

0 Essentials

Matrix/Vector

Vectors: Unit vector: $u^\top u = 1$ Orthogonal vectors: $u^\top v = 0$ **Range, Kernel, Nullity:** $range(\mathbf{A}) = \{\mathbf{z} | \exists \mathbf{x} : \mathbf{z} = \mathbf{A}\mathbf{x}\} = span(\text{columns of } \mathbf{A})$
 $rank(\mathbf{A}) = dim(range(\mathbf{A}))$ $kernel(\mathbf{A}) = \{\mathbf{x} : \mathbf{A}\mathbf{x} = \mathbf{0}\}$ (spans nullspace) $nullity(\mathbf{A}) = dim(kernel(\mathbf{A}))$
Ranks: $rank(XY) \leq rank(X) \forall X \in \mathbb{R}^{m \times n}, Y \in \mathbb{R}^{n \times k}$
eq. if $Y \in \mathbb{R}^{n \times n}, rank(Y) = n$ **Rank-nullity Theorem:** $dim(kernel(\mathbf{A})) + dim(range(\mathbf{A})) = n$

Orthogonal mat. $\mathbf{A}^{-1} = \mathbf{A}^\top$, $\mathbf{A}\mathbf{A}^\top = \mathbf{A}^\top \mathbf{A} = \mathbf{I}$, $\det(\mathbf{A}) \in \{+1, -1\}$, $\det(\mathbf{A}^\top \mathbf{A}) = 1$, preserves inner product, norm, distance, angle, rank, matrix orthogonality **Outer Product:** $\mathbf{u}\mathbf{v}^\top$, $(\mathbf{u}\mathbf{v}^\top)_{i,j} = \mathbf{u}_i \mathbf{v}_j$
Inner Product: $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y} = \sum_{i=1}^N \mathbf{x}_i \mathbf{y}_i$. $\langle \mathbf{x} \pm \mathbf{y}, \mathbf{x} \pm \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle \pm 2\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{y}, \mathbf{y} \rangle$

($\mathbf{u}_i^\top \mathbf{v}_j$) $\mathbf{v}_j = (\mathbf{v}_j \mathbf{v}_j^\top) \mathbf{u}_i$ Cross product: $\vec{a} \times \vec{b} = (a_2 b_3 - a_3 b_2, a_3 b_1 - a_1 b_3, a_1 b_2 - a_2 b_1)^\top$
Trace: $trace(\mathbf{X}\mathbf{Y}\mathbf{Z}) = trace(\mathbf{Z}\mathbf{X}\mathbf{Y})$
Transpose: $(\mathbf{A}^\top)^{-1} = (\mathbf{A}^{-1})^\top$, $(\mathbf{A}\mathbf{B})^\top = \mathbf{B}^\top \mathbf{A}^\top$, $(\mathbf{A} + \mathbf{B})^\top = \mathbf{A}^\top + \mathbf{B}^\top$

Cauchy-Schwarz inequality: $|\langle \mathbf{u}, \mathbf{v} \rangle| \leq \|\mathbf{u}\| \|\mathbf{v}\|$
Jensen inequality: for convex function f , non negative λ_i s.t. $\sum_{i=1}^n \lambda_i = 1$: $f(\sum_{i=1}^n \lambda_i x_i) \leq \sum_{i=1}^n \lambda_i f(x_i)$ Note: for concave, inequality sign switches **Convexity:** $f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y), \forall \theta \in [0, 1]$ **Least Squares equations:** $\arg \min_{\beta \in \mathbb{R}^{p+1}} \|\mathbf{y} - \mathbf{X}\beta\|^2, \hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$

Einstein matrix notation: $(\mathbf{A} \cdot \mathbf{B})_{ij} = \sum_{k=1}^n A_{ik} \cdot B_{kj}$
Kullback-Leibler: $KL(P||Q) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)}$

