Fast Low-Rank Modifications of the Think Singular Value Decomposition

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Linear Algebra and Its Applications

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Key words:

   singular value decomposition, sequential updating, subspace tracking

   1991 MSC: 49M27, 15A18, 15A23, 65F20

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1 The singular value decomposition

The singular value decomposition (SVD) diagonalizes a real matrix $\mathbf{X} \in \mathbb{R}^{p \times q}$ via left and right rotations by orthonormal matrices $\mathbf{U} \in \mathbb{R}^{p \times p}$ and $\mathbf{V} \in \mathbb{R}^{q \times q}$, e.g.,

$\mathbf{U}^\top \mathbf{X} \mathbf{V} = \mathbf{S}$ is diagonal and nonnegative. Equivalently, it decomposes $\mathbf{X}$ into a sum of rank-1 matrices generated by singular value *triplets*: $\mathbf{X} = \mathbf{U} \text{diag}(\mathbf{s}) \mathbf{V}^\top = \sum_i \mathbf{u}_i s_i \mathbf{v}_i^\top$ for singular values s_i on the diagonal of $\mathbf{S}$ and singular vectors $\mathbf{u}_i$ and $\mathbf{v}_i$ drawn from the columns of $\mathbf{U}$ and $\mathbf{V}$.

The rank-*r thin* SVD restricts this sum to the *r* triplets having the largest-magnitude singular values. We will write this $\mathbf{U} \text{diag}(\mathbf{s}) \mathbf{V}^\top \overset{r}{\leftarrow} \mathbf{X}$ with orthonormal subspace matrices $\mathbf{U} \in \mathbb{R}^{p \times r}$, $\mathbf{V} \in \mathbb{R}^{q \times r}$ and singular value vector $\mathbf{s} \in \mathbb{R}^r \geq 0$. In signal processing, this reduction of $\mathbf{X}$ to a product of thin matrices is interpreted as a form of lossy compression, with the subspace matrices acting as encoding and decoding operators. By the Schmidt (later Eckart-Young-Mirsky) theorem, the thin SVD is the optimal rank-*r* approximation of $\mathbf{X}$ under any unitarily invariant norm, including the Frobenius norm [1]. This licenses the additional interpretation of the thin SVD as a form of noise suppression, where $\mathbf{X}$ is presumed to be a low-rank data matrix containing measurements contaminated with additive Gaussian noise.

Computing a full SVD is fundamentally an $O(pq \cdot \min(p, q))$-time problem, making decompositions of extremely large matrices infeasible. Shortly after the introduction of a practical algorithm for computing the SVD on digital computers in the 1960s [2], research turned to problems of faster methods for computing approximations such as the thin SVD, as well as updating an SVD to incorporate new data (e.g., [3, 4]). In recent years the practical need for such methods has become acute and the literature has grown accordingly. Section 5 reviews the recent literature in light of the results presented below:

(1) A general identity for additive modifications of an SVD (section 2).

(2) Specializations of this identity to give SVD updates, downdates, and rank-1 modifications with reduced computational complexity (section 3).

(3) An expanded thin SVD and sequential updating scheme that offers a strictly linear-time thin SVD in a single pass through a data matrix (section 4).

The last result has practical value in online settings where data must be incorporated into the SVD as it arrives, typically because the data is too large to be stored or even buffered. For example, many computer vision algorithms call for a "running" thin SVD of a video stream—effectively a data matrix with $\approx 10^5$ rows and an inexhaustible supply of columns. Financial transaction streams and network activity streams are even more demanding.

2 Additive modifications

Let real matrix $\mathbf{X} \in \mathbb{R}^{p \times q}$ have rank r and economy SVD $\mathbf{U}\mathbf{S}\mathbf{V}^\top = \mathbf{X}$ with $\mathbf{S} \in \mathbb{R}^{r \times r}$. Let $\mathbf{A} \in \mathbb{R}^{p \times c}$, $\mathbf{B} \in \mathbb{R}^{q \times c}$ be arbitrary matrices of rank c. We are interested in the SVD of the sum

$$
\mathbf{X} + \mathbf{A}\mathbf{B}^\top = [\mathbf{U} \quad \mathbf{A}] \begin{bmatrix} \mathbf{S} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} [\mathbf{V} \quad \mathbf{B}]^\top,
\tag{1}
$$

expressed as modifications to $\mathbf{U}, \mathbf{S}, \mathbf{V}$. We are most interested in the case where $\mathrm{rank}(\mathbf{X} + \mathbf{A}\mathbf{B}^\top) \leq r + c < \min(p, q)$, so that $\mathbf{U}, \mathbf{V}, \mathbf{A}, \mathbf{B}$ are tall thin matrices. However, what follows is completely general.

