Multivariate Statistical Methods for Big Data Analysis and Process Improvement

Lecture 4: Calculating Loadings

Dr. Brandon Corbett

Course notes for ChE 765/SEP 767, McMaster University

But how do we calculate $\mathbf{p}_1$?!

Overview: how is a PCA model calculated?

We will look at 3 ways today:

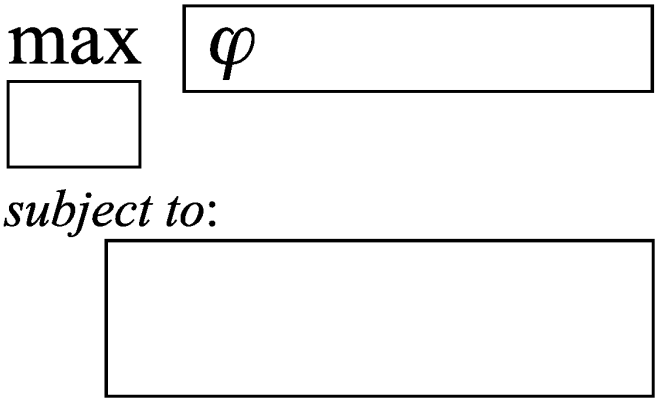
- Eigenvalue decomposition
- Singular value decomposition
- Non-linear iterative partial least-squares (NIPALS) algorithm
  - Used by most software packages

Why look at all the algorithms?

Each method highlights interesting properties of PCA

Optimization recap

Optimization problems are written in standard form:



PCA: optimization point of view

$$\max_{\square} \; \varphi$$

subject to:

$$\square$$

For PCA:

- What is a reasonable objective function?
- What are we searching for?
- Any constraints?

PCA: optimization derivation

Will be completed on the board. Brace yourselves for some math ...

- First component derivation
- Second component derivation

So what have we learnt?

What you have to know...

I won't test on the proof...

- PCA can be formulated as a **convex** optimization problem
  - Maximize variance captured
  - By changing loading vector
  - Subject to constraints (orthogonal to previous components and unit length)
- The solution to this problem results in an eigenvector/eigenvalue problem
- **KEY:** Loading vectors, $\mathbf{p}_1$ are the eigenvectors of the $\mathbf{X}^T\mathbf{X}$ matrix (covariance matrix)
  - $\left(\mathbf{X}^T\mathbf{X} - \lambda_a \mathbf{I}_k\right)\mathbf{p}_a = \mathbf{0}$
- Once we know $\mathbf{p}_a$ we can calculate $\mathbf{t_a}$
  - $\mathbf{t}_a = \mathbf{X}\mathbf{p}_a$

Nice but not mandatory to know: $\mathbf{t}_a^T\mathbf{t}_a = \lambda_a$

PCA: optimization derivation

- PCA is the eigendecomposition of $\mathbf{X}'\mathbf{X}$
- Note that $\mathbf{X}'\mathbf{X}$ is a real, symmetric matrix
- Eigendecomposition of a real, symmetric matrix:
  - can always be calculated
  - the eigenvectors are linearly independent (orthogonal)
    - $p_i \perp p_j$ for $i \neq j$
  - the eigenvalues are all real and nonnegative
  - which is good, because we showed that eigenvalue $\lambda_a = \mathcal{V}(\mathbf{t}_a) >= 0$
  - we forced $\lambda_1 > \lambda_2 > \ldots > \lambda_A$
  - sum of all eigenvalues $= \sum_{a=K}^{a} \lambda_a = \text{trace}(\mathbf{X}'\mathbf{X})$
  - for a centered $\mathbf{X}$ matrix, $\text{trace}(\mathbf{X}'\mathbf{X}) = \text{ssq}(\mathbf{X})$
  - that's the denominator used to calculate $R^2 = 1 - \frac{\text{Var}(\mathbf{E}_a)}{\text{Var}(\mathbf{X})}$

Eigenvalue summary

For long and thin matrices ($N > K$), compute the PCA model:

- loadings, p_a, are the eigenvectors of $\mathbf{X}'\mathbf{X}$ (a $K \times K$ matrix)
- once you have the eigenvectors, then $\mathbf{t}_a = \mathbf{X}\mathbf{p}_a$
- then calculate the predicted $\widehat{\mathbf{X}}_A = \mathbf{t}_1\mathbf{p}_1' + \mathbf{t}_2\mathbf{p}_2' + \ldots + \mathbf{t}_A\mathbf{p}_A'$
- residuals $= \mathbf{E}_A = \mathbf{X} - \widehat{\mathbf{X}}_A$
- eigenvalues are the variances of the scores, s_a^2
- sum of all eigenvalues $= \text{trace}(\mathbf{X}'\mathbf{X}) = \text{Var}(\mathbf{X})$
- finally, calculate $R^2 = 1 - \dfrac{\text{Var}(\mathbf{E}_A)}{\text{Var}(\mathbf{X})}$

Eigenvalue summary

Alternatively for short and wide matrices where $N < K$:

- scaled version of $\mathbf{t}_a$ = eigenvectors of $\mathbf{X}\mathbf{X}'$ (an $N \times N$ matrix)
- scaled loadings = $\mathbf{p}_a = \mathbf{X}\mathbf{t}_a$
- rescale loadings: $\mathbf{p}_a = \frac{\mathbf{p}_a}{\|\mathbf{p}_a\|}$
- recalculate scores again: $\mathbf{t}_a = \mathbf{X}\mathbf{p}_a$ (or just using the scaling factors above)

Singular Value Decomposition (SVD)

- $\mathbf{X} = \mathbf{U\Sigma V}' = \mathbf{TP}'$
- scores, $\mathbf{T} = \mathbf{U\Sigma}$ and the loadings, $\mathbf{P} = \mathbf{V}$

Disadvantages of Eigendecomposition and SVD

These two approaches suffer the same drawbacks:

- cannot handle missing data
- both methods calculate all components at once, even though we only require $A \ll K$

Further disadvantages of the eigendecomposition for *large* matrices:

- calculating $\mathbf{X}'\mathbf{X}$ can be difficult on large arrays
- also prone to numerical overflow for very large datasets
- we need to keep $\mathbf{X}$ available anyway to calculate the scores
- negates the intended benefit of the eigendecomposition

Any advantages?

- They teach us a lot about what PCA is doing
- All the properties of PCA can be derived from these decompositions
- Are slightly more accurate since calculate error is spread over all components*

* NIPALS algorithm error increases as we add more components.

NIPALS algorithm

- NIPALS: Non-linear *iterative* partial *least squares* algorithm
- NIPALS: Non-linear iterative projections using alternating least squares
- Why study it?
  - insight into what the loadings and scores mean
  - another look at orthogonality between components
  - handles missing data
  - used by all major software packages

Review of linear (least squares) regression

Terminology

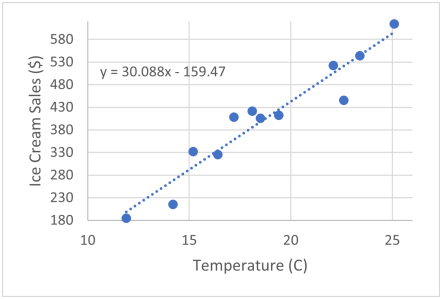
- x variable - independent
- y variable - dependent
- **Key phrase:** "Regress **y** onto **x**"

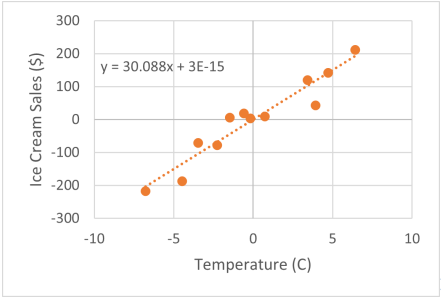
Equations

- $\hat{\mathbf{y}} = m\mathbf{x} + b$
- For mean centered data, $b = 0$!
- Reminder... what does "hat" on **y** mean?
- Formula for slope (derived later in course, but memorize now!):

$$m = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y}$$

Temp C	Ice cream sales ($)
14.2	215
16.4	325
11.9	185
15.2	332
18.5	406
22.1	522
19.4	412
25.1	614
23.4	544
18.1	421
22.6	445
17.2	408