Norms

- $\|\mathbf{x}\|_0 = |\{i | x_i \neq 0\}|$
- $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^N \mathbf{x}_i^2} = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$
- $\|\mathbf{u} - \mathbf{v}\|_2 = \sqrt{(\mathbf{u} - \mathbf{v})^\top (\mathbf{u} - \mathbf{v})}$
- $\|\mathbf{x}\|_p = (\sum_{i=1}^N |x_i|^p)^{\frac{1}{p}} ; \|\mathbf{x}\|_\infty = \max_{i=1, \dots, n} |x_i|$
- $\|\mathbf{M}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n \mathbf{m}_{i,j}^2} = \sqrt{\sum_{i=1}^{\min\{m,n\}} \sigma_i^2} = \|\sigma(\mathbf{A})\|_2 = \sqrt{trace(\mathbf{M}^\top \mathbf{M})}$
- $\|\mathbf{M}\|_G = \sqrt{\sum_{i,j} g_{ij} x_{ij}^2}$ (weighted Frobenius)
- $\|\mathbf{M}\|_1 = \sum_{i,j} |m_{i,j}|$
- $\|\mathbf{M}\|_2 = \sigma_{\max}(\mathbf{M}) = \|\sigma((\mathbf{M}))\|_\infty$ (spectral)
- $\|\mathbf{M}\|_p = \max_{\mathbf{v} \neq 0} \frac{\|\mathbf{M}\mathbf{v}\|_p}{\|\mathbf{v}\|_p}$
- $\|\mathbf{M}\|_* = \sum_{i=1}^{\min(m,n)} \sigma_i = \|\sigma(\mathbf{A})\|_1$ (nuclear)

Derivatives

$$\frac{\partial}{\partial \mathbf{x}} (\mathbf{b}^\top \mathbf{x}) = \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^\top \mathbf{b}) = \mathbf{b} \quad \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^\top \mathbf{x}) = 2\mathbf{x}$$
$$\frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^\top \mathbf{A} \mathbf{x}) = (\mathbf{A}^\top + \mathbf{A}) \mathbf{x} \quad \frac{\partial}{\partial \mathbf{x}} (\mathbf{b}^\top \mathbf{A} \mathbf{x}) = \mathbf{A}^\top \mathbf{b}$$
$$\frac{\partial}{\partial \mathbf{X}} (\mathbf{c}^\top \mathbf{X} \mathbf{b}) = \mathbf{c} \mathbf{b}^\top \quad \frac{\partial}{\partial \mathbf{X}} (\mathbf{c}^\top \mathbf{X}^\top \mathbf{b}) = \mathbf{b} \mathbf{c}^\top$$

$$\frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x} - \mathbf{b}\|_2) = \frac{\mathbf{x} - \mathbf{b}}{\|\mathbf{x} - \mathbf{b}\|_2} \quad \frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x}\|_2^2) = \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^\top \mathbf{x}) = 2\mathbf{x}$$
$$\frac{\partial}{\partial \mathbf{X}} (\|\mathbf{X}\|_F^2) = 2\mathbf{X} \quad \frac{\partial}{\partial \mathbf{x}} \log(x) = \frac{1}{x}$$

Eigendecomposition
 $\mathbf{A} \in \mathbb{R}^{N \times N}$ then $\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{-1}$ with $\mathbf{Q} \in \mathbb{R}^{N \times N}$.
if fullrank: $\mathbf{A}^{-1} = \mathbf{Q} \mathbf{\Lambda}^{-1} \mathbf{Q}^{-1}$ and $(\mathbf{\Lambda}^{-1})_{i,i} = \frac{1}{\lambda_i}$.

if \mathbf{A} symmetric: $\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^\top$ (\mathbf{Q} orthogonal). Eigenvalue λ : solve $\det(\mathbf{A} - \lambda \mathbf{I}) = 0$ Eigenvector \mathbf{v} : solve $(\mathbf{A} - \lambda \mathbf{I}) * \mathbf{v} = \vec{0}$

Probability / Statistics

- $P(x) := Pr[X = x] := \sum_{y \in Y} P(x, y) \bullet P(x|y) := Pr[X = x | Y = y] := \frac{P(x, y)}{P(y)}$, if $P(y) > 0 \bullet \forall y \in Y : \sum_{x \in X} P(x|y) = 1$ (property for any fixed y) $\bullet P(x, y) = P(x|y)P(y) \bullet \text{posterior } P(A|B) = \frac{\text{prior } P(A) \times \text{likelihood } P(B|A)}{\text{evidence } P(B)}$ (Bayes' rule) $\bullet P(x|y) = P(x) \Leftrightarrow P(y|x) = P(y)$ (iff X, Y independent)
- $P(x_1, \dots, x_n) = \prod_{i=1}^n P(x_i)$ (iff IID) \bullet Variance $Var[X] := E[(X - \mu_x)^2] := \sum_{x \in X} (x - \mu_x)^2 P(x) = E(X^2) - E(X)^2$ $Var(aX) = a^2 Var(X) \bullet$ expectation $\mu_x := E[X] := \sum_{x \in X} x P(x) \bullet E[X + Y] = E[X] + E[Y] \bullet$ standard deviation $\sigma_x := \sqrt{Var[X]}$