Let $\mathbf{P}$ be an orthogonal basis of the column-space of $(\mathbf{I} - \mathbf{U}\mathbf{U}^\top)\mathbf{A}$—the component of $\mathbf{A}$ that is orthogonal to $\mathbf{U}$—and set $\mathbf{R_A} \doteq \mathbf{P}^\top(\mathbf{I} - \mathbf{U}\mathbf{U}^\top)\mathbf{A}$. Note that $\mathrm{cols}(\mathbf{P}) = \mathrm{rows}(\mathbf{R_A}) = \mathrm{rank}((\mathbf{I} - \mathbf{U}\mathbf{U}^\top)\mathbf{A}) \leq c$, and may be zero. The relationships between

3

these matrices is summarized as

$$[\mathbf{U} \quad \mathbf{A}] = [\mathbf{U} \quad \mathbf{P}] \begin{bmatrix} \mathbf{I} \ \mathbf{U}^{\top}\mathbf{A} \\ \\ \mathbf{0} \ \mathbf{R_A} \end{bmatrix}. \tag{2}$$

Though similar to a QR decomposition, $\mathbf{R_A}$ need not be upper-triangular or square. Similarly, let $\mathbf{QR_B} = (\mathbf{I} - \mathbf{VV}^{\top})\mathbf{B}$. Substituting equation 2 into equation 1, we have

$$\mathbf{X} + \mathbf{AB}^{\top} = [\mathbf{U} \quad \mathbf{P}]\mathbf{K}[\mathbf{V} \quad \mathbf{Q}]^{\top}, \tag{3}$$

a product of two orthonormal matrices and

$$\mathbf{K} \doteq \begin{bmatrix} \mathbf{I} \ \mathbf{U}^{\top}\mathbf{A} \\ \\ \mathbf{0} \ \mathbf{R_A} \end{bmatrix} \begin{bmatrix} \mathbf{S} \ \mathbf{0} \\ \\ \mathbf{0} \ \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} \ \mathbf{V}^{\top}\mathbf{B} \\ \\ \mathbf{0} \ \mathbf{R_B} \end{bmatrix}^{\top} = \begin{bmatrix} \mathbf{S} \ \mathbf{0} \\ \\ \mathbf{0} \ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{U}^{\top}\mathbf{A} \\ \\ \mathbf{R_A} \end{bmatrix} \begin{bmatrix} \mathbf{V}^{\top}\mathbf{B} \\ \\ \mathbf{R_B} \end{bmatrix}^{\top}, \tag{4}$$

which is usually small, highly structured, and sparse. It follows immediately that diagonalizing $\mathbf{K}$ as $\mathbf{U}'^{\top}\mathbf{K}\mathbf{V}' = \mathbf{S}'$ gives rotations $\mathbf{U}'$ and $\mathbf{V}'$ of the extended subspaces $[\mathbf{U} \quad \mathbf{P}]$ and $[\mathbf{V} \quad \mathbf{Q}]$ such that

$$\mathbf{X} + \mathbf{AB}^{\top} = ([\mathbf{U} \quad \mathbf{P}]\mathbf{U}')\mathbf{S}'([\mathbf{V} \quad \mathbf{Q}]\mathbf{V}')^{\top} \tag{5}$$

is the desired SVD.

The rest of this paper develops scenarios where equation 5 provides a computationally attractive route to low-rank modifications of a thin SVD. For column updates and downdates of $\mathbf{X}$, the $\mathbf{K}$ matrix is sparse and easily diagonalized. Indeed, for low rank matrices and those having good low rank approximations, one can compute a thin SVD through sequential column updates in linear time.

4

3   Rank-1 modifications

Here we develop some special efficiencies offered by rank-1 modifications. For the SVD of $\mathbf{U}\mathbf{S}\mathbf{V}^\top + \mathbf{a}\mathbf{b}^\top$ with vectors $\mathbf{a} \in \mathbb{R}^p$ and $\mathbf{b} \in \mathbb{R}^q$, equation (2) can be effected in a partial step of the modified Gram-Schmidt algorithm:

$$\mathbf{m} \doteq \mathbf{U}^\top \mathbf{a}; \quad \mathbf{p} \doteq \mathbf{a} - \mathbf{U}\mathbf{m}; \quad R_a = \|\mathbf{p}\|; \quad \mathbf{P} = R_a^{-1} \cdot \mathbf{p} \tag{6}$$

and similarly

$$\mathbf{n} \doteq \mathbf{V}^\top \mathbf{b}; \quad \mathbf{q} \doteq \mathbf{b} - \mathbf{V}\mathbf{n}; \quad R_b = \|\mathbf{q}\|; \quad \mathbf{Q} = R_b^{-1} \cdot \mathbf{q}. \tag{7}$$

The rediagonalization problem of equation 4 simplifies to

$$\mathbf{K} = \begin{bmatrix} \mathbf{S} & \mathbf{0} \\ \mathbf{0} & 0 \end{bmatrix} + \begin{bmatrix} \mathbf{m} \\ \|\mathbf{p}\| \end{bmatrix} \begin{bmatrix} \mathbf{n} \\ \|\mathbf{q}\| \end{bmatrix}^\top, \tag{8}$$

a diagonal+rank-1 matrix, amenable to special treatment.

Table 1 shows how updating, downdating, and revising individual columns of the SVD are expressed as specializations of this scheme. Each offers further opportunities for reducing computation.

