Scientific Computing HW 3

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1. (a) Compute

$$\begin{aligned} P^T &= I^T - 2(uu^T)^T \\ &= I - 2(u^T)^T u^T \\ &= I - 2uu^T \\ &= P \end{aligned}$$

Using $u^T u = 1$,

$$\begin{aligned} P^2 &= (I - 2uu^T)(I - 2uu^T) \\ &= I^2 - 2Iuu^T - 2uu^T I + 4uu^T uu^T \\ &= I - 4uu^T + 4uu^T \\ &= I \end{aligned}$$

(b) Using $\operatorname{sign}(a)^2 = 1$ and $\operatorname{sign}(a)a = |a|$, compute

$$\tilde{u}^T x = \|x\|^2 + \operatorname{sign}(x_1)x_1\|x\| = \|x\|^2 + |x_1|\|x\|$$

$$\tilde{u}^T\tilde{u} = \|x\|^2 + \operatorname{sign}(x_1)^2\|x\|^2 + 2\operatorname{sign}(x_1)x_1\|x\| = 2\|x\|^2 + 2|x_1|\|x\|$$

Then compute

$$\begin{aligned} Px &= x - 2\frac{\tilde{u}^T x}{\tilde{u}^T\tilde{u}}\tilde{u} \\ &= x - \tilde{u} \\ &= -\operatorname{sign}(x_1)\|x\|e_1 \end{aligned}$$

(c) For convenience, write matrix entries as superscripts, reserving subscripts for the iteration described in the problem. We will prove using finite induction that for $1 \le j \le n$, the first j diagonal entries of A_j are

$$-\operatorname{sign}(A_0^{11})\|A_0(1:m,1)\|, \ldots, -\operatorname{sign}(A_{j-1}^{jj})\|A_{j-1}(j:m,j)\|$$

and that the entries below the first j diagonal entries are zero.

The case $j = 1$ is proven by $\text{House}(A_0(1:m,1))A_0(1:m,1) = -\operatorname{sign}(A_0^{11})\|A_0(1:m,1)\|e_1$, which is the first column of $A_1 = P_1 A_0$.

Assume the claim is true for j. Then (use $\sim$ to denote possibly nonzero entries)

$$A_j = \left[\begin{array}{ccc|c} -\operatorname{sign}(A_0^{11})\|A_0(1:m,1)\| & & \sim & \\ & \ddots & & \sim \\ & & -\operatorname{sign}(A_{j-1}^{jj})\|A_{j-1}(j:m,j)\| & \\ \hline \multicolumn{3}{c|}{0_{(m-j)\times j}} & \sim \end{array}\right]$$

From the algorithm,

$$P_{j+1} = \left[\begin{array}{c|c} I_{j\times j} & 0_{j\times(m-j)} \\ \hline 0_{(m-j)\times j} & \mathrm{House}(A_j(j+1:m, j+1)) \end{array}\right]$$

Then, by the fact $\mathrm{House}(A_j(j{+}1:m, j{+}1))A_j(j{+}1:m, j{+}1) = -\operatorname{sign}(A_j^{j+1,j+1})\|A_j(j+1:m, j+1)\|e_1$,

$$A_{j+1} = P_{j+1}A_j = \left[\begin{array}{ccc|c} -\operatorname{sign}(A_0^{11})\|A_0(1:m,1)\| & & \sim & \\ & \ddots & & \\ & & -\operatorname{sign}(A_j^{j+1,j+1})\|A_j(j+1:m,j+1)\| & \sim \\ \hline \multicolumn{3}{c|}{0_{(m-j-1)\times(j+1)}} & \sim \end{array}\right]$$

This closes the induction. Having proven the claim, setting $j = n$ gives

$$A_n = \left[\begin{array}{ccc} -\operatorname{sign}(A_0^{11})\|A_0(1:m,1)\| & & \sim \\ & \ddots & \\ & & -\operatorname{sign}(A_{n-1}^{nn})\|A_{n-1}(n:m,n)\| \\ \hline \multicolumn{3}{c}{0_{(m-n)\times n}} \end{array}\right]$$

To guarantee that A_n has positive diagonal entries, note that

$$-\operatorname{sign}(A_{j-1}^{jj})\|A_{j-1}(j:m,j)\| > 0 \iff -\operatorname{sign}(A_{j-1}^{jj}) > 0 \iff A_{j-1}^{jj} < 0$$

If $A_{j-1}^{jj} > 0$, change its sign before constructing P_j.