Lagrangian Multipliers

Minimize $f(\mathbf{x})$ s.t. $g_i(\mathbf{x}) \leq 0, i = 1, \dots, m$ (**inequality constr.**) and $h_i(\mathbf{x}) = \mathbf{a}_i^\top \mathbf{x} - b_i = 0$ or $h_i(\mathbf{x}) = \sum_w x_{w,i} - b_i = 0, i = 1, \dots, p$ (**equality constraint**)
 $L(\mathbf{x}, \alpha, \beta) := f(\mathbf{x}) + \sum_{i=1}^m \alpha_i g_i(\mathbf{x}) + \sum_{i=1}^p \beta_i h_i(\mathbf{x})$

1 Principal Component Analysis

$\mathbf{X} \in \mathbb{R}^{D \times N}$. N observations, K rank.

- Empirical Mean: $\bar{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n$.
- Center Data: $\bar{\mathbf{X}} = \mathbf{X} - [\bar{\mathbf{x}}, \dots, \bar{\mathbf{x}}] = \mathbf{X} - \mathbf{M}$.
- Cov.: $\Sigma = \frac{1}{N} \sum_{n=1}^N (\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^\top = \frac{1}{N} \bar{\mathbf{X}} \bar{\mathbf{X}}^\top$.
- Eigenvalue Decomposition: $\Sigma = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^\top$.
- Select $K < D$, only keep \mathbf{U}_K, λ_K .
- Transform data onto new Basis: $\bar{\mathbf{Z}}_K = \mathbf{U}_K^\top \bar{\mathbf{X}}$.
- Reconstruct to original Basis: $\tilde{\tilde{\mathbf{X}}} = \mathbf{U}_K \bar{\mathbf{Z}}_K$.
- Reverse centering: $\tilde{\mathbf{X}} = \tilde{\tilde{\mathbf{X}}} + \mathbf{M}$.

For compression save $\mathbf{U}_K, \bar{\mathbf{Z}}_K, \bar{\mathbf{x}}$.

$\mathbf{U}_k \in \mathbb{R}^{D \times K}, \Sigma \in \mathbb{R}^{D \times D}, \bar{\mathbf{Z}}_K \in \mathbb{R}^{K \times N}, \bar{\mathbf{x}} \in \mathbb{R}^{D \times N}$

Calculation of: $var(X) = \frac{1}{N} \sum_{n=1}^N (X_i - \bar{X})^2$

Iterative View

Residual r_i : $x_i - \tilde{x}_i = \mathbf{I} - \mathbf{u} \mathbf{u}^\top x_i$
Cov of r : $\frac{1}{n} \sum_{i=1}^n (\mathbf{I} - \mathbf{u} \mathbf{u}^\top) x_i x_i^\top (\mathbf{I} - \mathbf{u} \mathbf{u}^\top)^\top = (\mathbf{I} - \mathbf{u} \mathbf{u}^\top) \Sigma (\mathbf{I} - \mathbf{u} \mathbf{u}^\top)^\top = \Sigma - 2 \Sigma \mathbf{u} \mathbf{u}^\top + \mathbf{u} \mathbf{u}^\top \Sigma \mathbf{u} \mathbf{u}^\top = \Sigma - \lambda \mathbf{u} \mathbf{u}^\top$

- Find principal eigenvector of $(\Sigma - \lambda \mathbf{u} \mathbf{u}^\top)$
- which is the second eigenvector of Σ
- iterating to get d principal eigenvector of Σ

Power Method

Power iteration: $v_{t+1} = \frac{\mathbf{A} v_t}{\|\mathbf{A} v_t\|}, \lim_{t \rightarrow \infty} v_t = u_1$

Assuming $\langle u_1, v_0 \rangle \neq 0$ and $|\lambda_1| > |\lambda_j| (\forall j \geq 2)$

Reconstruction Proof Sketch

Given: $\tilde{X} = U_K U_K^\top \bar{X}$ To prove: squared reconstruction error is the sum of the lowest $D - K$ eigenvalues of Σ . $err = 1/N \sum_{i=1}^N \|\tilde{x}_i - \bar{x}_i\|_2^2 = 1/N \|\tilde{X} - \bar{X}\|_F^2 = 1/N \|(U_K U_K^\top - I_d) \bar{X}\|_F^2 = 1/N * trace((U_K U_K^\top - I_d) \bar{X} \bar{X}^\top (U_K U_K^\top - I_d)^\top) = 1/N * trace((U_K; 0] - U) \mathbf{\Lambda} ([U_K; 0] - U)^\top)$