Principal Component Analysis

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Dimensionality reduction

- it takes $n \times d$ memory to store data $\{x_i\}_{i=1}^n$ with $x_i \in \mathbb{R}^d$
- but many real data have repeated patterns
- can we represent each image compactly, but still preserve most of information?



Principal components

- patterns that capture the distinct features of the samples is called principal component (to be formally defined later)
- we can represent each sample as a weighted linear combination of the principal components, and just store the weights (As opposed to all pixel values)

Principal components:



average face



real face

10 principal components give a pretty good reconstruction of the face

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Principal Component Analysis (PCA) Representing data compactly



PCA formulation 1: direction of greatest variance

• given dataset $\{x_i\}_{i=1}^n$

we will assume that the data is centered at the origin, such that $\frac{1}{n}\sum_{i=1}^{n}x_i=0$

- otherwise, everything we do can be applied to the re-centered version of the data, i.e. $\{x_i \bar{x}\}_{i=1}^n$, with $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$
- we want to find the **direction** $u \in \mathbb{R}^d$ of greatest variance, and as we care about the direction, we will assume $||u||_2 = 1$
- we will justify why we care about greatest variance direction, later

PCA formulation 1: direction of greatest variance

- for a direction $u \in \mathbb{R}^d$ direction
 - $\begin{bmatrix} p_i = (u^T x_i) \\ u \in \mathbb{R}^d \end{bmatrix}$ is the projection of x_i onto u, i.e. the point on the direction of u that is closest to x_i
 - the length of the projection is $||p_i||_2 = u^T x_i$ mean of $\{p_i\}_{i=1}^n$ is zero, as $\sum_{i=1}^n p_i = \sum_{i=1}^n (u^T x_i)u = u^T \left(\sum_{i=1}^n x_i\right)u = 0$ • similarly, mean of $\{||p_i||_2\}_{i=1}^n$ is also zero • so, variance is $\frac{1}{n} \sum_{i=1}^n ||p_i||_2^2$ • variance maximizing direction is

- such variance maximizing directions are called the **principal components**
- 7 this is 1-dimensional PCA



The optimization problem in a matrix form

$$\underset{u \in \mathbb{R}^{\vee}}{\operatorname{arg\,max}} \frac{1}{n} \sum_{i=1}^{n} (u^{T} x_{i})^{2} = \underset{\tau=1}{\overset{n}{\underset{\tau=1}{\overset{n}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}{\underset{\tau=1}{\underset{\tau=1}{\overset{\tau=1}{\underset{\tau=1}$$

 \checkmark

• recall the data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$, and the optimization is

$$\arg \max_{u: \|u\|_2^2 = 1} u^T \mathbf{X}^T \mathbf{X} u$$

 assuming the data has zero mean, the covariance matrix of the data is defined as

$$\mathbf{C} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T = \frac{1}{n} \mathbf{X}^T \mathbf{X}$$

• which gives

$$\underset{u:\|u\|_2^2=1}{\operatorname{arg max}} u^T \mathbf{C} u$$

Given data points
$$\{X_i\}_{i=1}^n$$

Principal component UGR^d , $\|UU\|_{2}^{2}=1$ is the direction of maximum variance.
 $P_i = \operatorname{ProJu}(2\pi_i)$
 $= (UTx_i) \cdot U$
 $R R^d$
 $\|P_i\|_{2} = UTx_i$
 $\|P_i\|$

Given dataset EX: 31=1 Principal Component u GR, 114112=1 XC2] Maximum Variance. Pi = Proju(X:) $\leq (\chi_{\tau}^{\tau} u) \cdot U$ ٢ LIRd $\|P_{i}\|_{2} = \chi_{i}^{T} u$ $\| P_{1} \|_{2} = X_{1}^{T} u$ $\frac{1}{n}\sum_{i=1}^{n}(u^{T}x_{i})$ Maximize $1|u|_{2} = 1$ S£ n Zurxiru т л ц U IR IR R dxd Covariance Matrix