For example, to update $\mathbf{X}$ with a new column $\mathbf{c} \in \mathbb{R}^p$, one appends a row of zeros to $\mathbf{V}$ and then computes the rank-1 modification $\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = [\mathbf{X} \quad \mathbf{0}] + \mathbf{c}[0, \cdots, 0, 1]$. In this case, $\mathbf{n} = \mathbf{0}$, so equation 4 asks us only to rediagonalize the broken-arrow

5

operation	known	desired	$\mathbf{a}$	$\mathbf{b}^\top$
update	$\mathbf{US}[\mathbf{V}^\top \quad \mathbf{0}] = [\mathbf{X} \quad \mathbf{0}]$	$\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = [\mathbf{X} \quad \mathbf{c}]$	$\mathbf{c}$	$[0,\cdots,0,1]$
downdate	$\mathbf{USV}^\top = [\mathbf{X} \quad \mathbf{c}]$	$\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = \mathbf{X}$	$-\mathbf{c}$	$[0,\cdots,0,1]$
revise	$\mathbf{USV}^\top = [\mathbf{X} \quad \mathbf{c}]$	$\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = [\mathbf{X} \quad \mathbf{d}]$	$\mathbf{d}-\mathbf{c}$	$[0,\cdots,0,1]$
recenter	$\mathbf{USV}^\top = \mathbf{X}$	$\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = \mathbf{X}(\mathbf{I}-\frac{1}{q}\mathbf{11}^\top)$	$-\frac{1}{q}\mathbf{X1}$	$\mathbf{1}^\top \doteq [1,\cdots,1]$

Table 1

Common operations on the last column or on all columns expressed as rank-1 modifications of an SVD $\mathbf{USV}^\top = \mathbf{X}$ to give $\mathbf{U}'\mathbf{S}'\mathbf{V}'^\top = \mathbf{X} + \mathbf{ab}^\top$.

matrix

$$\mathbf{K} = \begin{bmatrix} \mathbf{S} & \mathbf{m} \\ \mathbf{0} & \|\mathbf{p}\| \end{bmatrix}, \tag{9}$$

which can be done in $O(r^2)$ time [5].

Similarly, one downdates the SVD by zeroing a column. In this case equation 4 simplifies to

$$\mathbf{K} = \begin{bmatrix} \mathbf{S} & \mathbf{0} \\ \mathbf{0} & 0 \end{bmatrix} \left(\mathbf{I} - \begin{bmatrix} \mathbf{Sn} \\ 0 \end{bmatrix} \begin{bmatrix} \mathbf{n} \\ \sqrt{1-\mathbf{n}^\top\mathbf{n}} \end{bmatrix}^\top \right), \tag{10}$$

$\mathbf{P}$ is unused, and $\mathbf{Q} = (\mathbf{b} - \mathbf{Vn})/\sqrt{1-\mathbf{n}^\top\mathbf{n}}$ is used only if updating $\mathbf{V}$. Note that downdating the ith column only requires knowing the ith row of $\mathbf{V}$.

4 An extended decomposition for reduced complexity

In a naïve implementation of the update, the QR-like decomposition of equation 2 takes $O(p(r+c)^2)$ time, the rediagonalization of equation 4 takes $O((r+c)^3)$ time, and the rotations of the subspaces takes $O((p+q)(c+r)^2)$ time. In the setting of a rank-1 update of a fixed-rank SVD, these times can be reduced to $O(pr)$, $O(r^2)$, and $O(r^3)$, respectively, by expanding the MGS as shown above, performing sparse diagonalizations, and deferring the costly subspace rotations as follows.

Instead of rotating the large singular vector matrices as prescribed in equation 5, we leave the SVD decomposed into the five matrices

$$\mathbf{U}_{p\times r} \cdot \mathbf{U}'_{r\times r} \cdot \mathbf{S}_{r\times r} \cdot \mathbf{V}'^{\top}_{r\times r} \cdot \mathbf{V}^{\top}_{q\times r}, \tag{11}$$

with orthonormal $\mathbf{U} \cdot \mathbf{U}'$, $\mathbf{V} \cdot \mathbf{V}'$, $\mathbf{U}$, and $\mathbf{U}'$ (but not $\mathbf{V}'$ or $\mathbf{V}$). The large outer matrices only record the span of the left and right subspaces and are built by appending columns to $\mathbf{U}$ and rows to $\mathbf{V}$. The transforms of these subspace bases that make $\mathbf{S}$ diagonal are maintained in the much smaller $\mathbf{U}'$, $\mathbf{V}'$ matrices. This makes the update much faster and eliminates the numerical error that would accumulate if the bases specified by the tall $\mathbf{U}$, $\mathbf{V}$ matrices were rotated on each update. The rest of this section details the updates of the left and right subspaces.