(d) From the iteration,

$$A_n = P_n P_{n-1} \dots P_1 A$$

From $P_j^2 = I$, we have $P_j^{-1} = P_j$, hence

$$(P_n P_{n-1} \dots P_1)^{-1} = P_1^{-1} P_2^{-1} \dots P_n^{-1} = P_1 P_2 \dots P_n$$

Which in turn gives a QR decomposition of A.

$$A = \underbrace{P_1 \dots P_n}_{=:Q} \underbrace{A_n}_{=:R}$$

2. (a) From the eigendecomposition $A = U\Lambda U^T$, we see U is orthogonal, so its columns $u_1, \ldots, u_n$ form an orthonormal basis of $\mathbb{R}^n$, and A has eigenpairs (λ_i, u_i). Define

$$\Sigma := \operatorname{diag}(\sigma_1, \ldots, \sigma_n), \quad \sigma_i := |\lambda_i|$$
$$V := \begin{bmatrix} v_1 & \ldots & v_n \end{bmatrix}, \quad v_i := s_i u_i, \quad s_i := \operatorname{sign}(\lambda_i)$$

Then we have

$$V = U \operatorname{diag}(s_1, \ldots, s_n), \quad V^T = \operatorname{diag}(s_1, \ldots, s_n) U^T, \quad \operatorname{diag}(s_1, \ldots, s_n)^2 = I_{n\times n}$$

The last equation comes from the fact that $\operatorname{sign}(x)^2 = 1$. Hence

$$\begin{aligned} V^T V &= \operatorname{diag}(s_1, \ldots, s_n) U^T U \operatorname{diag}(s_1, \ldots, s_n) \\ &= \operatorname{diag}(s_1, \ldots, s_n)^2 && U \text{ is orthogonal} \\ &= I_{n\times n} && \operatorname{diag}(s_1, \ldots, s_n)^2 = I_{n\times n} \end{aligned}$$

and

$$\begin{aligned} V V^T &= U \operatorname{diag}(s_1, \ldots, s_n)^2 U^T \\ &= U U^T && \operatorname{diag}(s_1, \ldots, s_n)^2 = I_{n\times n} \\ &= I_{n\times n} && U \text{ is orthogonal} \end{aligned}$$

Thus V is orthogonal.
Lastly, we check that $A = U\Sigma V^T$ by showing that the action of both sides agrees on the basis $u_1, \ldots, u_n$ of $\mathbb{R}^n$, i.e. $Au_i = U\Sigma V^T u_i$ for $1 \le i \le n$.

$$\begin{aligned} U\Sigma V^T u_i &= U\Sigma(s_i e_i) && \text{the } u_i\text{'s are orthonormal} \\ &= U(s_i|\lambda_i| e_i) \\ &= U(\lambda_i e_i) && \operatorname{sign}(x)|x| = x \\ &= \lambda_i u_i \\ &= A u_i && (\lambda_i, u_i) \text{ is an eigenpair of } A \end{aligned}$$

(b) Using the SVD $A = U\Sigma V^T$,

$$\begin{aligned} A^T A &= V\Sigma U^T U \Sigma V^T \\ &= V\Sigma^2 V^T && U^T U = I_{n\times n} \\ &= V \operatorname{diag}(\sigma_1^2, \ldots, \sigma_n^2) V^T \end{aligned}$$

This is an eigendecomposition of $A^T A$ with eigenpairs (σ_i^2, v_i).

