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List of symbols

 $\dot{=}$ Equality by definition

Approximate equality \approx

Proportional to

Set of natural numbers \mathbb{N}

 ${\rm I\!R}$ Set of real numbers

i:jSet of natural numbers between i and j. *I.e.*, $\{i, i+1, ..., j\}$

 $f:A\to B$ Function *f* that maps elements of set *A* to elements of

set B

1{predicate} Indicator function (1 if predicate is true, otherwise 0)

 $v \in \mathbb{R}^n$ *n*-dimensional vector

 $M \in \mathbb{R}^{m \times n}$ $m \times n$ matrix

 $\mathbf{T} \in \mathbb{R}^{d_1 imes \cdots imes d_n}$ Tensor

 M^{\top} Transpose of matrix *M*

 M^{-1} Inverse of matrix M

det(M)Determinant of M

 $\frac{\mathrm{d}}{\mathrm{d}x}f(x)$ Ordinary derivative of f(x) w.r.t. x at point $x \in \mathbb{R}$

 $\frac{\partial}{\partial x} f(x)$ Partial derivative of f(x) w.r.t. x at point $x \in \mathbb{R}^n$

 $\nabla_x f(x) \in \mathbb{R}^n$ Gradient of $f: \mathbb{R}^n \to \mathbb{R}$ at point $x \in \mathbb{R}^n$

 $\nabla_{\mathbf{x}}^2 f(\mathbf{x}) \in \mathbb{R}^{n \times n}$ Hessian of $f : \mathbb{R}^n \to \mathbb{R}$ at point $\mathbf{x} \in \mathbb{R}^n$

 $\theta \in \Theta$ Parametrization of a model, where Θ is a compact sub-

set of \mathbb{R}^K

 \mathcal{X} Input space

 \mathcal{Y} Output space

 $\mathcal{D} \subseteq \mathcal{X} \times \mathcal{Y}$ Labeled training data

Dimensionality reduction

The motivation behind dimensionality reduction is to find a low-dimensional representation of high-dimensional data. This can be split into two goals: (1) compressing the data, while preserving as much as possible of the relevant information, and (2) interpreting the data in low dimensionality is easier than high dimensionality.

¹ Often, the original raw representation is highdimensional and redundant, e.g., images, audio, time series.

 $m \ll n$.

Dimensionality reduction is often performed by an autoencoder, which typically has a bottleneck and aims to predict its input; see Figure 1. In general, we have an encoder F and a decoder G,

$$F: \mathbb{R}^n \to \mathbb{R}^m$$
, $G: \mathbb{R}^m \to \mathbb{R}^n$.

The reconstruction function is then the following function,

$$G \circ F : \mathbb{R}^n \to \mathbb{R}^n$$
,

which is ideally the identity function.

Linear autoencoders

To build a nice theory, we will only consider a single layer linear autoencoder, which means that we have the following functions,

$$F: x \mapsto z = Wx, \quad W \in \mathbb{R}^{m \times n}.$$

 $G: z \mapsto \hat{x} = Vz, \quad V \in \mathbb{R}^{n \times m}.$

The objective to minimize of the linear encoder is the following,

$$\mathcal{R}(W, V) = \mathcal{R}(P \doteq VW) \doteq \mathbb{E}\left[\frac{1}{2}||x - Px||^2\right].$$

Corollary. For centered data, *i.e.* E[x] = 0, optimal affine maps degenerate to linear ones.

Proof. Proof by contradiction. Let $a \neq 0$, then

$$\mathbb{E}\left[\|x - (Px + a)\|^{2}\right] = \mathbb{E}\left[\langle x - Px - a, x - Px - a\rangle\right]$$

$$= \mathbb{E}\left[\langle x - Px, x - Px\rangle + 2\langle x - Px, -a\rangle + \langle -a, -a\rangle\right]$$

$$= \mathbb{E}\left[\|x - Px\|^{2}\right] - 2\langle \underbrace{\mathbb{E}[x] - P\mathbb{E}[x]}_{=0}, a\rangle + \underbrace{\|a\|^{2}}_{>0}$$

$$> \mathbb{E}\left[\|x - Px\|^{2}\right].$$

Thus, the risk is strictly worse if $a \neq 0$.

Thus, we will assume that the data is centered, which makes the analysis easier, since we do not need to consider the affine case.

