Data Science Principal Component Analysis

Linear latent decomposition

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What is this lecture about?

- * Base representations may not be optimal (to be defined)
- * Latent models promise to exhibit the underlying (latent) factors that drive the process in question
- * This initial (but fundamental) definition of latent factors uses statistical correlation
- ⇒ It exhibits linear latent factors
- ⇒ Enables "simplification" of the data by sound decimation
 - * Also: we will study several interpretations

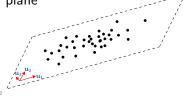
Reading: [1] (chap 12) and [3] (chap 3 and 10.3)

Intuition

Given $\mathcal{X} \subset \Omega$, we wish to decompose Ω into subspaces such that the projection of \mathcal{X} onto these subspaces retains the most "information".

Q: What information should we consider?

- \star Say $\mathfrak X$ is almost "contained" into a 2D plane in a 3D space
- * A relevant choice for our subspace is to chose a basis $\{u_1, u_2\}$ for the plane



Q: What characterizes $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$?

- ⇒ the fact that the data varies most along these directions
- \Rightarrow the fact that the data varies least orthogonally to these directions (\mathfrak{u}_3)

Formalization

Given \mathcal{X} , $\{\mathbf{u}_i\}_{i\in \mathbb{D}}$ is a new orthonormal basis of \mathbb{R}^D . The Principal Component \mathfrak{u}_1 is chosen such that the variance of the data projected over \mathbf{u}_1 is maximum. \mathbf{u}_2 is chosen using $\text{Proj}_{\mathbf{u}^{\perp}}(\mathfrak{X})$.

Model

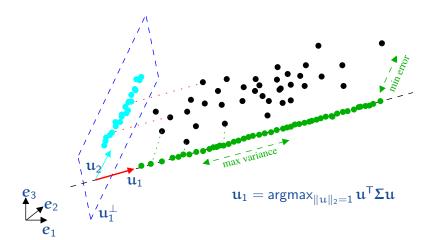
Given \mathcal{X} , the sample mean $(\overline{\mathbf{x}})$ and the variance of the data projected over \mathbf{u}_1 are

$$\overline{x} = \frac{1}{N} \sum_{i=1}^N x_i \quad \text{and} \quad \nu_{u_1} = \frac{1}{N} \sum_{i=1}^N (u_1^\mathsf{T} x_i - u_1^\mathsf{T} \overline{x})^2 = u_1^\mathsf{T} \Sigma u_1$$

where $\Sigma = \frac{1}{N} \sum_{i=1}^{N} (x_i - \overline{x})(x_i - \overline{x})^T$ is the data covariance matrix. Therefore

$$\mathbf{u}_1 = \underset{\mathbf{u}^\mathsf{T}\mathbf{u}=1}{\mathsf{argmax}} \, \mathbf{u}^\mathsf{T} \mathbf{\Sigma} \mathbf{u}$$

Intuition



Formalization

$$u_1 = \mathop{\mathsf{argmax}}_{u^T u = 1} u^T \mathbf{\Sigma} u \quad \Rightarrow \quad J(u) = u^T \mathbf{\Sigma} u + \lambda (1 - u^T u)$$

So that

$$\frac{\partial J(u)}{\partial u}|_{u=u_1}=0 \qquad \text{and} \qquad \frac{\partial J(u)}{\partial \lambda}|_{\lambda=\lambda_1}=0$$

Hence

$$\Sigma \mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \quad \Rightarrow \quad \mathbf{v}_{\mathbf{u}_1} = \mathbf{u}_1^\mathsf{T} \mathbf{\Sigma} \mathbf{u}_1 = \lambda_1$$

 $\Rightarrow (\mathfrak{u}_1,\lambda_1)$ is an eigenpair of the covariance matrix Σ

 \Rightarrow continuing with the decimation process, we obtain the set of Principal Components as the eigenpairs $\{(u_i, \lambda_i)\}_{i \in [\![D]\!]}$ of the covariance matrix Σ of data $\mathcal X$

$$\boldsymbol{\Lambda} = \left(\begin{array}{ccc} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_D \end{array} \right) = \left(\begin{array}{ccc} | & & | \\ \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_D \\ | & & | \end{array} \right)^\mathsf{T} \boldsymbol{\Sigma} \left(\begin{array}{ccc} | & & | \\ \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_D \\ | & & | \end{array} \right) = \boldsymbol{U}^\mathsf{T} \boldsymbol{\Sigma} \boldsymbol{U}$$

