easygsvd documentation

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The goal of this package is to provide a pure-Python, friendly interface to the generalized singular value decomposition (GSVD). Throughout this package, we assume that the matrices $A \in \mathbb{R}^{M \times N}$ and $L \in \mathbb{R}^{K \times N}$ satisfy the common kernel condition

$$\operatorname{rank}\left(\begin{bmatrix} A \\ L \end{bmatrix} \right) = N, \quad \text{or, equivalently,} \quad \ker(A) \cap \ker(L) = \{0_N\}. \tag{1}$$

See [1, 2, 3, 4] for more background on the GSVD than is provided here.

Description of the GSVD

The starting point for our description of the GSVD is contained in the following theorem regarding the "economic" GSVD.

Theorem 1 (Economic GSVD). *Let $A \in \mathbb{R}^{M \times N}$ and $L \in \mathbb{R}^{K \times N}$ with $\ker(A) \cap \ker(L) = \{0_N\}$. Let $r_A = \operatorname{rank}(A)$, $r_L = \operatorname{rank}(L)$, $n_A = \operatorname{nullity}(A)$, and $n_L = \operatorname{nullity}(L)$. Then, there exists an invertible matrix $X \in \mathbb{R}^{N \times N}$, semi-orthogonal matrices $\hat{U} \in \mathbb{R}^{M \times r_A}$ and $\hat{V} \in \mathbb{R}^{K \times r_L}$, a nonincreasing sequence $\{c_i\}_{i=1}^N \subseteq [0, 1]$ and a nondecreasing sequence $\{s_i\}_{i=1}^N \subseteq [0, 1]$ such that*

$$\hat{U}^T A X = \begin{bmatrix} \hat{C} & 0_{r_A \times n_A} \end{bmatrix}, \qquad \hat{V}^T L X = \begin{bmatrix} 0_{r_L \times n_L} & \hat{S} \end{bmatrix}, \tag{2}$$

where $\hat{C} = \operatorname{diag}(c_1, \ldots, c_{r_A})$ and $\hat{S} = \operatorname{diag}(s_{n_L+1}, \ldots, s_N)$. Here the c_i and s_i satisfy the properties:

- $c_i^2 + s_i^2 = 1$ *for each* $1 \leq i \leq N$.
- $c_i = 0$ *for* $i = r_A + 1, \ldots, N$ *and* $s_i = 0$ *for* $i = 1, \ldots, n_L$.
- $c_i = 1$ *for* $i = 1, \ldots, n_L$ *and* $s_i = 1$ *for* $i = r_A + 1, \ldots, N$,

In addition, we have the identities

$$X^T A^T A X = C^2, \quad X^T L^T L X = S^2, \quad X^T \left(A^T A + L^T L \right) X = I_N, \tag{3}$$

where $C = \operatorname{diag}(c_1, \ldots, c_N)$, $S = \operatorname{diag}(s_1, \ldots, s_N)$.

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Note that although there are N of the c_i and s_i, only r_A and r_L of them appear in the economic GSVD, respectively. For convenience, we define the *common-action rank*

$$r_\cap := \dim\left(\mathrm{col}(A^T) \cap \mathrm{col}(L^T)\right) \tag{4}$$

which satisfies the generalized rank-nullity condition

$$r_\cap + n_A + n_L = N \tag{5}$$

due to (1). We also define the *generalized singular values* of the pair (A, L) as the extended real-valued scalars

$$\gamma_i = \begin{cases} +\infty, & i \leq n_L, \\ c_i s_i^{-1}, & n_L < i \leq r_A, \\ 0, & r_A < i \leq N. \end{cases} \tag{6}$$

The generalized singular values are given in nonincreasing order, and for $i > n_L$ satisfy the generalized eigenvalue problem

$$(A^T A) x_i = \gamma_i^2 (L^T L) x_i \tag{7}$$

where x_i denotes the ith column of X appearing in the GSVD. Next, we define the "full" SVD.