$$\begin{array}{c} \max_{u} & \operatorname{uT}Cu & (a) \\ u \\ \mathrm{S.t.} & \operatorname{II}\operatorname{ull}_{2}^{2}=1. \\ & \operatorname{max} & \operatorname{uT}Cu \geq 0 \quad (b) \\ \mathrm{S.t.} & \overline{\operatorname{II}\operatorname{ull}_{2}^{2}} \leq 1 \\ \mathrm{Ckim:optimal} & \operatorname{ut}^{*} of(e) \text{ is the same as optimal} & \operatorname{ut}^{*} of(b) \\ & \operatorname{uT}Cu = \frac{1}{h} \sum_{\tau^{2}1}^{h} (\operatorname{uT} x_{\tau})^{2} \geq 0 \\ & \operatorname{max} & \operatorname{uT}Cu - \mathcal{H}\operatorname{II}\operatorname{ull}_{2}^{2} & (c) \leq \operatorname{unconstrained} \\ & \operatorname{ti}_{\lambda}(u) \\ \mathrm{Claim:} & \frac{2}{\lambda} GR^{\dagger} \quad \mathrm{s.t.} \quad u^{*} of(e) \quad \mathrm{is equal to} \quad u_{0}^{*}(b) \\ & \operatorname{strategy}: \operatorname{Identify} & \operatorname{u}^{*}(x) \quad \mathrm{of}(c). \\ & \operatorname{Lcheck} \quad \mathrm{which} \quad \mathcal{H} \quad \mathrm{fives} \quad \left\| \operatorname{u}^{*} \mathrm{ch} \right\|_{2}^{2} = 1 \end{array}$$

Gaal:
$$U^{*}(\lambda)$$
 of max $u^{T}Cu - A \|u\|_{2}^{2}$
 u
 \sqrt{u} $F_{A}(u) = 2 \cdot C \cdot u - 2\lambda \cdot u = 0$
 $\int \frac{G \cdot u = \lambda \cdot u}{\mu^{R} u}$
 $\frac{P}{R}$
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$$maximize_{u} u^{T} C u \qquad (a)$$

subject to $||u||_{2}^{2} = 1$

 we first claim that this optimization problem has the same optimal solution as the following inequality constrained problem

$$\begin{array}{l} \text{maximize}_{u} \ u^{T} \mathbf{C} u \\ \text{subject to} \quad \|u\|_{2}^{2} \leq 1 \end{array} \tag{b}$$

- the reason is that, because $u^T \mathbf{C} u \ge 0$ for all $u \in \mathbb{R}^d$ (which we will prove in a bit), the optimal solution of (b) has to have $||u||_2^2 = 1$
- if it did not have $||u||_2^2 = 1$, say $||u||_2^2 = 0.9$, then we can just multiply this u by a constant factor of $\sqrt{10/9}$ and increase the objective by a factor of 10/9 while still satisfying the constraints

- we are left to prove the following claim
- claim: $u^T \mathbf{C} u \ge 0$ where $\mathbf{C} = \frac{1}{n} \sum_{i=1}^n x_i x_i^T$
- proof:

$$u^{T}\mathbf{C}u = \frac{1}{n} \sum_{i=1}^{n} u^{T}(x_{i}x_{i}^{T})u$$
$$= \frac{1}{n} \sum_{i=1}^{n} (u^{T}x_{i})^{2} \ge 0$$

for any $u \in \mathbb{R}^d$

$$\begin{array}{ll} \text{maximize}_{u} \ u^{T} \mathbf{C} u & (b) \\ \text{subject to} & \|u\|_{2}^{2} \leq 1 \end{array}$$

- we are maximizing the variance, while keeping *u* small
- this can be reformulated as an unconstrained problem, with Lagrangian encoding, to move the constraint into the objective

$$\begin{array}{ll} \text{maximize}_{u} & u^{T}\mathbf{C}u - \lambda \|u\|_{2}^{2} \\ & \overbrace{F_{\lambda}(u)} \end{array} \tag{c}$$

- this encourages small *u* as we want, and we can make this connection precise: there exists a (unknown) choice of λ such that the optimal solution of (*c*) is the same as the optimal solution of (*b*)
- further, for this choice of λ , the optimal u has $||u||_2 = 1$