- * The variance $v_{\mathbf{u}_1}$ is expressed as a sum of squares $v_{\mathbf{u}_1} = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{u}_1^T(\mathbf{x}_i \overline{\mathbf{x}}))^2$
- \Rightarrow To maximize ν_{u_1} , terms $u_1^\mathsf{T}(x_i-\overline{x})$ should be collectively maximized
- \Rightarrow Since $(x_i \overline{x})$ is fixed, Pythagoras tells us it is equivalent to minimize the distance to the axis of projection (approximation error)
- ⇒ A Principal Component is a quadratic regression over the data

$$u_1 = \underset{\boldsymbol{u}^\top \boldsymbol{u} = \boldsymbol{1}}{\text{argmin}} \sum_{i=1}^N \| (\boldsymbol{x}_i - \overline{\boldsymbol{x}}) - [\boldsymbol{u}^\mathsf{T} (\boldsymbol{x}_i - \overline{\boldsymbol{x}})] \boldsymbol{u} \|_2^2 \ \Rightarrow \ \boldsymbol{\Sigma} u_1 = \lambda_1 u_1 \quad \text{ } \boldsymbol{\underline{\boldsymbol{v}}}$$

Maximize Projection Variance

⇔ Minimize Approximation Error



Physical interpretation

- * Consider a physical system \mathcal{X} with masses $m_i = 1$ at positions x_i
- * The inertia of the system w.r.t $a \in \Omega$ is $I_a(x) = \sum_{i=1}^N d^2(a, x_i)$
- * Huygens theorem tells us that if $g = \frac{1}{N} \sum_{i=1} x_i$ then

$$\mathrm{I}_{\alpha}(\mathfrak{X}) = d^2(\alpha,g) + \mathrm{I}_{g}(\mathfrak{X}) \qquad (\mathsf{Var}(\mathsf{X}) = \mathbb{E}[\mathsf{X}^2] - (\mathbb{E}\mathsf{X})^2)$$

* and if \mathbf{f} is a subspace of Ω going thru \mathbf{q} then

$$I_{\mathbf{J}\!\!f}(\mathfrak{X}) = \sum_{i=1}^N d^2(\mathbf{J}\!\!f, \mathbf{x}_i) \quad \text{where} \quad d(\mathbf{J}\!\!f, \mathbf{x}_i) = \|\mathbf{x}_i - \mathsf{Proj}_{\mathbf{J}\!\!f}(\mathbf{x}_i)\|$$

 \Rightarrow A Principal Component is a subspace of least inertia w.r.t \mathfrak{X}

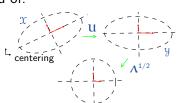
Structure of the latent space

The latent space with basis $\{u_i, \dots, u_D\}$ has the following properties:

- * By construction $\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_D$ and $\lambda\stackrel{\mathsf{def}}{=}\sum_{d=1}^D\lambda_d=\mathsf{Tr}(\Sigma)$
- * $\nu_{\mathbf{u}_d} = \lambda_d \Rightarrow \lambda$ represents the total variance \Rightarrow latent features are decorrelated $\mathbf{u}_d^\mathsf{T} \mathbf{u}_{d'} = 0$ (Λ is the diagonal latent covariance matrix)
- \star The basis $\{u_i, \cdots, u_D\}$ induces latent coordinates y_i for the data:

$$y_\mathfrak{i}(d) = \langle u_d, u_\mathfrak{i} - \overline{x} \rangle = u_d^\mathsf{T}(x_\mathfrak{i} - \overline{x}) \qquad \text{so that} \qquad y_\mathfrak{i} = U^\mathsf{T}(x_\mathfrak{i} - \overline{x})$$

- The transform is linear and composed of:
 - Centering on \bar{x}
 - Rotation using U
 - Scaling using
 ^{1/2}
 (whitening)

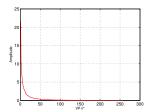


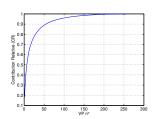
Structure of the model

- * The latent space preserves the variance (of the centered data)
- \Rightarrow the underlying data model is $X_i \sim f_{\chi} = \mathcal{N}(\overline{x}, \Sigma)$
- ⇒ PCA will not be relevant for non-Gaussian data (e.g clustered)

$$y_i = U^\mathsf{T}(x_i - \overline{x}) \qquad \text{so that} \qquad Uy_i = UU^\mathsf{T}(x_i - \overline{x}) = x_i - \overline{x}$$

 \Rightarrow at this stage, one purpose is to study the spectrum $\{\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_D\}$ of the data