NIPALS algorithm

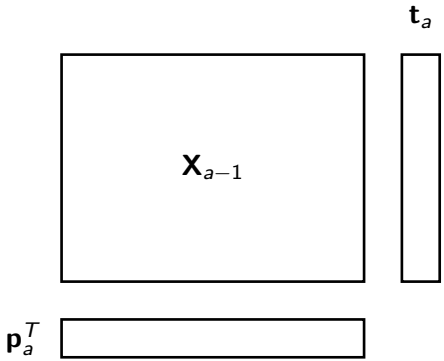
- Start with $\mathbf{X}$: preprocessed matrix of raw data
- More correctly, call it $\mathbf{X}_{a=0}$ or just $\mathbf{X}_0$
- to indicate that no components have been calculated yet

- We will break the algorithm into steps.

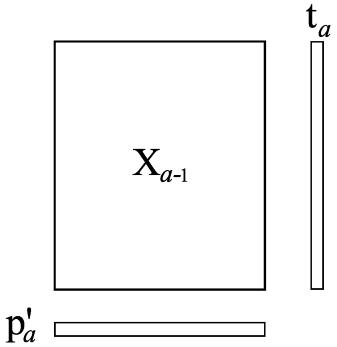
For $a = 1, 2, \ldots A$:

1. Select an arbitrary initial column for $\mathbf{t}_a$
2. In a while-loop, until convergence:
   - 2.1 Regress columns from $\mathbf{X}_{a-1}$ onto $\mathbf{t}_a$
   - 2.2 Normalize the loadings
   - 2.3 Regress rows from $\mathbf{X}_{a-1}$ onto $\mathbf{p}'_a$
3. Deflate component from $\mathbf{X}_{a-1}$ to calculate $\mathbf{X}_a$

End


$\mathbf{t}_a$
$\mathbf{X}_{a-1}$
$\mathbf{p}_a^T$

NIPALS algorithm



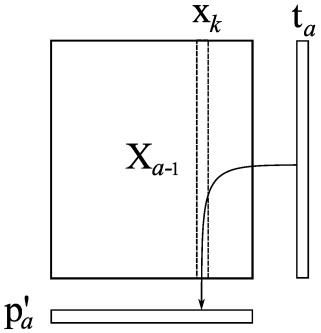
Step 1 Select an arbitrary initial column for $\mathbf{t}_a$

- Any column from $\mathbf{X}_0$
- A column of random numbers will also work
- Actually anything except a column of zeros works

NIPALS algorithm

Step 2.1 Regress every column from $\mathbf{X}_{a-1}$ (called $\mathbf{x}_k$) onto $\mathbf{t}_a$

- regress $\mathbf{x}_k$ onto $\mathbf{t}_a$ (terminology: "*regress a* $\mathbf{y}$ *onto an* $\mathbf{x}$")
- store regression coefficient as entry in $p_{k,a}$



- Recall LS for centered data: $\hat{\mathbf{y}} = \beta\mathbf{x}$, and $\widehat{\beta} = \dfrac{\mathbf{x}'\mathbf{y}}{\mathbf{x}'\mathbf{x}}$
- In this case: $p_{k,a} = \dfrac{\mathbf{t}_a'\mathbf{x}_k}{\mathbf{t}_a'\mathbf{t}_a}$

NIPALS algorithm

Step 2.1

- Repeat regression for every column in $\mathbf{X}_{a-1}$
- Can calculate regressions in one go:

$$\mathbf{p}'_a = \frac{1}{\mathbf{t}'_a \mathbf{t}_a} \cdot \mathbf{t}'_a \mathbf{X}_{a-1}$$

  - $\mathbf{t}_a$ is an $N \times 1$ column vector
  - $\mathbf{X}_{a-1}$ is an $N \times K$ matrix
  - $\mathbf{p}_a$ is a $K \times 1$ column vector

NIPALS algorithm

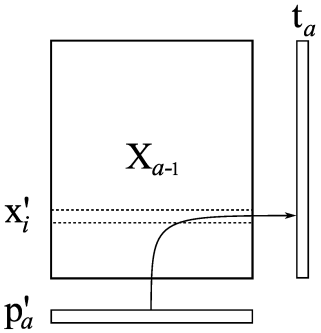
Step 2.2 Normalize the loadings

- $\mathbf{p}'_a$ won't have unit length (magnitude)
- Rescale it to magnitude 1.0
- $\mathbf{p}'_a = \frac{1}{\sqrt{\mathbf{p}'_a \mathbf{p}_a}} \cdot \mathbf{p}'_a = \frac{\mathbf{p}'_a}{\|\mathbf{p}'_a\|}$