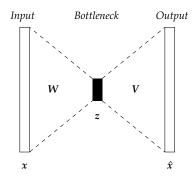


Figure 1. Diagram of a single layer linear autoen-

Note that while the optimal linear reconstruction map *P* is unique, its parametrization W, V is not unique, since for any invertible matrix $A \in \mathbb{R}^{m \times m}$, we can construct an optimal parametrization,

$$VW = VIW = V(AA^{-1})W = (VA)(A^{-1}W),$$

with $A^{-1}W$, VA. The weight matrices are non-identifiable.

Since P cannot be any $n \times n$ matrix, we want to know how the composition of $W \in \mathbb{R}^{m \times n}$ and $V \in \mathbb{R}^{n \times m}$ characterizes the matrix P and which constraints they impose. The answer to this is that the weight matrices impose a rank constraint on P,

$$rank(\mathbf{P}) = \min\{rank(\mathbf{W}), rank(\mathbf{W})\} \le \min\{m, n\} = m.$$

Thus, when optimizing for P, we are constrained to matrices with rank less or equal to m.

Projection 1.2

The rank constraint and linearity of P means that the image (column space) of **P** is a linear subspace $\mathcal{U} \subseteq \mathbb{R}^n$ of dimension at most m. We will break the solution to our problem into two parts: (1) finding the optimal subspace \mathcal{U} , and (2) finding the optimal mapping to that subspace.²

Finding the optimal mapping to a subspace. We will first focus on (2); given subspace \mathcal{U} , we need to determine the optimal linear map P^* , such that

$$P^* = \underset{P}{\operatorname{argmin}} \|x - Px\|^2, \quad \operatorname{col}(P) = \mathcal{U}.$$

Definition 1 (Orthogonal projection). A linear transformation P: $\mathcal{V} \to \mathcal{V}$ is called an orthogonal projection onto \mathcal{U} if $\forall x \in \mathcal{V}$:

- 1. Projection: $P(x) \in \mathcal{U}$;
- 2. *Orthogonality*: $null(P) \perp col(P)$, which is equivalent to the following holding, $\langle P(x), y \rangle = \langle x, P(y) \rangle$ (self-adjointness);
- 3. Idempotency: P(P(x)) = P(x).

Definition 2. The orthogonal projection to a linear subspace $\mathcal{U} \subseteq \mathbb{R}^n$ is defined as

$$\Pi_{\mathcal{U}}: \mathbb{R}^n \to \mathcal{U}, \quad \Pi_{\mathcal{U}}(\mathbf{x}) = \operatorname*{argmin}_{\mathbf{x}' \in \mathcal{U}} \|\mathbf{x} - \mathbf{x}'\|.$$

 2 We do not search for the weight matrices W, V, since they are not unique, but P is unique.

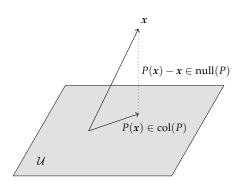


Figure 2. Orthogonal projection of x onto subspace plane \mathcal{U} .

Proof. We need to show that the definition of $\Pi_{\mathcal{U}}$ indeed is an orthogonal projection by showing that it adheres to the properties of Definition 1.

- 1. Projection: This is true by definition of the values that the argmin are allowed to take on;
- 2. *Idempotency*: For all $u \in \mathcal{U}$, $\Pi_{\mathcal{U}}(u) = \operatorname{argmin}_{x' \in \mathcal{U}} \|u x'\| = u$. Thus, $\Pi_{\mathcal{U}} = \Pi_{\mathcal{U}} \circ \Pi_{\mathcal{U}};$
- 3. *Orthogonality*: We need to show that $\Pi_{\mathcal{U}}(x) x \in \mathcal{U}^{\perp}$. Decompose it into $u\in\mathcal{U}$ and $u^\perp\in\mathcal{U}^\perp$ by $\Pi_\mathcal{U}(x)-x=u+u^\perp.$ Then, we only need to show that u = 0.