Theorem 2 (Full SVD)**.** *The semi-orthogonal matrices $\hat{U}$ and $\hat{V}$ can be extended to orthogonal matrices*

$$U := \begin{bmatrix} \hat{U} & U_\perp \end{bmatrix} \in \mathbb{R}^{M\times M}, \quad V := \begin{bmatrix} \hat{V} & V_\perp \end{bmatrix} \in \mathbb{R}^{K\times K} \tag{8}$$

such that

$$U^T A X = \begin{bmatrix} \hat{C} & 0_{r_A \times n_A} \\ 0_{(M-r_A)\times r_A} & 0_{(M-r_A)\times n_A} \end{bmatrix}, \quad V^T L X = \begin{bmatrix} 0_{r_L \times n_L} & \hat{S} \\ 0_{(K-r_L)\times n_L} & 0_{(K-r_L)\times r_L} \end{bmatrix}. \tag{9}$$

It is possible to directly express A and L in terms of either the full or economic GSVDs as

$$A = U \begin{bmatrix} \hat{C} & 0_{r_A \times n_A} \\ 0_{(M-r_A)\times r_A} & 0_{(M-r_A)\times n_A} \end{bmatrix} X^{-1}, \quad L = V \begin{bmatrix} 0_{r_L \times n_L} & \hat{S} \\ 0_{(K-r_L)\times n_L} & 0_{(K-r_L)\times r_L} \end{bmatrix} X^{-1}. \tag{10}$$

The GSVD reveals the four fundamental subspaces of both A and L.

Theorem 3 (Fundamental subspaces revealed by GSVD)**.** *Let $Y := X^{-T}$ and $\check{C} :=$* $\mathrm{diag}(c_{n_L+1}, \ldots, c_{r_A})$*, $\check{S} :=$* $\mathrm{diag}(s_{n_L+1}, \ldots, s_{r_A})$ *which includes only the scalars c_i and s_i which are not equal to zero or one. Introduce the partitionings*

$$X = \begin{array}{c} \begin{array}{ccc} n_{\mathbf{L}} & r_\cap & n_{\mathbf{A}} \end{array} \\ \begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} \end{array}, \quad Y = \begin{array}{c} \begin{array}{ccc} n_{\mathbf{L}} & r_\cap & n_{\mathbf{A}} \end{array} \\ \begin{bmatrix} Y_1 & Y_2 & Y_3 \end{bmatrix} \end{array}$$

$$U = \begin{array}{c} \begin{bmatrix} U_1 & U_2 \end{bmatrix} \\ \begin{array}{cc} n_{\mathbf{L}} & r_\cap \end{array} \end{array}, \quad V = \begin{array}{c} \begin{bmatrix} V_2 & V_3 \end{bmatrix} \\ \begin{array}{cc} r_\cap & n_{\mathbf{A}} \end{array} \end{array}$$

Then,

$$A \begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} = \begin{bmatrix} U_1 & U_2\check{C} & 0_{M\times n_A} \end{bmatrix}, \tag{11}$$

$$L \begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} = \begin{bmatrix} 0_{K\times n_L} & V_2\check{S} & V_3 \end{bmatrix}, \tag{12}$$

$$A^T \begin{bmatrix} U_1 & U_2 \end{bmatrix} = \begin{bmatrix} Y_1 & Y_2\check{C} \end{bmatrix}, \tag{13}$$

$$L^T \begin{bmatrix} V_2 & V_3 \end{bmatrix} = \begin{bmatrix} Y_2\check{S} & V_3 \end{bmatrix}, \tag{14}$$

and we have the following characterizations of the four fundamental subspaces related to A and L:

$$\ker(A) = \mathrm{col}(X_3), \qquad \ker(L) = \mathrm{col}(X_1), \tag{15}$$

$$\ker(A^T) = \mathrm{col}(U_\perp), \qquad \ker(L^T) = \mathrm{col}(V_\perp), \tag{16}$$

$$\mathrm{col}(A) = \mathrm{col}(\hat{U}), \qquad \mathrm{col}(L) = \mathrm{col}(\hat{V}), \tag{17}$$

$$\mathrm{col}(A^T) = \mathrm{col}\left(\begin{bmatrix} Y_1 & Y_2 \end{bmatrix}\right), \qquad \mathrm{col}(L^T) = \mathrm{col}\left(\begin{bmatrix} Y_2 & Y_3 \end{bmatrix}\right). \tag{18}$$