4.1 Updating the left subspace

Let $\mathbf{K}$ and $\mathbf{p}$ be defined as above, and let orthogonal $\mathbf{C}$, $\mathbf{D} \in \mathbb{R}^{(r+1)\times(r+1)}$ diagonalize $\mathbf{K}$ as $\mathbf{C}\mathbf{S}'\mathbf{D}^{\top} = \mathbf{K}$. From equation 5, the left-side update must satisfy $\mathbf{U}_{new}\mathbf{U}'_{new} = [\mathbf{U}_{old} \quad \mathbf{p}]\mathbf{U}'_{old}\mathbf{C}$. If $\mathbf{K}$ has rank r (i.e. the update is not rank-increasing), then $\mathbf{C}$ has

the form $\mathbf{C} = \begin{bmatrix} \mathbf{C}_{1:r,1:r} & \mathbf{0} \\ \\ \mathbf{0} & 1 \end{bmatrix}$ and the left of side equation 11 is simply updated

$$\mathbf{U}' \leftarrow \mathbf{U}' \mathbf{C}_{1:r,1:r}. \tag{12}$$

Otherwise the rank-increasing update is

$$\mathbf{U}' \leftarrow \begin{bmatrix} \mathbf{U}' & \mathbf{0} \\ \\ \mathbf{0} & 1 \end{bmatrix} \mathbf{C}; \qquad \mathbf{U} \leftarrow [\mathbf{U} \quad \mathbf{p}]. \tag{13}$$

The appends preserve orthogonality of $\mathbf{U}$ because $\mathbf{U}^{\top}\mathbf{p} = \mathbf{0}$ by construction.

Over thousands or millions of updates, the multiplications may erode the orthogonality of $\mathbf{U}'$ through numerical error, albeit slowly because these matrices remain small. Loss of orthogonality can be contained and corrected by occasionally forming the small product $\mathbf{U}'\mathbf{S}' \in \mathbb{R}^{r \times r}$, refactoring via SVD, and premultiplying the resulting right subspace into $\mathbf{V}'$. It is an open question how often this is necessary to guarantee a certain overall level of numerical precision; it does not change the overall complexity.

4.2 *Updating the right subspace*

The right-side updates are somewhat more complicated because updates add *rows* to $\mathbf{V}$ while guaranteeing that the *columns* of the product $\mathbf{V}\mathbf{V}'$ are orthogonal. From

equation 5, the right-side update must satisfy

$$\mathbf{V}_{new}\mathbf{V}'_{new} = \begin{bmatrix} \mathbf{V}_{old}\mathbf{V}'_{old} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \mathbf{D}. \tag{14}$$

To do so, it is convenient to calculate and update a small pseudo-inverse matrix $\mathbf{V}'^{+}$. When the update is rank-increasing, the right-hand side update is simply

$$\mathbf{V}'_{new} \leftarrow \begin{bmatrix} \mathbf{V}'_{old} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \mathbf{D}; \quad (\mathbf{V}'^{+})_{new} \leftarrow \mathbf{D}^{\top} \begin{bmatrix} (\mathbf{V}'^{+})_{old} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix}; \quad \mathbf{V}_{new} \leftarrow \begin{bmatrix} \mathbf{V}_{old} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \tag{15}$$

because $\begin{bmatrix} \mathbf{V}\mathbf{V}' & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \mathbf{D} = \begin{bmatrix} \mathbf{V} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{V}' & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \mathbf{D}$ and $\mathbf{D}$ is orthogonal.

When the rank does not increase, the last column of $\mathbf{D}$ represents an unused subspace dimension and should be suppressed. This licenses another optimization: Split $\mathbf{D} \in \mathbb{R}^{(r+1)\times r} \rightarrow \begin{bmatrix} \mathbf{W} \in \mathbb{R}^{r\times r} \\ \mathbf{w} \in \mathbb{R}^{1\times r} \end{bmatrix}$ where submatrix $\mathbf{W}$ is a linear transform that will be applied to $\mathbf{V}'$, and row-vector $\mathbf{w}$ is the subspace projection of the new data vector. The resulting right-side update

$$\mathbf{V}'_{new} \leftarrow \mathbf{V}'_{old}\mathbf{W}; \quad (\mathbf{V}'^{+})_{new} \leftarrow \mathbf{W}^{+}(\mathbf{V}'^{+})_{old}; \quad \mathbf{V}_{new} \leftarrow \begin{bmatrix} \mathbf{V}_{old} \\ \mathbf{w}(\mathbf{V}'^{+})_{new} \end{bmatrix} \tag{16}$$

can be verified by substitution into equation 14.

Conveniently, the pseudo-inverse $\mathbf{W}^+$ can be computed in $O(r^2)$-time using only matrix-vector and vector-vector products via the identity

$$\mathbf{W}^+ = \mathbf{W}^\top + \frac{\mathbf{w}^\top}{1 - \|\mathbf{w}\|^2}(\mathbf{w}\mathbf{W}^\top), \tag{17}$$

which is a special case of the following result for submatrices of an orthonormal matrix:

