Singular Value Decomposition (SVD)

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Orthonormal Basis

Definition (Orthonormal Basis).

A set of vector $\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k\} \subset \mathbb{R}^n$ $(k \leq n)$ forms an orthonormal basis (of some space or subspace) if:

- unit ℓ_2-norm: $||\mathbf{v}_i||_2 = 1$ for all i,
- orthogonal to each other: $\mathbf{v}_i^T \mathbf{v}_j = 0$ for all $i \neq j$.

SVD and Truncated SVD

Singular Value Decomposition (SVD)

- Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be any matrix.
- Rank: $r = \mathrm{rank}(\mathbf{A})$. $(r \leq m, n)$
- SVD: $\mathbf{A} = \sum_{i=1}^{r} \boxed{\sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T}$

A rank-1 matrix

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- Rank: $r = \mathrm{rank}(\mathbf{A})$. $(r \leq m, n)$
- SVD: $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$
  - Singular values: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$.
  - Left singular vectors: $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_r\} \subset \mathbb{R}^m$ forms an orthonormal basis.
  - Right singular vectors: $\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_r\} \subset \mathbb{R}^n$ forms an orthonormal basis.

Truncated SVD

- Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be any matrix.
- Rank: $r = \mathrm{rank}(\mathbf{A})$. $(r \leq m, n)$
- SVD: $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$
- **Truncated SVD**: for $0 < k < r$, $\mathbf{A}_k = \sum_{i=1}^{k} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$
  - $\mathbf{A}_k$ is the best rank-k approximation to $\mathbf{A}$.
  - $\mathbf{A}_k = \mathrm{argmin}_{\mathbf{B}} \; \left|\left|\mathbf{A} - \mathbf{B}\right|\right|_F^2 ; \quad s.t. \quad \mathrm{rank}(\mathbf{B}) \leq k.$

Matrix Frobenius Norm

- Let $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{m \times n}$ be any matrix.
- Frobenius norm: $||\mathbf{A}||_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2}$.
  - A generalization of the ℓ_2-vector norm to matrix.
- Property: $||\mathbf{A}||_F = \sqrt{\sum_{i=1}^{r} \sigma_i^2}$.
  - σ_i is the i-th singular value of $\mathbf{A}$.

Error of Truncated SVD

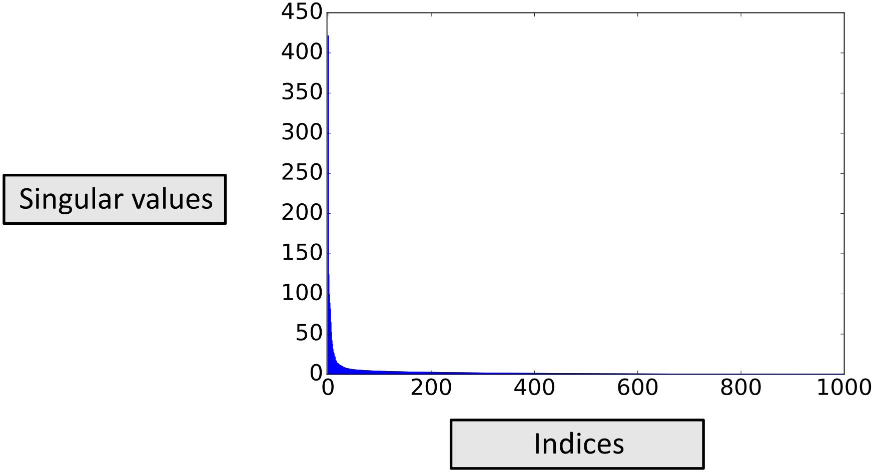
- SVD: $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$
- Truncated SVD: for $0 < k < r$, $\mathbf{A}_k = \sum_{i=1}^{k} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$.
- Error of the truncated SVD:

$$\left|\left|\mathbf{A} - \mathbf{A}_k\right|\right|_F^2 = \underbrace{\sum_{i=k+1}^{r} \sigma_i^2}_{\text{Bottom (the smallest) singular values}}.$$