Additionally,

$$\mathbb{R}^N = \mathrm{col}(X_1) \oplus \mathrm{col}(X_2) \oplus \mathrm{col}(X_3), \tag{19}$$

and

$$\mathrm{col}(A^T) \cap \mathrm{col}(L^T) = \mathrm{col}(Y_2). \tag{20}$$

Note that we have not defined matrices U_3 and V_1 — this is done to ensure that in the partitioning U_2 and V_2 have the same number of columns. Since $Y = X^{-T}$, the X_i and Y_i satisfy the conditions

$$\sum_{i=1}^{3} X_i Y_i^T = XY^T = I_N, \quad Y_i^T X_j = \begin{cases} I, & i = j, \\ 0, & i \neq j. \end{cases} \tag{21}$$

The matrices A and L can be expressed directly in terms of the economic GSVD as

$$A = U_1 Y_1^T + U_2 \check{C} Y_2^T, \quad L = V_2 \check{S} Y_2^T + V_3 Y_3^T. \tag{22}$$

Performing the GSVD

Performing the GSVD of the matrix pair (A, L) is simple:

```
gsvd_result = gsvd(A, L, tol=1e-12, full_matrices=False)
```

The tolerance parameter `tol` is a threshold used to determine the numerical rank of A, and the `full_matrices` option is used to determine whether or not $U_\perp$ and $V_\perp$ are computed (this can be expensive if M and/or K are very large, and is not needed for most uses of the GSVD). The output of `gsvd` is a `GSVDResult` object which provides an interface to the computed GSVD.

Interfacing with the GSVD

Any of the quantities defined in the description of the GSVD can be accessed as attributes of the `GSVDResult` object:

```python
gsvd_result.A # A
gsvd_result.L # L

gsvd_result.U1 # U1
gsvd_result.U2 # U2
gsvd_result.V2 # V2
gsvd_result.V3 # V3
gsvd_result.Uhat # Uhat = [U1, U2]
gsvd_result.Vhat # Vhat = [V2, V3]
gsvd_result.Uperp # only available if full_matrices=True
gsvd_result.Vperp # only available if full_matrices=True
gsvd_result.U # U = [U1, U2, Uperp], only available if full_matrices=True
gsvd_result.V # V = [V2, V3, Vperp], only available if full_matrices=True

gsvd_result.X # X
gsvd_result.X1 # X1, first n_L columns of X
gsvd_result.X2 # X2, middle r_int columns of X
gsvd_result.X3 # X3, last n_A columns of X
gsvd_result.Y # Y
gsvd_result.Y1 # Y1, first n_L columns of Y
gsvd_result.Y2 # Y2, middle r_int columns of Y
gsvd_result.Y3 # Y3, last n_A columns of Y

gsvd_result.c = c # all N c's
gsvd_result.s = s # all N s's
gsvd_result.c_hat # first r_A c's
gsvd_result.s_hat # last r_L s's
gsvd_result.c_check # middle r_int c's
gsvd_result.s_check # middle r_int s's

gsvd_result.gamma # all N generalized SVs
gsvd_result.gamma_check # middle r_int generalized SVs (finite and nonzero)
```

We provide easy access to orthogonal projectors onto the fundamental subspaces:

```python
# valid_subspaces = ["col(A)", # "col(A.T)", "ker(A)", "ker(A.T)",
#                    "col(L)", "col(L.T)", "ker(L)", "ker(L.T)"]
gsvd_result.get_orthogonal_projector("col(A)", matrix=True)
```

The parameter `matrix` controls whether or not the projector is returned as a matrix. If `matrix=False` is passed, instead of a matrix a `scipy.sparse.linalg.LinearOperator` object is returned represented the projection.[1]

In addition to the orthogonal projectors, we also provide access to certain oblique projectors. Given a splitting $\mathbb{R}^N = \mathcal{X} \oplus \mathcal{Y}$, the oblique projection onto a subspace $\mathcal{X}$

[1]All operations are implemented to be efficient in the regime $N \ll M, K$.

along a subspace $\mathcal{Y}$ is defined as the unique operator $\mathcal{E}_{\mathcal{X}}^{\mathcal{Y}}$ satisfying

$$\forall x \in \mathcal{X} \quad \mathcal{E}_{\mathcal{X}}^{\mathcal{Y}} x = x, \qquad \forall y \in \mathcal{Y} \quad \mathcal{E}_{\mathcal{X}}^{\mathcal{Y}} y = 0_N, \qquad \forall z \in \mathbb{R}^N \quad \mathcal{E}_{\mathcal{X}}^{\mathcal{Y}} z \in \mathcal{X}. \tag{23}$$

