathbf{m}}) - \overline{\mathbf{m}}^*\mathbf{N}\overline{\mathbf{m}}. \end{aligned} \tag{21}$$

As $n_k > 0$ for all $k = 0, 1, \ldots, K$, $\mathbf{N}$ is positive definite, and so the quadratic form $\mathbf{x}^*\mathbf{N}\mathbf{x}$ has a minimum of zero when $\mathbf{x} = \mathbf{0}$. Therefore $F(\mathbf{a})$ is minimized for $\mathbf{a} = \overline{\mathbf{m}}$ and has a minimum of

$$F(\overline{\mathbf{m}}) = -\overline{\mathbf{m}}^*\mathbf{N}\overline{\mathbf{m}} = -\sum_{k=0}^{K} n_k ||\overline{m}_k||^2. \tag{22}$$

So $\mathbf{A}_M$ is the Frobenius-optimal structured matrix $\mathbf{A}$ approximating $\mathbf{M}$. It has a squared Frobenius norm of

$$\begin{aligned} ||\mathbf{A}_M - \mathbf{M}||_F^2 &= \sum_{k=0}^{K} \sum_{\mathcal{A}_k} ||m_{ij}||^2 - \sum_{k=0}^{K} n_k ||\overline{m}_k||^2 \\ &= \sum_{k=0}^{K} n_k \left(\sum_{\mathcal{A}_k} \frac{||m_{ij}||^2}{n_k} - ||\overline{m}_k||^2 \right) \\ &= \sum_{k=0}^{K} n_k \sigma_k^2 \end{aligned} \tag{23}$$

where

$$\sigma_k^2 = \frac{1}{n_k} \sum_{\mathcal{A}_k} (m_{ij} - \overline{m}_k)^2$$

is the variance of the m_{ij} for the index set $\mathcal{A}_k$. □

3.1 Examples

Two well-known examples of structural matrices are Toeplitz matrices and Hankel matrices. Toeplitz matrices have an index function

$$f(i, j) = j - i$$

Hankel matrices take

$$f(i,j) = i + j$$

Another approach to Toeplitz approximation is to embed a Toeplitz matrix in a larger circulant one.

Toeplitz matrices are matrices of the form

$$\mathbf{T} = \begin{bmatrix} t_0 & t_1 & t_2 & \dots & t_{n-2} & t_{n-1} \\ t_{-1} & t_0 & t_1 & \dots & t_{n-3} & t_{n-2} \\ t_{-2} & t_{-1} & t_0 & \dots & t_{n-4} & t_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ t_{2-n} & t_{3-n} & t_{4-n} & \dots & t_0 & t_1 \\ t_{1-n} & t_{2-n} & t_{3-n} & \dots & t_{-1} & t_0 \end{bmatrix} \tag{24}$$

Hankel matrices are matrices of the form

$$\mathbf{H} = \begin{bmatrix} h_0 & h_1 & h_2 & \dots & h_{n-2} & h_{n-1} \\ h_1 & h_2 & h_3 & \dots & h_{n-1} & h_n \\ h_2 & h_3 & h_4 & \dots & h_n & h_{n+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{n-2} & h_{n-1} & h_n & \dots & h_{2n-4} & h_{2n-3} \\ h_{n-1} & h_n & h_{n+1} & \dots & h_{2n-3} & h_{2n-2} \end{bmatrix} \tag{25}$$

References

[1] Tony F Chan. An optimal circulant preconditioner for toeplitz systems. *SIAM Journal on Scientific and Statistical Computing*, 9(4):766–771, 1988.

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[3] Ulf Grenander and Gabor Szegö. *Toeplitz forms and their applications*. University of California Press, 1958.