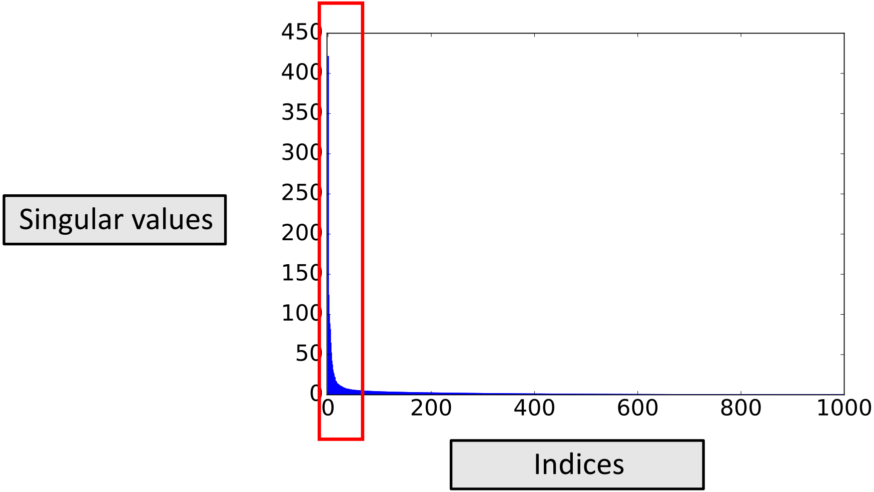
SVD: Example

Original image (1000×1500)

SVD: Example

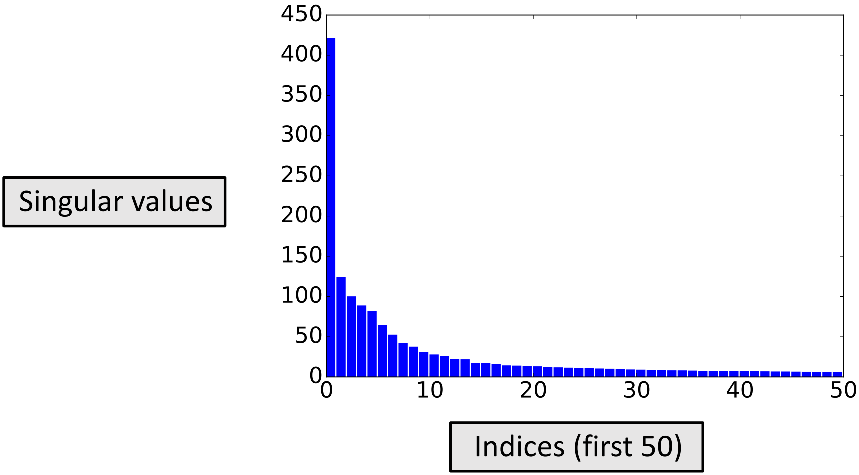

Singular values
450
400
350
300
250
200
150
100
50
0
0
200
400
600
800
1000
Indices

SVD: Example



Singular values
450
400
350
300
250
200
150
100
50
0
0
200
400
600
800
1000
Indices

SVD: Example



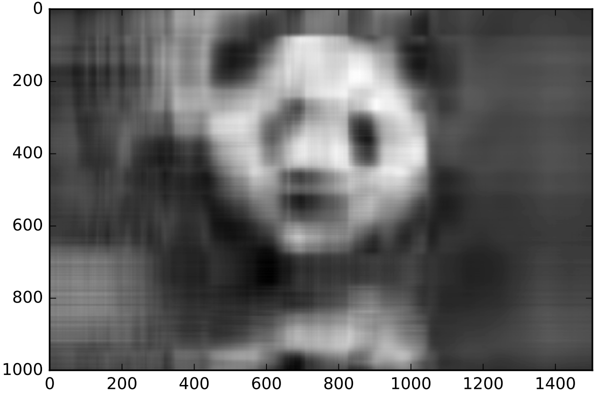
Singular values
450
400
350
300
250
200
150
100
50
0
0
10
20
30
40
50
Indices (first 50)

SVD: Example

Original image (1000×1500)