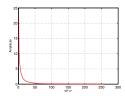




Decomposition via PCA

MNIST partial dataset: N = 7291 images 16×16 (8bits) $\Rightarrow D = 256$

























 $cr(\Delta_e)=44\%$

 $cr(\Delta_c)=48\%$

cr(∆,,)=51%

 $cr(\Delta_o)=54\%$ $cr(\Delta_q)=57\%$

Data Science: Principal Component Analysis

DS03 - 12

Approximation via PCA

Low-rank approximation from the Eckart and Young theorem:

If
$$\Sigma = U \Lambda U^T$$
 and for $K < D$ define $\Sigma_K \stackrel{\text{def}}{=} \sum_{d=1}^K \lambda_d u_d u_d^T$ then

$$\underset{\mathsf{rank}(S)=K}{\mathsf{argmin}} \| \boldsymbol{\Sigma} - \boldsymbol{S} \|_F^2 = \boldsymbol{\Sigma}_K \qquad \mathsf{and} \qquad \| \boldsymbol{\Sigma} - \boldsymbol{\Sigma}_K \|_F^2 = \sum_{d=K+1}^D \lambda_d$$

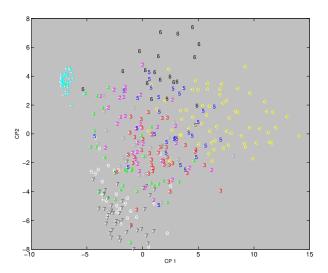
 $\Rightarrow \Sigma_{K}$ is the closest K-rank matrix to Σ

Truncation (of \mathbf{U} and $\boldsymbol{\Lambda}$)

$$\boldsymbol{\Sigma}_{K} = \left(\begin{array}{ccc} | & & | \\ \boldsymbol{u}_{1} & \cdots & \boldsymbol{u}_{K} \\ | & & | \end{array} \right) \left(\begin{array}{ccc} \lambda_{1} & & \boldsymbol{0} \\ & \ddots & \\ \boldsymbol{0} & & \lambda_{K} \end{array} \right) \left(\begin{array}{ccc} | & & | \\ \boldsymbol{u}_{1} & \cdots & \boldsymbol{u}_{K} \\ | & & | \end{array} \right)^{\mathsf{T}} = \boldsymbol{U}_{K} \boldsymbol{\Lambda}_{K} \boldsymbol{U}_{K}^{\mathsf{T}}$$

Visualization via PCA

 $ilde{m{\emptyset}}$ MNIST partial dataset: $m{\mathsf{K}} = 2 \Rightarrow ilde{m{\mathfrak{y}}}_{i} \in \mathbb{R}^{2}$



Geometry of PCA

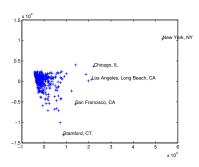
The quality of reconstruction can be measured by

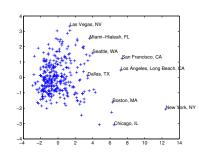
- * the relative contribution of each dimension to the variance $c_d=\frac{\lambda_d}{\sum_k \lambda_k}$
- ⇒ depends on the distribution of the spectrum
 - * the projection ratio of each data x_i over a latent factor $ho_d(x_i) = \frac{\langle u_d, x_i \rangle^2}{\|\mathbf{x}\|^2} = \cos^2(\angle(u_d, x_i))$
- \Rightarrow the closer $\rho_d(x_i)$ is to 1, the more x_i lies on u_d
- \Rightarrow The above can be grouped (summed) to evaluate wrt a subspace $\{u_1,u_2,\cdots\}$

Geometry of PCA

Every original data comes with its unit (scale), that we can estimate via σ_d^2 the sample variance along original dimension d. PCA is more effective is all scales are similar.

 \Rightarrow we create the scaling matrix $S = \text{diag}[\sigma_1^2, \cdots, \sigma_d^2]$ and we define the metric $d_S^2(x,y) = (x-y)^T S^{-1}(x-y) \Rightarrow$ in that metric space, the covariance matrix Σ_S is also rescaled (into the correlation matrix) and used as a base for PCA.