We also define the M-weighted orthogonal complement of a subspace $\mathcal{X}$ as

$$\mathcal{X}^{\perp_M} = \{x \in \mathbb{R}^N \,:\, \forall y \in \mathcal{X} \; x^T M^T M y = 0\}. \tag{24}$$

In terms of the GSVD matrices, we have

$$\mathcal{E}_{\ker(L)}^{\ker(L)^{\perp_A}} = X_1 Y_1^T, \qquad \mathcal{E}_{\ker(L)^{\perp_A}}^{\ker(L)} = X_2 Y_2^T + X_3^T Y_3^T, \tag{25}$$

$$\mathcal{E}_{\ker(A)}^{\ker(A)^{\perp_L}} = X_3 Y_3^T, \qquad \mathcal{E}_{\ker(A)^{\perp_L}}^{\ker(A)} = X_1 Y_1^T + X_2 Y_2^T. \tag{26}$$

```
# valid_options = [
#     1, # projection onto ker(L) along ker(L)^{perp_A}
#     2, # projection onto ker(L)^{perp_A} along ker(L)
#     3, # projection onto ker(A) along ker(A)^{perp_L}
#     4, # projection onto ker(A)^{perp_L} along ker(A)
# ]
gsvd_result.get_oblique_projector(which=1, matrix=True)
```

Alongside the oblique projectors, we also give access to the oblique pseudoinverses $L_A^\dagger$ and $A_L^\dagger$. These are defined as the unique operators satisfying

$$\forall z \in \operatorname{col}(L) \quad L_A^\dagger z = \underset{x \in \mathbb{R}^N \,:\, Lx = z}{\arg\min} \; \|x\|_{A^T A}, \quad \forall z \in \operatorname{col}(L)^\perp \quad L_A^\dagger z = 0_N, \tag{27}$$

$$\forall z \in \operatorname{col}(A) \quad A_L^\dagger z = \underset{x \in \mathbb{R}^N \,:\, Ax = z}{\arg\min} \; \|x\|_{L^T L}, \quad \forall z \in \operatorname{col}(A)^\perp \quad A_L^\dagger z = 0_N, \tag{28}$$

and can be written explicitly in terms of the GSVD quantities as

$$L_A^\dagger = X_2 \check{S}^{-1} V_2^T + X_3 V_3^T, \quad A_L^\dagger = X_1 U_1^T + X_2 \check{C}^{-1} U_2^T. \tag{29}$$

The quantities

$$A L_A^\dagger = U_2 \check{\Gamma} V_2^T, \quad L A_L^\dagger = U_2 \check{\Gamma}^{-1} V_2^T. \tag{30}$$

where here $\check{\Gamma} = \operatorname{diag}(\gamma_{n_L+1}, \ldots, \gamma_{r_A})$ is comprised of the generalized singular values which are finite and nonzero. The oblique pseudoinverse may be used for bringing a regularized least squares problem into standard form [5, 6]:

$$x^\star := \underset{x \in \mathbb{R}^N}{\arg\min} \; \|Ax - b\|_2^2 + \lambda \|Lx\|_2^2 \tag{31}$$

$$= L_A^\dagger \left(\underset{z \in \mathbb{R}^K}{\arg\min} \|A L_A^\dagger z - b\|_2^2 + \lambda \|z\|_2^2 \right) + X_1 U_1^T b \tag{32}$$

$$= A_L^\dagger \left(\underset{z \in \mathbb{R}^M}{\arg\min} \|z - b\|_2^2 + \lambda \|L A_L^\dagger z\|_2^2 \right). \tag{33}$$

References

[1] Charles F Van Loan. "Generalizing the singular value decomposition". In: *SIAM Journal on numerical Analysis* 13.1 (1976), pp. 76–83.

[2] Christopher C Paige and Michael A Saunders. "Towards a generalized singular value decomposition". In: *SIAM Journal on Numerical Analysis* 18.3 (1981), pp. 398–405.

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