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• our strategy is to analytically describe $u(\lambda)$ that is optimal solution of (c), and find λ such that $||u(\lambda)||_2^2 = 1$

• to find such λ and the corresponding u, we solve the unconstrained optimization, by setting the gradient to zero

 $\nabla F_{\lambda}(u) = 2\mathbf{C}u - 2\lambda u = 0$

• the candidate solution satisfies: $Cu = \lambda u$, i.e. an eigenvector of C

maximize_{*u*}
$$u^T \mathbf{C} u - \lambda \| u \|_2^2$$

 $F_{\lambda}(u)$

- let $(\lambda^{(1)}, u^{(1)})$ denote the largest eigenvalue and corresponding eigenvector of **C**, with norm one, i.e. $||u^{(1)}||_2^2 = 1$
- one property of the largest eigenvalue is that
 - $u^T \mathbf{C} u \leq \lambda^{(1)} ||u||_2^2$ and the maximum is achieved with $u = u^{(1)}$
- we claim that for

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- $\lambda > \lambda^{(1)}$, the optimal solution is u = 0 with objective value zero
- $\lambda < \lambda^{(1)}$, one optimal solution is $u = cu^{(1)}$ with $c = \infty$, with objective value infinity
- $\lambda = \lambda^{(1)}$, one optimal solution is $u = u^{(1)}$, with objective value zero

The solution maximize_{*u*} $u^T C u - \lambda ||u||_2^2$

• if
$$\lambda < \lambda^{(1)}$$
 then one can take $u = cu^{(1)}$, which gives $F_{\lambda}(u) = \lambda^{(1)}c^2 - \lambda c^2 = (\lambda^{(1)} - \lambda)c^2$

and we can now take c as large as we want to make the objective unbounded (and hence optimal u has norm unbounded)

>0

• if $\lambda > \lambda^{(1)}$ then one can show that the optimal u = 0, as for any u with norm c,

$$F_{\lambda}(u) \leq \lambda^{(1)}c^2 - \lambda c^2 = (\underbrace{\lambda^{(1)} - \lambda}_{< o})c^2$$

and taking c = 0 maximizes the objective

- hence, only $\lambda = \lambda^{(1)}$ gives optimal u with unit norm, i.e. $||u||_2^2 = 1$ and the optimal solution is $u = u^{(1)}$
- finally, we found the optimal solution of maximize_u $u^T C u$ **subject to** $||u||_2^2 = 1$

which is the eigenvector $u^{(1)}$ corresponding to the top eigenvalue $\lambda^{(1)}$ of ${f C}$

The principal component analysis

- so far we considered finding ONE principal component $u \in \mathbb{R}^d$
- it is the eigenvector corresponding to the maximum eigenvalue of the covariance matrix

$$\mathbf{C} = \frac{1}{n} \mathbf{X}^T \mathbf{X} \in \mathbb{R}^{d \times d}$$

- We can use Singular Value Decomposition (SVD) to find such eigen vector
- note that is the data is not centered at the origin, we should recenter the data before applying SVD
- in general we define and use multiple principal components
- if we need r principal components, we take r eigenvectors corresponding to the largest r eigenvalues of ${\bf C}$

$$av_{f} M \tilde{l}_{n} \sum_{i=1}^{n} ||X_{i} - P_{i}||_{2}^{2}$$

$$= \sum_{i=1}^{n} \frac{||X_{i} - u(u^{T} x_{i})||_{2}^{2}}{|X_{i}|^{2} - 2X_{i}^{T} u u^{T} X_{i}}$$

$$= \sum_{i=1}^{n} \frac{||X_{i}||^{2} - 2X_{i}^{T} u u^{T} X_{i}}{|X_{i}|^{2} + X_{i}^{T} u u^{T} u^{T} X_{i}}$$