Proof by contradiction. Let $u \neq 0$, then

$$\|\Pi_{\mathcal{U}}(x) - x\|^2 = \underbrace{\|u\|^2}_{>0} + \|u^{\perp}\|^2 + 2\underbrace{\langle u, u^{\perp} \rangle}_{=0}$$

$$> \|u^{\perp}\|^2$$

$$= \|\underbrace{\Pi_{\mathcal{U}}(x) - u}_{\in \mathcal{U}} - x\|^2,$$

which contradicts with

$$\|\Pi_{\mathcal{U}}(x) - x\| = \min_{x' \in \mathcal{U}} \|x' - x\| \le \|\tilde{u} - x\|, \quad \forall \tilde{u} \in \mathcal{U}.$$

Hence, $\Pi_{\mathcal{U}}(x) - x \in \mathcal{U}^{\perp}$ and is unique;

4. Linearity: We need to show homogeneity,

$$\Pi_{\mathcal{U}}(\alpha \mathbf{x}) = \underset{\mathbf{x}'' \in \mathcal{U}}{\operatorname{argmin}} \|\alpha \mathbf{x} - \mathbf{x}''\|$$

$$= \underset{\alpha \mathbf{x}' \in \mathcal{U}}{\operatorname{argmin}} \|\alpha \mathbf{x} - \alpha \mathbf{x}'\|$$

$$= \alpha \underset{\mathbf{x}' \in \mathcal{U}}{\operatorname{argmin}} |\alpha| \|\mathbf{x} - \mathbf{x}'\|$$

$$= \alpha \underset{\mathbf{x}' \in \mathcal{U}}{\operatorname{argmin}} \|\mathbf{x} - \mathbf{x}'\|$$

$$= \alpha \underset{\mathbf{x}' \in \mathcal{U}}{\operatorname{argmin}} \|\mathbf{x} - \mathbf{x}'\|$$

$$= \alpha \Pi_{\mathcal{U}}(\mathbf{x}).$$

And, we need to show additivity,

So, we know that $\Pi_{\mathcal{U}}$ is an orthogonal projection. Now, we want to find the matrix *P* representing that linear transformation.

Given an orthonormal basis U of U, we can compute the optimal projection matrix,

$$P = UU^{\top}$$
.

Note that in this case W and V share parameters, and UU^{\top} is the optimal weight matrix if we enforce parameter sharing via $V = W^{\top}$.

Proof. The image of the projection matrix is \mathcal{U} ,

$$Px = \left(\sum_{i=1}^m u_i u_i^{\top}\right) x = \sum_{i=1}^m u_i u_i^{\top} x = \sum_{i=1}^m \langle u_i, x \rangle u_i.$$

Self-adjointness,

$$P^{\top} = (UU^{\top})^{\top} = UU^{\top} = P.$$

Idempotency,

$$PP = U \underbrace{U^{\top}U}_{I_{m}} U^{\top} = UU^{\top} = P.$$

Orthogonality, TODO

In general, we do not have an orthonormal basis for U. In a nonorthonormal basis V for \mathcal{U} , we can recover the projection matrix,

$$P = VV^+, \quad V^+ \doteq (V^\top V)^{-1}V^\top.$$

Note that V^+ is the left Moore-Penrose pseudo-inverse of V.

Proof. **P** is the projection matrix of \mathcal{U} ,

$$PV = VV^+V = V(V^\top V)^{-1}V^\top V = V.$$

Together with the rank constraint, this yields $Pu^{\perp} = 0$ for all $u^{\perp} \in \mathcal{U}^{\perp}$.

Self-adjointness,

$$\mathbf{P}^{\top} = \left(\mathbf{V} \left(\mathbf{V}^{\top} \mathbf{V}\right)^{-1} \mathbf{V}^{\top}\right)^{\top} = \mathbf{V} \left(\mathbf{V}^{\top} \mathbf{V}\right)^{-1} \mathbf{V}^{\top} = \mathbf{P}.$$

Idempotency,

$$PP = V(V^{\top}V)^{-1}V^{\top}V(V^{\top}V)^{-1}V^{\top} = VV^{+} = P.$$

Finding the optimal subspace. Now we need to find out which subspace of dimension m or less is optimal to project onto. First, we need to rewrite the objective function to find a new interpretation,

$$\mathcal{R}(\mathbf{P}) = \frac{1}{2} \mathbb{E} \left[\| \mathbf{x} - \mathbf{P} \mathbf{x} \|^2 \right]$$

$$= \frac{1}{2} \mathbb{E} \left[\langle \mathbf{x}, \mathbf{x} \rangle + 2 \langle \mathbf{x}, -\mathbf{P} \mathbf{x} \rangle + \langle -\mathbf{P} \mathbf{x}, -\mathbf{P} \mathbf{x} \rangle \right]$$