Proposition: Let tall matrix $\mathbf{D} = \begin{bmatrix} \mathbf{W} \\ \mathbf{Y} \end{bmatrix}$ have orthonormal columns, such that $\mathbf{D}^\top \mathbf{D} = \mathbf{W}^\top \mathbf{W} + \mathbf{Y}^\top \mathbf{Y} = \mathbf{I}$. Let $\mathbf{U}^\top \mathbf{Y} \mathbf{V} = \mathbf{S}$ be a diagonalization of $\mathbf{Y}$ with $\mathbf{U}^\top \mathbf{U} = \mathbf{V}^\top \mathbf{V} = \mathbf{I}$ and $\mathbf{S}$ having positive values on its diagonal. Then

$$\mathbf{W}^+ = \mathbf{W}^\top + \mathbf{V}\mathbf{S}^2(\mathbf{I} - \mathbf{S}^2)^+ \mathbf{V}^\top \mathbf{W}^\top \tag{18}$$

with

$$\mathbf{W}^+ = \mathbf{W}^\top + \mathbf{Y}^\top(\mathbf{I} - \mathbf{Y}\mathbf{Y}^\top)^+ \mathbf{Y}\mathbf{W}^\top \tag{19}$$

when $\mathbf{Y}$ is a square or wide matrix and

$$\mathbf{W}^+ = \mathbf{W}^\top + \frac{\mathbf{y}^\top}{1 - \|\mathbf{y}\|^2}(\mathbf{y}\mathbf{W}) \tag{20}$$

when $\mathbf{y} = \mathbf{Y}$ is a row vector.

This is essentially the Sherman-Woodbury-Morrison formula applied to the cosine-sine decomposition. Readers desiring more detail can find a proof in the appendix.

The expanded update eliminates the costliest and numerically most vulnerable steps of the update—the rotation and re-orthogonalization of $\mathbf{U}, \mathbf{V}$. The time complexity falls to $O(pr + r^3)$ for each update, with an overall complexity of $O(pqr + qr^3) = O(pqr)$ for the entire thin SVD, assuming that the desired rank is small relative to the matrix, specifically $r = O(\sqrt{p})$. For a high-dimensional low-rank matrices, we effectively have a *linear-time* SVD algorithm. If, furthermore, the data is streamed through the CPU, the update requires only $O((p + q)r)$ space to store the current SVD and data vector, i.e., it is sublinear in the number of data matrix elements.

The predicted linear scaling behavior is borne out empirically in trials with large dense random matrices: The proposed incremental SVD exhibits linear scaling behavior with size and rank (see figure 1 for details) and is orders of magnitude faster than Lanczos methods (as implemented in Matlab 5 and 6). Part of the dramatic speed-up may be attributed to the fact that the working storage of the proposed method can be kept entirely in the CPU's onboard cache, while the Lanczos methods make heavy use of the computer's bus. The two algorithms illustrate a trade-off between speed and accuracy: The multi-pass Lanczos method achieves slightly better numerical accuracy but the single-pass incremental method is orders of magnitude faster.

5   Related work

Modern thin SVD and SVD updating methods are generally based on symmetric eigenvalue perturbations or projections of the problem into subspaces. Many of these methods can be derived as special cases of the framework given in section 2.
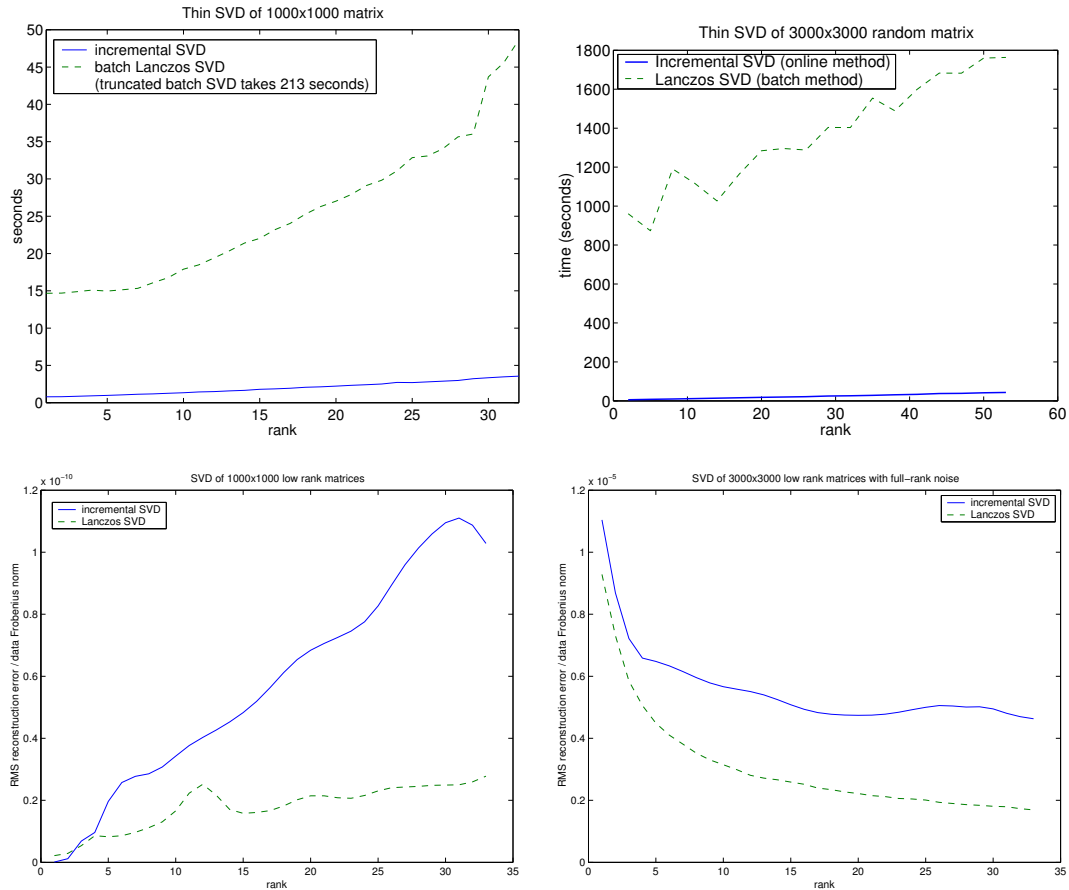
Figure 1. Run-time (top) and matrix reconstruction error (bottom) of sequential SVD updating (solid line) versus batch Lanczos (dashed line), as a function of the number of singular vector/value triplets computed from a random matrix. Each datapoint represents the average of 100 trials. The sequential update shows clear linear scaling and speed advantages. The experiment graphed at left employed low-rank matrices; at right, full-rank matrices having reasonable low-rank approximations. The proposed method exhibits similar speed/scaling advantages over other updating algorithms (e.g., [7, 8]), but produces more accurate results. Experiments were performed in Matlab 5 and 6 on an AlphaServer with a 600MHz CPU, 10G RAM, and a fast crossbar bus.