NIPALS algorithm

Step 2.3 Regress every row in $\mathbf{X}$ onto $\mathbf{p}'_a$

- regress $\mathbf{x}_i$ onto $\mathbf{p}'_a$
- store regression coefficient as entry in $t_{i,a}$



- Recall LS for centered data: $\hat{\mathbf{y}} = \beta\mathbf{x}$, and $\widehat{\beta} = \dfrac{\mathbf{x}'\mathbf{y}}{\mathbf{x}'\mathbf{x}}$
- $t_{i,a} = \dfrac{\mathbf{p}'_a\mathbf{x}_i}{\mathbf{p}'_a\mathbf{p}_a}$

NIPALS algorithm

Step 2.3

- Repeat regression for every row in $\mathbf{X}_{a-1}$
- In practice: $\mathbf{t}_a = \dfrac{1}{\mathbf{p}_a'\mathbf{p}_a} \cdot \mathbf{X}_{a-1}\mathbf{p}_a$
  - $\mathbf{t}_a$ is an $N \times 1$ column vector
  - $\mathbf{X}_{a-1}$ is an $N \times K$ matrix
  - $\mathbf{p}_a$ is an $K \times 1$ column vector

NIPALS algorithm

Back to **step 2.** Have we converged?

- $\mathbf{t}_a$ compared to $\mathbf{t}_a$ from previous iteration
- Stop if change less than $\sqrt{\text{eps}} \approx 1.5 \times 10^{-8}$
- Could also compare change in $\mathbf{p}_a$ to previous iteration

- Safety net: also stop if number of iterations > 300

At convergence:

- $\mathbf{t}_a$ and $\mathbf{p}_a$ jointly form the a^{th} component
- Store them as columns in matrix $\mathbf{T}$ and $\mathbf{P}$ respectively

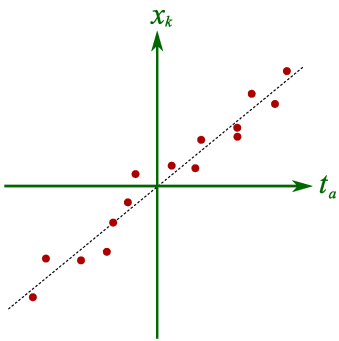
NIPALS algorithm

Finally, **step 3** Deflate the $\mathbf{X}_{a-1}$ matrix

- Deflation removes the part we can explain
- $\mathbf{E}_a = \mathbf{X}_{a-1} - \mathbf{t}_a \mathbf{p}_a'$
- $\mathbf{E}_a$ = residuals *after* fitting the a^{th} component
- Then let $\mathbf{X}_a = \mathbf{E}_a$ and repeat from step 1 for $a + 1$
- e.g. for $a = 1$: $\mathbf{X}_{a-1} = \mathbf{X}_0$ = preprocessed raw data
- e.g. for $a = 2$: $\mathbf{X}_1$ = residuals after 1 component = data matrix used to calculate 2^{nd} component

What happens at convergence?

Let's review the regressions calculated on the last iteration:



- **Step 2.1** Regress every column from $\mathbf{X}_{a-1}$ onto $\mathbf{t}_a$
- $p_{k,a} = \dfrac{\mathbf{t}_a' \mathbf{x}_k}{\mathbf{t}_a' \mathbf{t}_a}$
- What will regression look like for a strong relationship?
- Weak/no relationship?
- Meaning of the loading $p_{k,a}$ should be apparent now
- Regression can be used to predict: $\hat{\mathbf{x}}_k = \mathbf{t}_a' p_{k,a}$

On your own: interpret **step 2.3** when we regress rows in $\mathbf{X}_{a-1}$ onto $\mathbf{p}_a$

What happens after convergence?