$$= av_{f} m \tilde{l}_{n} \sum_{i=1}^{n} - X_{i}^{T} u u^{T} X_{i}$$

$$= av_{f} m \tilde{l}_{n} \sum_{i=1}^{n} - X_{i}^{T} u u^{T} X_{i}$$

$$= av_{f} m ax \sum_{i=1}^{n} u^{T} X_{i} X_{i}^{T} u$$

$$\int_{U} P_{i} = U(u^{T}x_{i})$$

$$\int_{U} S_{i} \in ||U^{U}|_{2}^{2} = 1$$

$$\int_{U} U^{T}u$$

Alternate view of PCA: minimizing reconstruction error $\chi \in \mathbb{R}^{n \times d}$, $\mathcal{U} = [u_1 - u_r] \in \mathbb{R}^{n \times d}$ we would like to have a set of orthogonal directions $u_1, \ldots, u_r \in \mathbb{R}^d$, with $||u_i||_2 = 1$ for all j, such that each data can be represented as linear combination of those direction vectors, i.e.

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0

$$x_i \approx p_i = a_i[1]u_1 + \dots + a_i[r]u_r$$

- those directions that minimize the average reconstruction error for a dataset is called the **principal components**
- given a choice of u_1, \ldots, u_r , the best representation p_i of x_i is the projection of the point onto the subspace spanned by u_i 's, i.e.

$$p_i = \sum_{j=1}^r (u_j^T x_i) u_j$$

the goal is to find u_1, \ldots, u_r to minimize the reconstruction error $\sum ||x_i - p_i||^2$



Variance maximization vs. reconstruction error minimization

• both give the same principal components as optimal solution



Alternate view of PCA: minimizing reconstruction error

minimize
$$\frac{1}{n} \sum_{i=1}^{n} ||x_i - p_i||^2$$

$$\mathbf{p}_i = \sum_{j=1}^r (u_j^T x_i) u_j = \mathbf{U} \mathbf{U}^T x_i$$

where
$$\mathbf{U} = [u_1 \ u_2 \ \cdots \ u_r] \in \mathbb{R}^{d \times r}$$

minimize $\frac{1}{n} \sum_{i=1}^n ||x_i - \mathbf{U}\mathbf{U}^T x_i||^2$
subject to $\mathbf{U}^T \mathbf{U} = \mathbf{I}_{r \times r}$

 we will not formally prove it, but the optimal solution of this problem is the *r* principal components

Principal Component Analysis

- input: data points $\{x_i\}_{i=1}^n$, target dimension $r \ll d$
- output: *r*-dimensional subspace
- algorithm:

• compute mean
$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

• compute covariance matrix

$$\mathbf{C} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T$$

• let (u_1, \ldots, u_r) be the set of (normalized) eigenvectors with corresponding to the largest r eigenvalues of ${\bf C}$

• return
$$\mathbf{U} = \begin{bmatrix} u_1 & u_2 & \cdots & u_r \end{bmatrix}$$

• further the data points can be represented compactly via $a_i = \mathbf{U}^T (x_i - \bar{x}) \in \mathbb{R}^r$

reconstruction

- given principal component $\mathbf{U} \in \mathbb{R}^{d \times r}$ and $\bar{x} \in \mathbb{R}^{d}$, each data point is represented in a lower dimension as $a_i = \mathbf{U}^T (x_i - \bar{x})$
- then the reconstruction of the data point is

$$p_i = \bar{x} + \sum_{j=1}^{\infty} a_i[j]u_j = \bar{x} + \mathbf{U}a_i$$

the reconstruction error is

$$\begin{aligned} \|x_i - p_i\|_2^2 &= \|(x_i - \bar{x}) - (p_i - \bar{x})\|_2^2 \\ &= \|(x_i - \bar{x}) - \mathbf{U}a_i\|_2^2 \end{aligned}$$

Matrix completion for recommendation systems



- users provide ratings on a few movies, and we want to predict the missing entries in this ratings matrix, so that we can make recommendations
- without any assumptions, the missing entries can be anything, and no prediction is possible

 $= \mathbf{U}a_i$

- however, the ratings are not arbitrary, but people with similar tastes rate similarly
- such structure can be modeled using low dimensional representation of the data as follows
- we will find a set of principal component vectors $\mathbf{U} = \begin{bmatrix} u_1 & u_2 & \cdots & u_r \end{bmatrix} \in \mathbb{R}^{d \times r}$
- such that that ratings $x_i \in \mathbb{R}^d$ of user *i*, can be represented as $x_i = a_i[1]u_1 + \cdots + a_i[r]u_r$

for some lower-dimensional $a_i \in \mathbb{R}^r$ for i-th user and some $r \ll d$