(c) Via the "basis extension theorem" and the Gram–Schmidt process, we can extend the linearly independent orthonormal set $u_1, \ldots, u_n$ to an orthonormal basis $u_1, \ldots, u_n, u_{n+1}, \ldots, u_m$ of $\mathbb{R}^m$. Since AA^T is $m \times m$, it requires an $m \times m$ eigendecomposition.

$$\begin{aligned} AA^T &= U\Sigma V^T V \Sigma U^T \\ &= U\Sigma^2 U^T \\ &= \left[\begin{array}{c|c|c|c} U & u_{n+1} & \ldots & u_m \end{array}\right] \left[\begin{array}{c|c} \Sigma^2 & 0_{n\times(m-n)} \\ \hline 0_{(m-n)\times n} & 0_{(m-n)\times(m-n)} \end{array}\right] \left[\begin{array}{c} U^T \\ \hline u_{n+1}^T \\ \hline \vdots \\ \hline u_m^T \end{array}\right] \end{aligned}$$

This is an eigendecomposition of AA^T with eigenpairs (σ_i^2, u_i) for $1 \le i \le n$ and $(0, u_i)$ for $n+1 \le i \le m$.

(d) From A being full rank, the least squares solution to $Ax = b$ is $x^* = (A^TA)^{-1}A^Tb$. From the SVD $A = U\Sigma V^T$ and the fact A is full rank (so that A^TA and Σ are nonsingular),

$$A^TA = V\Sigma^2V^T \implies (A^TA)^{-1} = V(\Sigma^{-1})^2V^T$$

Hence

$$\begin{aligned} x^* &= (A^TA)^{-1}A^Tb \\ &= V(\Sigma^{-1})^2V^TV\Sigma U^Tb \\ &= V(\Sigma^{-1})^2SU^Tb \\ &= V\Sigma^{-1}U^Tb \end{aligned}$$

(e) We use the fact that $\|A\|_2$ equals the largest singular value of A. From the SVD $A = U\Sigma V^T$ and the fact A is nonsingular (Σ is nonsingular), we have $A^{-1} = V\Sigma^{-1}U^T$, an SVD of A^{-1}. Assume the singular values of A are arranged in decreasing order, $\sigma_1 \geq \cdots \geq \sigma_n > 0$. Then Σ^{-1} gives the singular values of A^{-1}, which arranged in decreasing order are $\frac{1}{\sigma_n} \geq \cdots \geq \frac{1}{\sigma_1}$. Thus $\left\|A^{-1}\right\|_2 = \frac{1}{\sigma_n}$.

(f) Throughout we use the fact that $Av_i = \sigma_iu_i$ for $1 \leq i \leq n$, and that for vectors $w_1, \ldots, w_k$, $\text{span}(w_1, \ldots, w_k)$ is the smallest subspace containing $w_1, \ldots, w_k$.

We first show that $\text{null}(A) = \text{span}(v_{r+1}, \ldots, v_n)$.

- Let $x \in \text{null}(A)$. Using the basis $v_1, \ldots, v_n$, write

  $$x = \sum_{i=1}^{n} c_iv_i$$

  for some $c_1, \ldots, c_n \in \mathbb{R}$. This, along with $Ax = 0$ and $Av_i = \sigma_iu_i$, gives

  $$\sum_{i=1}^{r} c_i\sigma_iu_i = 0$$

  Since the u_i's are linearly independent, $c_i\sigma_i = 0$, hence $c_i = 0$, for $1 \leq i \leq r$. Thus

  $$x = \sum_{i=r+1}^{n} c_iv_i \in \text{span}(v_{r+1}, \ldots, v_n)$$

  We conclude $\text{null}(A) \subset \text{span}(v_{r+1}, \ldots, v_n)$.
- For $r + 1 \leq i \leq n$, we have $Av_i = \sigma_iu_i = 0$, so $v_i \in \text{null}(A)$. Then $\text{null}(A)$ is a subspace of $\mathbb{R}^n$ containing $v_{r+1}, \ldots, v_n$, hence $\text{span}(v_{r+1}, \ldots, v_n) \subset \text{null}(A)$.

Then we show that $\text{range}(A) = \text{span}(u_1, \ldots, u_r)$.

- Let $y \in \text{range}(A)$. Then $y = Ax$ for some $x \in \mathbb{R}^n$. Using the basis $v_1, \ldots, v_n$, write

  $$x = \sum_{i=1}^{n} c_iv_i$$

  for some $c_1, \ldots, c_n \in \mathbb{R}$. This, along with $Av_i = \sigma_iu_i$, gives

  $$y = Ax = \sum_{i=1}^{r} c_i\sigma_iu_i \in \text{span}(u_1, \ldots, u_r)$$

  Thus $\text{range}(A) \subset \text{span}(u_1, \ldots, u_r)$.
- For $1 \leq i \leq r$, using the fact $Av_i = \sigma_iu_i$, we have $u_i = A\left(\frac{1}{\sigma_i}v_i\right) \in \text{range}(A)$. Then $\text{range}(A)$ is a subspace of $\mathbb{R}^m$ containing $u_1, \ldots, u_r$, hence $\text{span}(u_1, \ldots, u_r) \subset \text{range}(A)$.