Businger [3] proposed an update adapted from QR-decomposition updates based on annihilations via Givens rotations. Bunch and Nielsen [4], Gu and Eisenstat [5] developed updates based on symmetric eigenvalue updates of the data's gram ma-

trix. As remarked in a Gu and Eisenstat [9] downdating paper, all such methods can be as expensive as computing a new SVD from scratch. Noting that updating a thin SVD offers more attractive economies, Berry et al. [10] proposed to project the updating problem into a previously estimated low-rank subspace, but the resulting updates ignore any component of new data that lies outside that subspace. This was remediated by Zha and Simon [11]; their solution requires a full SVD of a dense matrix on each update. Witter and Berry [12] also introduced a related downdate. Chandrasekaran et al. [7], Levy and Lindenbaum [8] proposed sequential eigenspace (left subspace) updates based on analyses that, with some algebra, can be rendered as special cases of equation 5 (with binary-valued $\mathbf{B}$). The Levy and Lindenbaum [8] method takes linear time for $r \ll \min(p, q)$ but appears to exhibit quadratic scaling well before $r = \sqrt{p}$. All of these methods require expensive multiplications of large subspace matrices, making them considerably slower than our proposed method, and also making loss of orthogonality an important numerical issue. In addition, the eigenspace updates (e.g., Chandrasekaran et al. [7], Levy and Lindenbaum [8]) presume centered (zero-mean) data; if the data stream does not comply one would need to use the recentering operator given in table 1 of this paper in conjunction with an estimator of the data mean.

6   Discussion: Approximation, sublinear, and tracking algorithms

The $O(pqr)$ time complexity result of section 4 rests on the assumption that the rank of the thin SVD holds at $r \leq O(\sqrt{p})$. If the data stream has higher numerical rank, it may eventually be desirable to suppress rank-increasing updates by some form of truncation. One possibility is to ignore the component of an update the lies outside the current subspace by setting $\|\mathbf{p}\| \to 0$ in equation 9 and using the

13

optimizations that follow. The optimal greedy tactic is to allow a rank-increasing update but immediately discard the new low-order singular value triplet. Clearly if a matrix has rank$> r$ then either truncating tactic will eventually discard variance that would be retained in an optimal low-rank approximation of the data matrix.

It is worth asking how suboptimal a greedy truncation scheme can be. In principle, an adversary could order a data stream such that some significant data trends only appear late in the stream, where they may be partly lost to truncation. One obvious strategy for such poorly behaved data streams is to exploit the low complexity of the update to compute a thin SVD of higher rank than ultimately desired, thereby allocating more memory to accommodate novel directions of variance in the data stream. The excess singular value triplets can be discarded later. On the other hand, if the vectors are random samples from a stationary data source, then on average the thin SVD will orient to approximate the true singular vectors and values, even if r is set too small. This can be established and quantified using the same central-limit-theorem arguments that justify approximate SVDs made by randomly sampling a subset of rows and/or columns from a large matrix (see Frieze et al. [15]). Indeed, the fast update can be combined with random sampling to give sublinear algorithms for massive data streams.

If the data source is nonstationary (like the adversary above), the update is trivially adapted to subspace tracking by causing the singular values to decay between updates: $\mathbf{s} \to \lambda\mathbf{s}$ for $0 < \lambda < 1$. This allows the subspace to rotate toward new directions of variance in the data stream, which would otherwise by dwarfed by the "weight of experience" already recorded by the singular values. Similarly, the rank capacity r can be adjusted online in response to data vectors having a significant component outside the estimated subspace.