After convergence of $\mathbf{t}_a$ and $\mathbf{p}_a$:

- $\mathbf{p}'_a = \dfrac{\mathbf{t}'_a \mathbf{X}_{a-1}}{\mathbf{t}'_a \mathbf{t}_a}$
- Drop the "a" subscripts for now; transpose the entire equation
- Rewrite step 2.1 as: $\mathbf{p} = \dfrac{\mathbf{X}'\mathbf{t}}{\mathbf{t}'\mathbf{t}}$
- Rewrite step 2.3 as: $\mathbf{t} = \dfrac{\mathbf{X}\mathbf{p}}{\mathbf{p}'\mathbf{p}}$
- Note that $\mathbf{p}'\mathbf{p} = 1.0$
- Substitute $\mathbf{t}$ into equation for $\mathbf{p}$ gives $\mathbf{p} = \dfrac{\mathbf{X}'\mathbf{X}\mathbf{p}}{\mathbf{t}'\mathbf{t}}$
- Rearrange to $(\mathbf{X}'\mathbf{X} - \mathbf{t}'\mathbf{t}\mathbf{I}_K)\,\mathbf{p} = \mathbf{0}$ where $\mathbf{I}_K$ is a $K \times K$ identity matrix

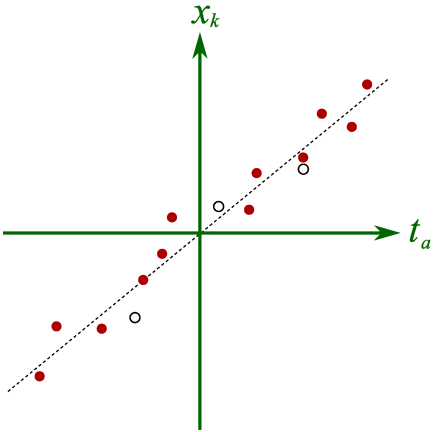
This shows (again) that:

- $\mathbf{p}$ is an eigenvector of $\mathbf{X}'\mathbf{X}$
- The eigenvalue is $\lambda = \mathbf{t}'\mathbf{t}$, which we interpret/know as the variance of $\mathbf{t}$

NIPALS notes

- Convergence is fast if the eigenvalues are well separated
- Two close eigenvalues leads to very slow convergence, followed by very fast convergence for the next one
- The algorithm handles missing data (next)

NIPALS algorithm: concept of handling missing data



Missing values are ignored and do not influence the slope calculation.

More details:

- Nelson, Taylor, MacGregor (paper 68)
- Arteaga and Ferrer (paper 20)

 39

Outliers

Discussion

What will an outlier do to a PCA model?

NIPALS summary

Advantages:

- Calculates one component at a time
- Handles missing data
- It converges (sometimes slowly)

Disadvantages:

- Round off errors may accumulate if you go very far (not usually a problem on modern computers)

Notes:

- Also called the Power algorithm for computing eigenvalues of a square matrix
- Excellent on large data sets (large N *and* large K)
- Google used this algorithm for their first search engine (called PageRank)
  - http://ilpubs.stanford.edu:8090/422/
  - Ipsen, Ilse, and Wills, "*Analysis and Computation of Google's PageRank*", 7th IMACS International Symposium on Iterative Methods in Scientific Computing, Fields Institute, Toronto, Canada, 5-8 May 2005

Flipping signs

In NIPALS, SVD or eigendecompositions:

- $\hat{\mathbf{X}}_1 = \mathbf{t}_1\mathbf{p}_1' = (-\mathbf{t}_1)(-\mathbf{p}_1')$
- Both the scores and loadings may flip sign
- Depends on the computer, initial guesses, algorithm implementation
- Not a problem: model interpretation is still consistent
- Not a problem: model's performance is identical

Just be aware when comparing results from different users/software/computers.

Last class: Flipping signs

In NIPALS, SVD or eigendecompositions:

- $\hat{\mathbf{X}}_1 = \mathbf{t}_1\mathbf{p}_1' = (-\mathbf{t}_1)(-\mathbf{p}_1')$
- Both the scores and loadings may flip sign
- Depends on the computer, initial guesses, algorithm implementation
- Not a problem: model interpretation is still consistent
- Not a problem: model's performance is identical

Just be aware when comparing results from different users/software/computers.