From $\text{range}(A) = \text{span}(u_1, \ldots, u_r)$ and the u_i's being linearly independent, we see that $u_1, \ldots, u_r$ form a basis of $\text{range}(A)$, hence $\text{rank}(A) = r$.

3. The claim is that (here we omit the subscript for the 2–norm)

$$\min_{Ax=b} \|x\| = \|x^*\|$$

First we see that x^* solves $Ax = b$.

$$Ax^* = AA^T(AA^T)^{-1}b = b$$

Now let x solve $Ax = b$. Then

$$Ax = Ax^* \implies A(x - x^*) = 0$$

From this,

$$(x - x^*)^T x^* = (x - x^*)^T A^T (AA^T)^{-1} b = (A(x - x^*))^T (AA^T)^{-1} b = 0$$

In turn, we get

$$\|x\|^2 = \|(x - x^*) + x^*\|^2 = \|x - x^*\|^2 + \|x^*\|^2 + 2(x - x^*)^T x^* = \|x - x^*\|^2 + \|x^*\|^2 \geq \|x^*\|^2$$

Hence $Ax^* = b$, with $\|x\| \geq \|x^*\|$ whenever $Ax = b$. This establishes the claim.

4. (a) From the Schur decomposition $A = QTQ^*$, we have $AQ = QT$. If (λ, v) is an eigenpair of T, write $Tv = \lambda v$, so that $AQv = QTv = \lambda Qv$, hence (λ, Qv) is an eigenpair of A.

   (b) Since T is upper triangular, its eigenvalues are the diagonal entries $\lambda_1, \lambda_2, \lambda_3$.
   Moreover, $Te_1 = \lambda_1 e_1$, confirming (λ_1, v_1) as an eigenpair with $v_1 = e_1$.
   Seeking an eigenpair of the form (λ_2, v_2) with $v_2 = [a, 1, 0]^T$, compute

$$Tv_2 = \begin{bmatrix} \lambda_1 a + t_{12} \\ \lambda_2 \\ 0 \end{bmatrix}, \quad \lambda_2 v_2 = \begin{bmatrix} \lambda_2 a \\ \lambda_2 \\ 0 \end{bmatrix}$$

   Equating the first components,

$$\lambda_1 a + t_{12} = \lambda_2 a \implies (\lambda_2 - \lambda_1) = t_{12} \implies a = \frac{t_{12}}{\lambda_2 - \lambda_1}$$

   Seeking an eigenpair of the form (λ_3, v_2) with $v_3 = [b, c, 1]^T$, compute

$$Tv_3 = \begin{bmatrix} \lambda_1 b + t_{12} c + t_{13} \\ \lambda_2 c + t_{23} \\ \lambda_3 \end{bmatrix}, \quad \lambda_3 v_3 = \begin{bmatrix} \lambda_3 b \\ \lambda_3 c \\ \lambda_3 \end{bmatrix}$$

   Equating the second components,

$$\lambda_2 c + t_{23} = \lambda_3 c \implies (\lambda_3 - \lambda_2)c = t_{23} \implies c = \frac{t_{23}}{\lambda_3 - \lambda_2}$$

   Equating the first components,

$$\lambda_1 b + t_{12} c + t_{13} = \lambda_3 b \implies (\lambda_3 - \lambda_1)b = t_{12} c + t_{13} \implies b = \frac{t_{12} c}{\lambda_3 - \lambda_1} + \frac{t_{13}}{\lambda_3 - \lambda_1}$$

   Using the formula for c,

$$b = \frac{t_{12} t_{23}}{(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)} + \frac{t_{13}}{\lambda_3 - \lambda_1}$$