14

7 Acknowledgments

References

[1] L. Mirsky. Symmetric gauge functions and unitarily invariant norms. *Quart. J. Math. Oxford*, 11:50–59, 1960.

[2] Gene Golub and Arthur van Loan. *Matrix Computations*. Johns Hopkins U. Press, 1996.

[3] P. Businger. Updating a singular value decomposition. *BIT*, 10:376–385, 1970.

[4] J. R. Bunch and C. P. Nielsen. Updating the singular value decomposition. *Numer. Math.*, 31:111–129, 1978.

[5] M. Gu and S. C. Eisenstat. A stable and fast algorithm for updating the singular value decomposition. Tech. Report YALEU/DCS/RR-966, Department of Computer Science, Yale University, New Haven, CT, 1993.

[6] G. W. Stewart. An updating algorithm for subspace tracking. *IEEE Trans. Signal Processing*, 40:1535–1541, 1992.

[7] S. Chandrasekaran, B. S. Manjunath, Y. F. Wang, J. Winkeler, and H. Zhang. An eigenspace update algorithm for image analysis. *Graphical models and image processing: GMIP*, 59(5):321–332, 1997.

[8] A. Levy and M. Lindenbaum. Sequential Karhunen-loeve basis extraction and its application to images. Technical Report CIS9809, Technion, 1998.

[9] M. Gu and S. Eisenstat. Downdating the singular value decomposition. *SIAM J. Matrix Analysis and Applications*, 16:793–810, 1995.

[10] Michael Berry, Susan Dumais, and Todd Letsche. Computational methods for intelligent information access. In *Proc. Supercomputing'95*, 1995.

[11] Hongyuan Zha and Horst D. Simon. On updating problems in latent semantic indexing. *SIAM Journal on Scientific Computing*, 21(2):782–791), 1999.

[12] Dian I. Witter and Michael W. Berry. Downdating the latent semantic indexing model for conceptual information retrieval. *The Computer Journal*, 41 (1998), 1998.

[13] Matthew Brand. Incremental singular value decomposition of uncertain data. In *Proceedings, European Conference on Computer Vision*, Lecture Notes on Computer Science, pages 707–720. Springer-Verlag, 2002.

[14] Matthew Brand. Fast online SVD revisions for data mining and recommending. In *Proceedings, SIAM International Conference on Data Mining*, 2003.

[15] Alan M. Frieze, Ravi Kannan, and Santosh Vempala. Fast Monte-Carlo algorithms for finding low-rank approximations. In *IEEE Symposium on Foundations of Computer Science*, pages 370–378, 1998.

A Proof of partitioned pseudo-inverse update

Without loss of generality, suppress any all-zero rows in $\mathbf{W}$ and $\mathbf{Y}$ so that the singular value decompositions $\mathbf{U}_1\mathbf{S}_1\mathbf{V}_1^\top = \mathbf{W} \in \mathbb{R}^{r_1 \times c}$ and $\mathbf{U}_2\mathbf{S}_2\mathbf{V}_2^\top = \mathbf{Y} \in \mathbb{R}^{r_2 \times c}$ have no zero-valued singular values. Restating the orthogonal sum in terms of the SVDs, we have $\mathbf{V}_1\mathbf{S}_1^2\mathbf{V}_1^\top = \mathbf{W}^\top\mathbf{W} = \mathbf{I} - \mathbf{Y}^\top\mathbf{Y} = \mathbf{I} - \mathbf{V}_2\mathbf{S}_2^2\mathbf{V}_2^\top$. Pre- and postmultiplying by $\mathbf{V}_1^\top, \mathbf{V}_1$ gives $\mathbf{S}_1^2 = \mathbf{I} - \mathbf{V}_1^\top\mathbf{V}_2\mathbf{S}_2^2\mathbf{V}_2^\top\mathbf{V}_1$ and similarly $\mathbf{S}_2^2 = \mathbf{I} - \mathbf{V}_2^\top\mathbf{V}_1\mathbf{S}_1^2\mathbf{V}_1^\top\mathbf{V}_2$. The fact that diagonality is preserved by $\mathbf{V}_1^\top\mathbf{V}_2 \in \mathbb{R}^{r_1 \times r_2}$ and its transpose implies that $\mathbf{V}_1^\top\mathbf{V}_2$ has at most one nonzero element in each row and column. This in turn implies that every column in $\mathbf{V}_1$ is orthogonal to at least $r_2 - 1$ columns in $\mathbf{V}_2$,