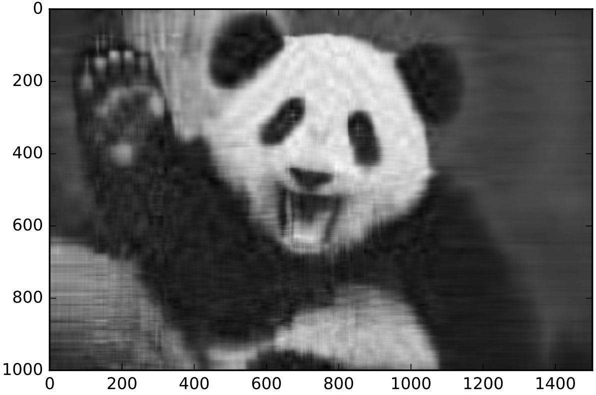
SVD: Example

Rank-5 truncated SVD



SVD: Example

Rank-20 truncated SVD



SVD: Example

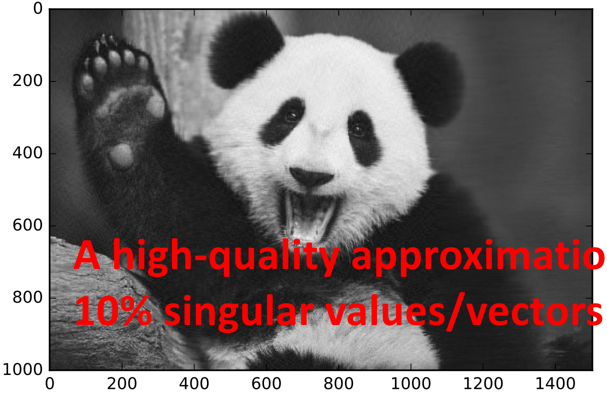
Rank-50 truncated SVD

SVD: Example

Rank-100 truncated SVD

SVD: Example

Rank-100 truncated SVD



A high-quality approximation using 10% singular values/vectors!

SVD: Example

- The original matrix
  - Shape: 1000×1500
  - #Entries: 1.5M
- The rank-100 truncated SVD
  - Shape: 100×1, 100×1500, and 1000×100
  - #Entries: 0.25M
- Truncated SVD saves 83% storage

Power Iteration for Computing Truncated SVD

A Property

Theorem. If $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T$ is the SVD of $\mathbf{A}$, then $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T$.

Proof.

- $\mathbf{A}^T \mathbf{A} = \left(\sum_{i=1}^{r} \sigma_i \, \mathbf{u}_i \, \mathbf{v}_i^T\right)^T \left(\sum_{j=1}^{r} \sigma_j \, \mathbf{u}_j \, \mathbf{v}_j^T\right) = \left(\sum_{i=1}^{r} \sigma_i \, \mathbf{v}_i \, \mathbf{u}_i^T\right)\left(\sum_{j=1}^{r} \sigma_j \, \mathbf{u}_j \, \mathbf{v}_j^T\right)$.

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- $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_i \, \mathbf{v}_i^T + \sum_{i \neq j} \sigma_i \, \sigma_j \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_j \, \mathbf{v}_j^T$.

Using $\left(\sum_i \mathbf{x}_i{}^T\right) \left(\sum_j \mathbf{x}_j\right) = \sum_i \mathbf{x}_i{}^T \, \mathbf{x}_i + \sum_{i \neq j} \mathbf{x}_i{}^T \, \mathbf{x}_j$.

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- $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_i \, \mathbf{v}_i^T + \sum_{i \neq j} \sigma_i \, \sigma_j \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_j \, \mathbf{v}_j^T$.
- $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T + \sum_{i \neq j} \sigma_i \, \sigma_j \, \mathbf{v}_i \, 0 \, \mathbf{v}_j^T$.

Using the properties of orthonormal basis: $\mathbf{u}_i^T \mathbf{u}_i = 1$ and $\mathbf{u}_i^T \mathbf{u}_j = 0$ for $i \neq j$.

A Property

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- $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_i \, \mathbf{v}_i^T + \sum_{i \neq j} \sigma_i \, \sigma_j \, \mathbf{v}_i \, \mathbf{u}_i^T \mathbf{u}_j \, \mathbf{v}_j^T$.
- $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T$

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Eigenvalue decomposition of $\mathbf{A}^T \mathbf{A}$.

Implication: To compute the top singular values σ_i and right singular vectors $\mathbf{v}_i$, we can do **eigenvalue decomposition** instead of **SVD**.

Power Iteration for Truncated SVD

Goal: Compute the top 1 eigenvalue/eigenvector of $\mathbf{A}^T\mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T$.

Algorithm:

1. Randomly initialize a vector $\mathbf{x}_0$ (with unit ℓ_2-norm);
2. Repeat the power iteration: $\mathbf{x}_q \leftarrow \mathbf{A}^T\mathbf{A}\,\mathbf{x}_{q-1}$ and $\mathbf{x}_q \leftarrow \mathbf{x}_q / \left\|\mathbf{x}_q\right\|_2$.

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Merely 2 matrix-vector multiplications.
Very Cheap!

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Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

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Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \, \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.

- Every vector can be written as a linear combination of the orthonormal basis.
- Because $\mathbf{x}_0$ is randomly initialized, $|\alpha_1| = \mathbf{x}_0^T\mathbf{v}_1 = \Omega(1/n)$ with high probability.

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- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \, \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.
- $\mathbf{x}_q \propto (\mathbf{A}^T \mathbf{A})^q \, \mathbf{x}_0$

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- $\mathbf{x}_q \propto (\mathbf{A}^T\mathbf{A})^q \, \mathbf{x}_0$

- It can be proved that $(\mathbf{A}^T\mathbf{A})^q = \sum_{i=1}^{r} \sigma_i^{2q} \, \mathbf{v}_i \, \mathbf{v}_i^T$.