   (c) By parts (a) and (b), eigenvectors of A are

$$Qv_1 = Qe_1 = q_1$$

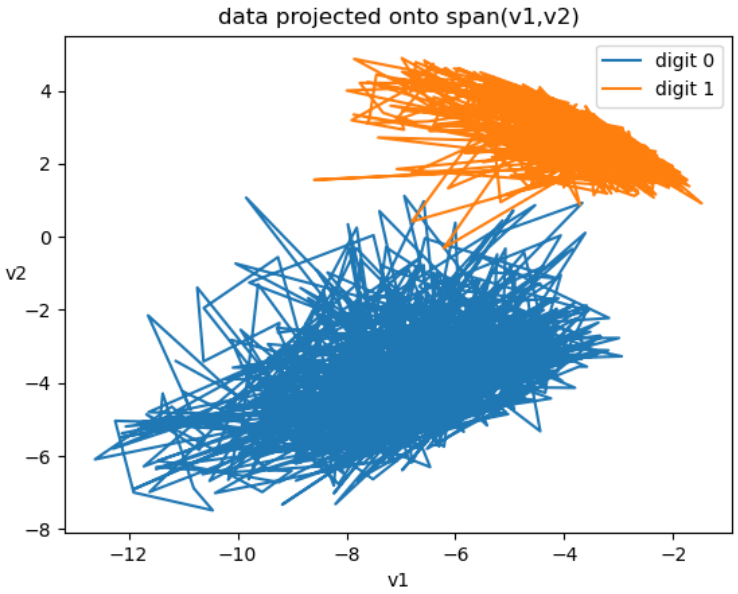
$$Qv_2 = aq_1 + q_2$$

$$Qv_3 = bq_1 + cq_2 + q_3$$

   where

$$a = \frac{t_{12}}{\lambda_2 - \lambda_1}, \quad b = \frac{t_{12} t_{23}}{(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)} + \frac{t_{13}}{\lambda_3 - \lambda_1}, \quad c = \frac{t_{23}}{\lambda_3 - \lambda_2}$$

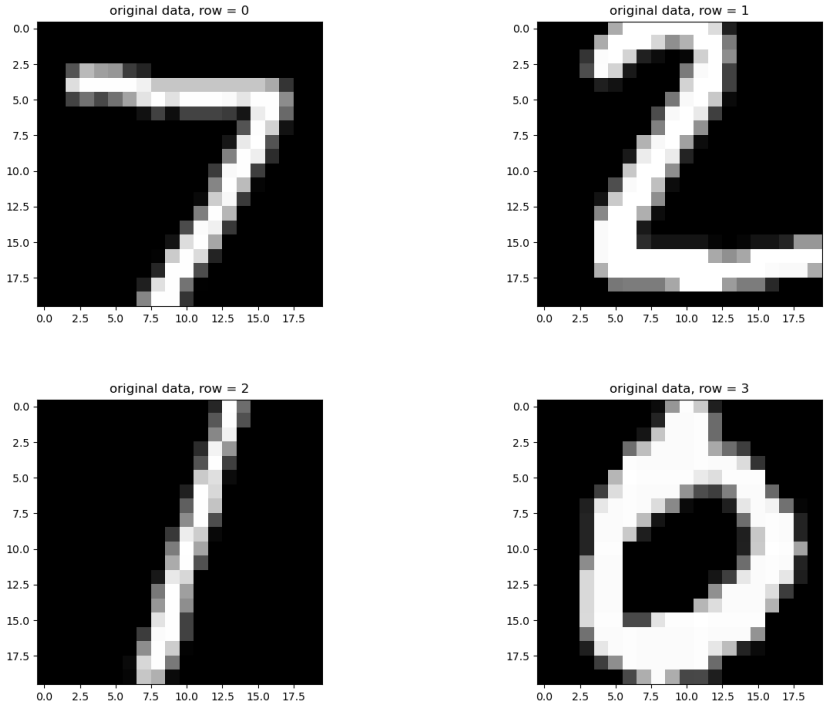
5. Code: `https://github.com/RokettoJanpu/scientific-computing-1-redux/blob/main/hw3.ipynb`

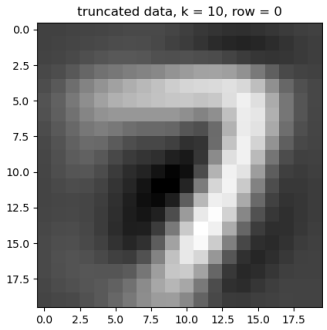


(a)

Indeed, 0s and 1s cluster in this space.