16

and vice versa, making $r_1r_2 - \min(r_1, r_2)$ orthogonality relationships between $\mathbf{V}_1$ and $\mathbf{V}_2$ and $r_1(r_1 - 1)/2 + r_2(r_2 - 1)/2$ orthogonality relationships within $\mathbf{V}_1$ and $\mathbf{V}_2$. Since $r_1 + r_2 \geq c$, this exhausts all the $c(c-1)/2$ possible orthogonalities in a c-dimensional basis, therefore any pair of columns $\{\mathbf{v}_i \in \mathbf{V}_1, \mathbf{v}_j \in \mathbf{V}_2\}$ that is not orthogonal must be identical (up to a flippable sign). I.e. $\mathbf{v}_1^\top \mathbf{v}_2 \neq 0 \Rightarrow \mathbf{v}_1 = \pm \mathbf{v}_2$. After making appropriate sign flips, the concatenation $[\mathbf{V}_1, \mathbf{V}_2] \in \mathbb{R}^{c \times (r_1 + r_2)}$ is an orthogonal basis of $\mathbb{R}^c$ with duplicate columns, and the product $\mathbf{V}_1^\top \mathbf{V}_2 \in \{0, 1\}^{r_1 \times r_2}$ can be viewed as a submatrix of a permutation matrix, having some all-zero rows or columns along its shorter axis. It follows that the equality $\mathbf{S}_1^2 = \mathbf{I} - \mathbf{V}_1^\top \mathbf{V}_2 \mathbf{S}_2^2 \mathbf{V}_2^\top \mathbf{V}_1$ can be separated into independent equations $s_i^2 = 1 - s_j^2$ for singular values $s_i \in \mathrm{diag}(\mathbf{S}_1)$ and $s_j \in \mathrm{diag}(\mathbf{S}_2)$ where $(\mathbf{V}_1^\top \mathbf{V}_2)_{ij} = \mathbf{v}_i^\top \mathbf{v}_j = 1$, while those singular values not put into correspondence by $\mathbf{V}_1^\top \mathbf{V}_2$ are unitary, i.e. if $(\mathbf{V}_1^\top \mathbf{V}_2)_{ij} = 0$ for all j, then $s_i = 1$. Pseudo-inverting both sides of each independent scalar equation we obtain $(s_i^2)^+ = (1 - s_j^2)^+ = s_j^2(1 - s_j^2)^+ + 1$ for all s_j within the spectral radius of an orthogonal matrix, including $s_j = 1 \Rightarrow s_i = 0$. and $s_j \neq 1$. The correspondences between the singular vectors and singular values is summarized by the following chain of equalities for the symmetric pseudo-inverse:

$$\mathbf{V}_1(\mathbf{S}_1^+)^2\mathbf{V}_1^\top = (\mathbf{W}^\top \mathbf{W})^+ = (\mathbf{I} - \mathbf{Y}^\top \mathbf{Y})^+ \tag{A.1}$$
$$= (\mathbf{I} - \mathbf{V}_2\mathbf{S}_2^2\mathbf{V}_2^\top)^+ \tag{A.2}$$
$$= \mathbf{V}_2\mathbf{S}_2^2(\mathbf{I} - \mathbf{S}_2^2)^+\mathbf{V}_2^\top + \mathbf{I} \tag{A.3}$$

To verify, pre- and post-multiply by $\mathbf{V}_1^\top, \mathbf{V}_1$ or $\mathbf{V}_2^\top, \mathbf{V}_2$ to recover the separate pseudo-inverse equalities. This is then substituted into an expansion of the asymmetric pseudo-inverse,

$$\mathbf{W}^+ = (\mathbf{W}^\top \mathbf{W})^+\mathbf{W}^\top \tag{A.4}$$
$$= (\mathbf{I} + (\mathbf{W}^\top \mathbf{W})^+ - \mathbf{I})\mathbf{W}^\top \tag{A.5}$$
$$= \mathbf{W}^\top + ((\mathbf{W}^\top \mathbf{W})^+ - \mathbf{I})\mathbf{W}^\top \tag{A.6}$$

$$= \mathbf{W}^\top + (\mathbf{V}_2 \mathbf{S}_2^2 (\mathbf{I} - \mathbf{S}_2^2)^+ \mathbf{V}_2^\top + \mathbf{I} - \mathbf{I}) \mathbf{W}^\top, \tag{A.7}$$

to prove the proposition. For the special case of $r_2 \leq c$,

$$\mathbf{V}_2 \mathbf{S}_2 (\mathbf{I} - \mathbf{S}_2^2)^+ \mathbf{S}_2 \mathbf{V}_2^\top = \mathbf{V}_2 \mathbf{S}_2 \mathbf{U}_2^\top \mathbf{U}_2 (\mathbf{I} - \mathbf{S}_2^2)^+ \mathbf{U}_2^\top \mathbf{U}_2 \mathbf{S}_2 \mathbf{V}_2^\top \tag{A.8}$$
$$= \mathbf{Y}^\top \mathbf{U}_2 (\mathbf{I} - \mathbf{S}_2 \mathbf{V}_2^\top \mathbf{V}_2 \mathbf{S}_2)^+ \mathbf{U}_2^\top \mathbf{Y} \tag{A.9}$$
$$= \mathbf{Y}^\top (\mathbf{I} - \mathbf{U}_2 \mathbf{S}_2 \mathbf{V}_2^\top \mathbf{V}_2 \mathbf{S}_2 \mathbf{U}_2^\top)^+ \mathbf{Y} \tag{A.10}$$
$$= \mathbf{Y}^\top (\mathbf{I} - \mathbf{Y} \mathbf{Y}^\top) \mathbf{Y} \tag{A.11}$$

where $\mathbf{U}_2$ enters the pseudo-inverse without generating extra terms because it is square. ∎