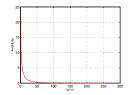




Approximation via PCA

 \bigcirc MNIST partial dataset: N = 7291 images 16 \times 16 (8bits) \Rightarrow D = 256

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Practical PCA

Given $\mathfrak{X} \in \Omega$

- \star Compute the sample mean $\overline{\mathbf{x}}$
- * Center the data $x_i \leftarrow (x_i \overline{x})$ and form centered data matrix X
- \star $\Sigma = \frac{1}{N}XX^{\mathsf{T}}$ and $\Sigma = U\Lambda U^{\mathsf{T}}$

← △ Exact transform so far

- ⋆ Select the number of components K
- \star Define \mathbf{U}_K , Λ_K and compute $\{\tilde{\mathbf{y}}_i\}_{i\in [\![N]\!]}$ and/or $\{\tilde{\mathbf{x}}_i\}_{i\in [\![N]\!]}$





Choice of K

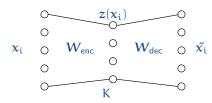
- 1. K = d, the target dimension $\Rightarrow \tilde{y}_i \in \mathbb{R}^d$
- 2. Require $Var(\mathcal{Y}) = \tau.Var(\mathcal{X}) \quad \Rightarrow \quad K \text{ such that } \frac{\sum_{d=1}^{K} \lambda_d}{\sum_{d=1}^{D} \lambda_d} \geqslant \tau$
- 3. Train K such that $\mathcal{L}(\mathcal{X}) \leqslant \varepsilon$ (e.g $\mathcal{L}(\mathcal{X}) = \sum_{i} \|x_{i} \tilde{x}_{i}\|^{2}$)

PCA and linear AutoEncoders

A linear AE is a simple structure

 \star $W_{\rm enc}$ and $W_{\rm dec}$: encoder and decoder weights

$$z(x_{\mathfrak{i}}) = W_{\mathsf{enc}} x_{\mathfrak{i}} \quad \ ilde{x}_{\mathfrak{i}} = W_{\mathsf{dec}} z(x_{\mathfrak{i}})$$



We optimize the weight matrices

$$\theta^* = \operatorname*{argmin}_{W_1,W_2} \sum_{i=1}^N \frac{1}{2} \sum_{d=1}^D (x_i[d] - \tilde{x}_i[d])^2 = \operatorname*{argmin}_{\operatorname{rank}(W) = K} \|X - WZ\|_F^2$$

Using again the Eckart and Young theorem with $X = U \Psi V^T$ then the solution is $W_{\text{dec}} \mathbf{Z} = \mathbf{U}_{\mathsf{K}} \mathbf{\Psi}_{\mathsf{K}} \mathbf{V}_{\mathsf{K}}^{\mathsf{T}}$.

Setting
$$oldsymbol{W}_{\mathsf{dec}} = oldsymbol{\mathsf{U}}_{\mathsf{K}} oldsymbol{\mathsf{\Psi}}_{\mathsf{K}}$$
 , then clearly $oldsymbol{W}_{\mathsf{enc}} = oldsymbol{\mathsf{\Psi}}_{\mathsf{K}}^{-1} oldsymbol{\mathsf{U}}_{\mathsf{K}}^{\mathsf{T}}$

 $W_{enc}X = Z = V^T = V^T(X^TX)^{-1}(X^TX) = V^T(V\Psi\Psi V^T)^{-1}(V\Psi U^T)X = \Psi_{\nu}^{-1}U_{\nu}^TX$

Note: $W_{\text{dec}} = W_{\text{dec}} = \text{Id}_{D}$ cannot be a solution if K < D and W_{enc} is not the inverse of W_{dec}

PCA and linear AutoEncoders

A linear AE is a simple structure

 \star $W_{\rm enc}$ and $W_{\rm dec}$: encoder and decoder weights

$$z(x_{\mathfrak{i}}) = W_{\text{enc}} x_{\mathfrak{i}} \quad \ \tilde{x}_{\mathfrak{i}} = W_{\text{dec}} z(x_{\mathfrak{i}})$$

We optimize the weight matrices

$$X = U\Psi V^\mathsf{T} \text{ and } W_\mathsf{dec} = U\Psi \text{ and } W_\mathsf{enc} = \Psi^{-1}U^\mathsf{T} \Rightarrow \tilde{x}_\mathfrak{i} = U_\mathsf{K} U_\mathsf{K}^\mathsf{T} x_\mathfrak{i}$$

Relation to PCA (centered data)