$$= \frac{1}{2} \mathbb{E} \left[\| \mathbf{x} \|^2 \right] + \frac{1}{2} \mathbb{E} \left[\| \mathbf{P} \mathbf{x} \|^2 \right] - \mathbb{E} \left[\langle \mathbf{x}, \mathbf{P} \mathbf{x} \rangle \right]$$

$$= \frac{1}{2} \mathbb{E} \left[\| \mathbf{x} \|^2 \right] + \frac{1}{2} \mathbb{E} \left[\| \mathbf{P} \mathbf{x} \|^2 \right] - \mathbb{E} \left[\langle \mathbf{x}, \mathbf{P}^2 \mathbf{x} \rangle \right]$$

$$= \frac{1}{2} \mathbb{E} \left[\| \mathbf{x} \|^2 \right] + \frac{1}{2} \mathbb{E} \left[\| \mathbf{P} \mathbf{x} \|^2 \right] - \mathbb{E} \left[\| \mathbf{P} \mathbf{x} \|^2 \right]$$

$$= \frac{1}{2} \mathbb{E} \left[\| \mathbf{x} \|^2 \right] - \frac{1}{2} \mathbb{E} \left[\| \mathbf{P} \mathbf{x} \|^2 \right].$$

Because our data is centered, we know the following,

$$\operatorname{Var}[x] = \mathbb{E}\left[\|x\|^{2}\right] - \|\underbrace{\mathbb{E}[x]}_{=0}\|^{2}$$

$$= \mathbb{E}\left[\|x\|^{2}\right].$$

$$\operatorname{Var}[Px] = \mathbb{E}\left[\|Px\|^{2}\right] - \|\mathbb{E}[Px]\|^{2}$$

$$= \mathbb{E}\left[\|Px\|^{2}\right] - \|P\underbrace{\mathbb{E}[x]}_{=0}\|^{2}$$

$$= \mathbb{E}\left[\|Px\|^{2}\right].$$

$$\mathcal{R}(\mathbf{P}) = \frac{1}{2}(\operatorname{Var}[\mathbf{x}] - \operatorname{Var}[\mathbf{P}\mathbf{x}]) \propto -\frac{1}{2}\operatorname{Var}[\mathbf{P}\mathbf{x}].$$

Hence, minimizing $\mathcal{R}(P)$ is equivalent to maximizing the variance Var[Px].

We can further simplify this expression to find a sufficient statistic for the objective function,

$$-\frac{1}{2} \operatorname{Var}[\mathbf{P}\mathbf{x}] = -\frac{1}{2} \mathbb{E} \left[\|\mathbf{P}\mathbf{x}\|^{2} \right]$$

$$= -\frac{1}{2} \mathbb{E} \left[\langle \mathbf{x}, \mathbf{P}\mathbf{x} \rangle \right]$$

$$= -\frac{1}{2} \mathbb{E} \left[\operatorname{tr} \left(\mathbf{x}^{\top} \mathbf{P}\mathbf{x} \right) \right]$$

$$= -\frac{1}{2} \operatorname{tr} \left(\mathbb{E} \left[\mathbf{P}\mathbf{x}\mathbf{x}^{\top} \right] \right)$$

$$= -\frac{1}{2} \operatorname{tr} \left(\mathbf{P} \mathbb{E} \left[\mathbf{x}\mathbf{x}^{\top} \right] \right).$$

Idempotency of projection matrices.

$$\langle x, P^2 x \rangle = \langle Px, Px \rangle.$$

$$||Px||^2 = \langle Px, Px \rangle = \langle x, P^2x \rangle = \langle x, Px \rangle.$$

Cyclic property of trace.

 $\mathbb{E}[xx^{\top}]$ is a sufficient statistic for $\mathcal{R}(\mathbf{P})$.

The optimal projection is fully determined by the covariance matrix $\mathbb{E}[xx^{\top}]$, together with $\mathbb{E}[x]$ for centering.

Principal component analysis

Theorem 3 (Spectral theorem). Any symmetric and positive semidefinite matrix Σ can be non-negatively diagonalized with an orthogonal matrix,

$$\Sigma = Q\Lambda Q^{\top}, \quad \Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n),$$

where $\lambda \ge \cdots \ge \lambda_n \ge 0$ and Q is orthogonal.