- for example, $u_1 \in \mathbb{R}^d$ means how horror movie fans like each of the d movies,
- and $a_i[1]$ means how much user i is fan of horror movies

- let $\mathbf{X} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \in \mathbb{R}^{d \times n}$ be the ratings matrix, and assume it is fully observed, i.e. we know all the entries
- then we want to find $\mathbf{U} \in \mathbb{R}^{d \times r}$ and $\mathbf{A} = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix} \in \mathbb{R}^{r \times n}$ that approximates \mathbf{X}



which can be solved using PCA (i.e. SVD)

- in practice, we only observe ${f X}$ partially
- let $S_{\text{train}} = \{(i_{\ell}, j_{\ell})\}_{\ell=1}^{N}$ denote N observed ratings for user i_{ℓ} on movie j_{ℓ}



- let v_i^T denote the *j*-th row of **U** and a_i denote *i*-th column of **A**
- then user *i*'s rating on movie *j*, i.e. \mathbf{X}_{ji} is approximated by $v_j^T a_i$, which is the inner product of v_j (a column vector) and a column vector a_i
- we can also write it as $\langle v_j, a_i \rangle = v_j^T a_i$

- a natural approach to fit v_j 's and $a'_i s$ to given training data is to solve $\text{minimize}_{\mathbf{U},\mathbf{A}} \sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} v_j^T a_i)^2$
- this can be solved, for example via gradient descent or alternating minimization
- this can be quite accurate, with small number of samples

sampled matrix



low-rank matrix X

Gradient descent output UA



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



0.25% sampled

sampled matrix



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



low-rank matrix X



Gradient descent output UA



0.50% sampled

sampled matrix



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



low-rank matrix X



Gradient descent output UA



0.75% sampled

sampled matrix



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



low-rank matrix X



Gradient descent output UA



1.00% sampled

sampled matrix



low-rank matrix X

squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



Gradient descent output UA



1.25% sampled

sampled matrix



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



low-rank matrix X



Gradient descent output UA



1.50% sampled

sampled matrix



squared error $(\mathbf{X}_{ji} - (\mathbf{UA})_{ji})^2$



low-rank matrix X

Gradient descent output UA



1.75% sampled

minimize_{U,A}
$$\sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

• Gradient descent on $\{v_j\}_{j=1}^d$ and $\{a_i\}_{i=1}^n$ can be implemented via

$$v_j^{(t)} \leftarrow v_j^{(t-1)} - 2\eta \sum_{i \in S_j} ((v_j^{(t-1)})^T a_i^{(t-1)} - \mathbf{X}_{ji}) a_i^{(t-1)}$$

for all $j \in \{1, ..., d\}$, where S_j is the set of users who rated movie j and

$$a_i^{(t)} \leftarrow a_i^{(t-1)} - 2\eta \sum_{j \in S_i} ((v_j^{(t-1)})^T a_i^{(t-1)} - \mathbf{X}_{ji}) v_j^{(t-1)}$$

for all $i \in \{1, ..., n\}$, where S_i is the set of movies that were rated by user i

minimize_{U,A}
$$\sum_{(i,j)\in S_{\text{train}}} (\mathbf{X}_{ji} - v_j^T a_i)^2$$

- alternating minimization
 - repeat

- fix v_i 's and find optimal a'_i s
 - for each *i*, set the gradient to zero: $2\sum_{j\in S_i} ((v_j^{(t-1)})^T a_i - \mathbf{X}_{ji}) v_j^{(t-1)} = 0$, which gives

$$a_i \left(\sum_{j \in S_i} v_j v_j^T \right) = \sum_{\substack{j \in S_i \\ j \in S_i}} \mathbf{X_{ij}} v_j$$
$$a_i = \left(\sum_{j \in S_i} v_j v_j^T \right)^{-1} \sum_{j \in S_i} \mathbf{X_{ij}} v_j$$

• fix $a'_i s$ and find optimal v_j 's (similarly)