- * PCA: $\Sigma = \frac{1}{N}XX^{\mathsf{T}} = \mathbf{U}\Lambda\mathbf{U}^{\mathsf{T}}$ so that $\tilde{x}_i = \mathbf{U}_{\mathsf{K}}\mathbf{U}_{\mathsf{K}}^{\mathsf{T}}x_i$
- * AE: $X = U\Psi V^T \Rightarrow \Sigma = \frac{1}{N}XX^T = \frac{1}{N}U\Psi^2U^T$ and $\tilde{x}_i = U_KU_K^Tx_i$
- $\Rightarrow \Lambda = \frac{1}{N} \Psi^2 = (\frac{1}{\sqrt{N}} \Psi) (\frac{1}{\sqrt{N}} \Psi)$ so that $PCA(X) \leftrightarrow AE(\frac{1}{\sqrt{N}} X)$
 - ⇒ A linear AE performs a PCA if the data is centered and scaled

 $z(x_i)$

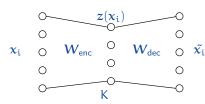
K

PCA and linear AutoEncoders

A linear AE is a simple structure

 \star W_{enc} and W_{dec} : encoder and decoder weights

$$z(\mathbf{x}_{i}) = \mathbf{W}_{\mathsf{enc}} \mathbf{x}_{i} \quad \ \tilde{\mathbf{x}}_{i} = \mathbf{W}_{\mathsf{dec}} z(\mathbf{x}_{i})$$



We optimize the weight matrices

⇒ A linear AE performs a PCA if the data is centered and scaled

- * If adding hidden layers, the latent space becomes non-linear
- ⇒ non-linear AutoEncoders
 - Changing the loss function (ELBO) enables sparsity in the latent space
- ⇒ Variational AutoEncoders (VAE)

 $\underline{ ext{Note}}: W_{ ext{dec}} = W_{ ext{dec}} = \mathsf{Id}_D \ \ ext{cannot} \ \ ext{be a solution if } \ \mathsf{K} < D \ \ ext{and} \ \ W_{ ext{enc}} \ \ ext{is not} \ \ ext{the inverse of } W_{ ext{dec}}$

Alternative formulations

- * Probabilistic PCA reformulates PCA with an explicit latent distribution $\mathbb{P}(z) = \mathcal{N}(0, \mathsf{Id}_{\mathsf{K}})$ and the conditional model is $\mathbb{P}(x|z) = \mathcal{N}(Wz + \mu + \sigma^2 \mathrm{Id}_D)$ so that
 - the model accomodates "measurement noise" (with variance σ^2)
 - the model can run in a generative mode
 - parameters can be estimated via Maximum Likelihood
 - an EM algorithm (see later) can be derived for saving computations
 - Bayesian PCA reverts the conditional so as to find K by training
- * Kernel PCA embarks a nonlinear mapping $\phi(x_i)$ via a kernel function $k(x_i, x_i) = \phi(x_i)^T \phi(x_i)$ to perform PCA within a more favorable space
- * Local PCA perform PCA on data neighborhoods to consider the local intrinsic dimensionality only
- \triangle The limitation of PCA is often the decomposition of Σ in $O(D^3)$

Summary

- ⋆ PCA is part of the linear latent models
- * PCA applies on centered data and uses variance as a criteral for decomposition
- PCA is an exact complete decomposition into decorrelated components
- ⋆ PCA assumes a Normal distribution of the data
- * PCA can be equivalently formulated as a regression
- * PCA offers a sound decimation strategy based on a low rank approximation
- * PCA can be used for denoising via a Gaussian noise model
- ⋆ PCA is equivalent to a linear AutoEncoder
- * PCA may be given a stochastic formulation
- * PCA may be generalized to the non-linear case via kernels

Example questions [mostly require formal – mathematical – answers]

- ★ Explain how PCA uses variance as a criterion
- * Show that variance maximization is equivalent to error minimization
- Show how PCA uses the Eckart-Young theorem
- ★ Given some data, how do you apply PCA?
- ★ What information does it provide you with?
- * How do you reconstruct data with K < D components?
- * How do you select the components to keep?
- * Can you apply PCA on any data?
- ⋆ Is it relevant to apply PCA on any data?
- * How can I apply PCA over clustered data?
- * Show that PCA is equivalent to a linear AE

Note: Make sure you can explain in detail what is: linear transform, orthogonal matrix, coordinate, rank, mean, variance, projection, eigen decomposition, trace, Frobenius norm, Lagrange Multiplier

References I

- [1] Christopher M. Bishop. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag, Berlin, Heidelberg, 2006. (available online).
- [2] Avrim Blum, John Hopcroft, and Ravindran Kannan. Foundations of Data Science. Cambridge University Press, 2020. (available online).
- [3] Richard O. Duda, Peter E. Hart, and David G. Stork. *Pattern Classification*. Wiley, New York, 2 edition, 2001.