(b)

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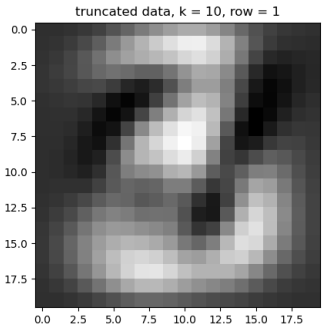
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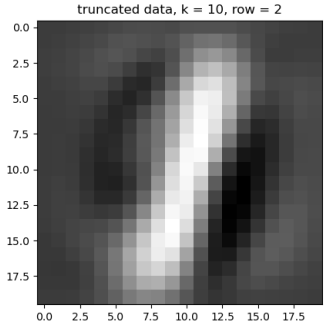
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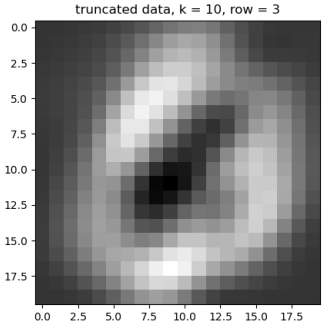
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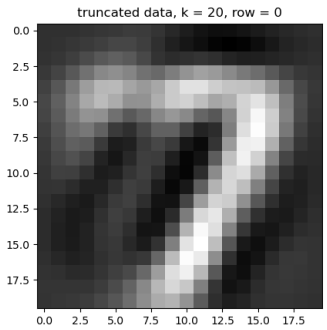
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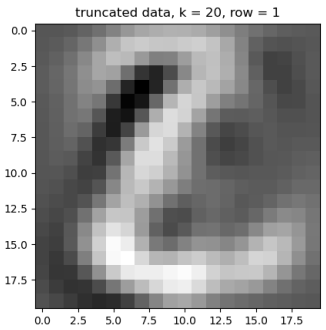
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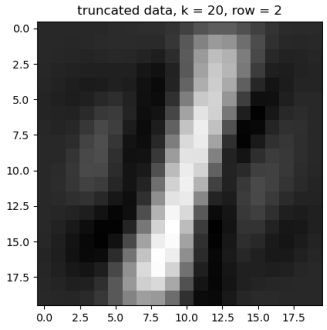
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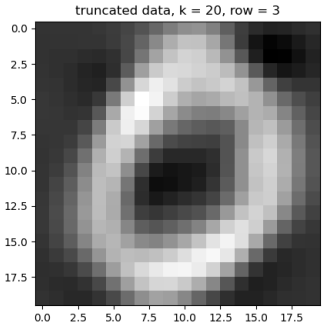
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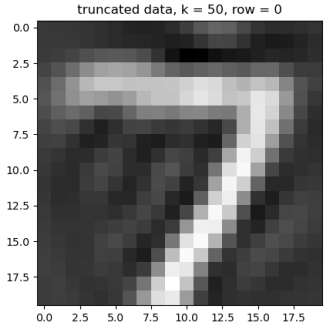
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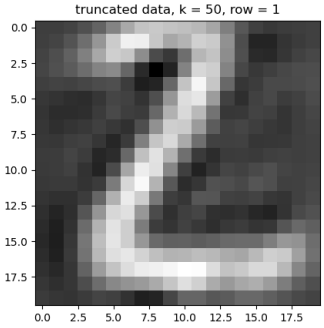
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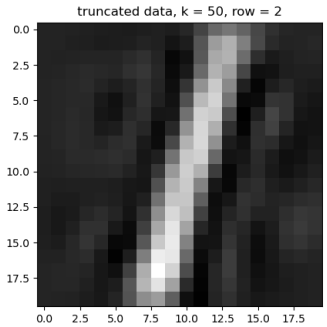
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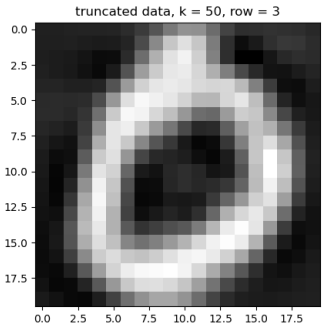
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