Power Iteration for Truncated SVD

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Algorithm:

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Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.
- $\mathbf{x}_q \propto (\mathbf{A}^T\mathbf{A})^q \mathbf{x}_0 = \left(\sum_{i=1}^{r} \sigma_i^{2q} \mathbf{v}_i \mathbf{v}_i^T\right)\left(\sum_{j=1}^{n} \alpha_j \mathbf{v}_j\right) = \sum_{i=1}^{r} \alpha_i \sigma_i^{2q} \mathbf{v}_i$.

- It can be proved that $(\mathbf{A}^T\mathbf{A})^q = \sum_{i=1}^{r} \sigma_i^{2q} \mathbf{v}_i \mathbf{v}_i^T$.

Power Iteration for Truncated SVD

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Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \, \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.
- $\mathbf{x}_q \propto \sum_{i=1}^{r} \alpha_i \, \sigma_i^{2q} \, \mathbf{v}_i$.

Power Iteration for Truncated SVD

Goal: Compute the top 1 eigenvalue/eigenvector of $\mathbf{A}^T\mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \mathbf{v}_i \mathbf{v}_i^T$.

Algorithm:

1. Randomly initialize a vector $\mathbf{x}_0$ (with unit ℓ_2-norm);
2. Repeat the power iteration: $\mathbf{x}_q \leftarrow \mathbf{A}^T\mathbf{A}\,\mathbf{x}_{q-1}$ and $\mathbf{x}_q \leftarrow \mathbf{x}_q / \left\|\mathbf{x}_q\right\|_2$.

Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.
- $\mathbf{x}_q \propto \sum_{i=1}^{r} \alpha_i \sigma_i^{2q} \mathbf{v}_i$.
- $\mathbf{x}_q \propto \sum_{i=1}^{r} \alpha_i \left(\frac{\sigma_i}{\sigma_1}\right)^{2q} \mathbf{v}_i = \alpha_1 \mathbf{v}_1 + \sum_{i=2}^{r} \alpha_i \left(\frac{\sigma_i}{\sigma_1}\right)^{2q} \mathbf{v}_i$.

Power Iteration for Truncated SVD

Goal: Compute the top 1 eigenvalue/eigenvector of $\mathbf{A}^T\mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T$.

Algorithm:

1. Randomly initialize a vector $\mathbf{x}_0$ (with unit ℓ_2-norm);
2. Repeat the power iteration: $\mathbf{x}_q \leftarrow \mathbf{A}^T\mathbf{A}\,\mathbf{x}_{q-1}$ and $\mathbf{x}_q \leftarrow \mathbf{x}_q / \left\|\mathbf{x}_q\right\|_2$.

Convergence Analysis ($\mathbf{x}_q$ converges to $\mathbf{v}_1$):

- $\mathbf{x}_0 = \sum_{i=1}^{n} \alpha_i \, \mathbf{v}_i$. Here $|\alpha_1| = \Omega(1/n)$ with high probability.
- $\mathbf{x}_q \propto \sum_{i=1}^{r} \alpha_i \, \sigma_i^{2q} \, \mathbf{v}_i$.
- $\mathbf{x}_q \propto \sum_{i=1}^{r} \alpha_i \left(\frac{\sigma_i}{\sigma_1}\right)^{2q} \mathbf{v}_i = \alpha_1 \mathbf{v}_1 + \underbrace{\sum_{i=2}^{r} \alpha_i \left(\frac{\sigma_i}{\sigma_1}\right)^{2q} \mathbf{v}_i}_{\text{It converge to 0 because } \frac{\sigma_i}{\sigma_1} < 1.}$.

Power Iteration for Truncated SVD

Goal: Compute the top k eigenvalue/eigenvector of $\mathbf{A}^T \mathbf{A} = \sum_{i=1}^{r} \sigma_i^2 \, \mathbf{v}_i \, \mathbf{v}_i^T$.

Algorithm:

1. Randomly initialize a matrix $\mathbf{X}_0 \in \mathbb{R}^{n \times k}$ (entries are i.i.d. standard Gaussian);
2. Orthogonalize the columns: $\mathbf{X}_0 \leftarrow \mathrm{orth}(\mathbf{X}_0)$;
3. Repeat the power iteration:
   - **i.** $\mathbf{X}_q \leftarrow \mathbf{A}^T \mathbf{A} \, \mathbf{X}_{q-1}$;
   - ***ii.*** $\mathbf{X}_q \leftarrow \mathrm{orth}(\mathbf{X}_q)$.