Remark. Q is composed of ordered eigenvectors of Σ , and Λ is composed of ordered eigenvalues of Σ .

Theorem 4 (PCA theorem). The variance maximizing projection matrix **P** for a covariance matrix $\mathbb{E}[xx^{\top}] = Q\Lambda Q^{\top}$ as in the spectral theorem is given by

$$P = UU^{\top}, \quad U = Q \begin{bmatrix} I_m \\ 0 \end{bmatrix}.$$

Proof.

$$Var[Px] = tr(P\mathbb{E}[xx^{\top}])$$

$$= tr(UU^{\top}Q\Lambda Q^{\top})$$

$$= tr((Q^{\top}U)(Q^{\top}U)^{\top}\Lambda).$$

This term is maximized by $\mathbf{Q}^{\mathsf{T}}\mathbf{U} = \begin{bmatrix} \mathbf{I}_m & \mathbf{0} \end{bmatrix}^{\mathsf{T}}$.

 $P = UU^{\top}, \mathbb{E}[xx^{\top}] = Q\Lambda Q^{\top}.$

Cyclic property.

Learning algorithms 1.4

Eigenvalue decomposition of the (symmetric) sample covariance matrix has $\mathcal{O}(n^3)$ complexity. Furthermore, the complexity of computing $\mathbb{E}[xx^{\top}]$ is $\mathcal{O}(Nn^2)$.³ This is quite costly, thus we need to search for algorithms that have lower runtime complexity.

³ Typically, $N \gg n$.

Power method. The power method is a recursive algorithm for computing principal eigenvectors. It initializes a vector at random $v^{(0)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. Then, it iteratively improves this guess,

$$v^{(t+1)} = \frac{Av^{(t)}}{\|Av^{(t)}\|}.$$

The computational complexity of this algorithm is $\mathcal{O}(Tn^2)$.

Lemma 5. Let u_1 be the unique principal eigenvector of a diagonalizable matrix A with eigenvalues $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n \geq 0$. If $\langle v_0, u_1 \rangle \neq 0$, then

$$\lim_{t\to\infty} \boldsymbol{v}^{(t)} = \boldsymbol{u}_1.$$

Proof. We can decompose vectors as a linear combination of eigenvectors, $v^{(0)} = \sum_{i=1}^{n} \alpha_{i} u_{i}$. Then,

$$\begin{split} \boldsymbol{v}^{(k)} &\propto \boldsymbol{A}^k \boldsymbol{v}^{(0)} \\ &= \sum_{i=1}^n \alpha_i \lambda_i^k \boldsymbol{u}_i \\ &\propto \alpha_1 \boldsymbol{u}_1 + \sum_{i=2}^n \alpha_i \bigg(\frac{\lambda_i}{\lambda_1}\bigg)^k \boldsymbol{u}_i. \end{split} \qquad \qquad \text{Divide by λ_1.}$$

 $\lambda_i/\lambda_1 < 1$ for i > 1, thus the sum goes to o and $v^{(k)} \to u_1$.

We can use this algorithm to also compute the next principal eigenvectors by factoring out u_1 and then doing the algorithm again to recover u_{2} , and continue doing that until we have the m principal eigenvectors.

Thus, the total complexity of finding the m principal eigenvectors is $\mathcal{O}(Tmn^2)$. However, this does not get rid of the $\mathcal{O}(Nn^2)$ complexity for computing the sample covariance matrix.

Gradient descent. By treating the autoencoder as a neural network, we can use deep learning techniques, such as gradient descent. Gradient descent iteratively updates the weights by

$$\mathbf{P}^{(t+1)} = \mathbf{P}^{(t)} - \eta \nabla_{\mathbf{P}} \mathcal{R}(\mathbf{P}).$$

The gradient is computed by $(P - I)xx^{\top}$. The problem with this is that we cannot constrain P to be a projection. Thus, we actually need to update *V* and *W*. Thus, by the chain rule for matrix derivatives,

$$\nabla_{W} \mathcal{R}(W, V) = (P - I) x x^{\top} W^{\top}$$
$$\nabla_{V} \mathcal{R}(W, V) = V^{\top} (P - I) x x^{\top}.$$

The complexity for *T* iterations is then $\mathcal{O}(T(m+k)n^2)$, where *k* is the batch size.

Non-linear autoencoders 1.5

We can get much better performance by considering non-linearities, and we can easily use gradient descent to work with non-linear architectures.