Linear Algebra: Part II

Math Tools: Week 2

Overview

1. Eigenvectors and eigenvalues
    1. Quick review of matrix-vector multiplication
    2. General applications

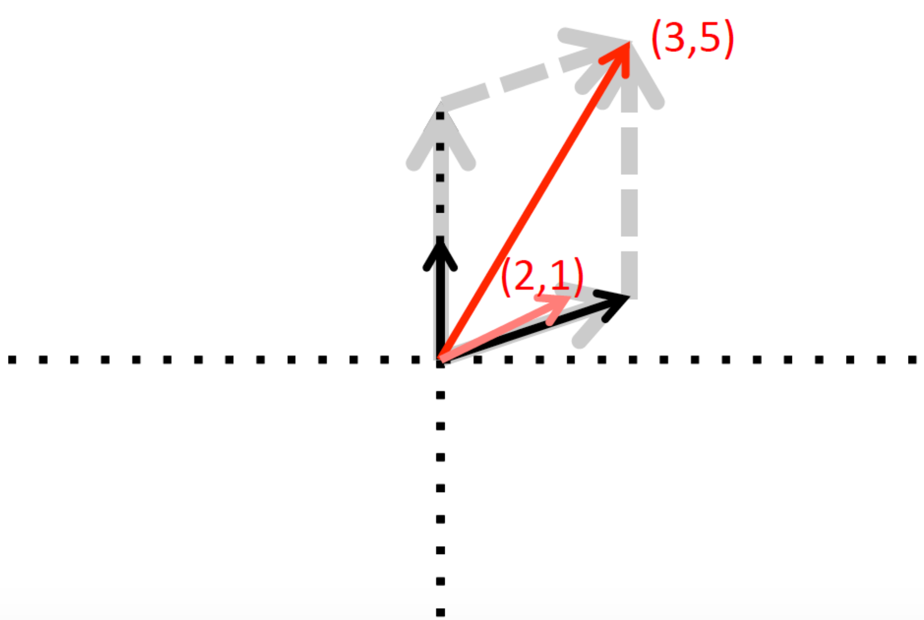
2. PCA
    1. Mathematical derivation
    2. Example

3. SVD
    1. Applications

Recall from last week: What do matrices do to vectors?

Outer product interpretation

$$\begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = 2 \begin{bmatrix} 0 \\ 2 \end{bmatrix} + 1 \begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \end{bmatrix} + \begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$



Columns of M 'span the plane'

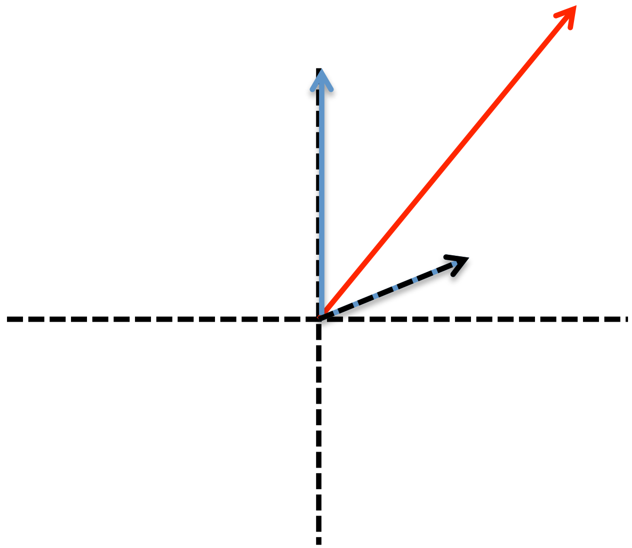
→ Different combinations of the columns of M can give you any vector in this plane

New vector is rotated and scaled

Recall from last week: What do matrices do to vectors?

Inner product interpretation

$$\begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} 0 & 3 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \\ \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$



Rows of M also 'span the plane'

Inner product multiplication can be thought of as a shorthand way to do several inner products

New vector is rotated and scaled

Relating this to eigenvalues and eigenvectors

$$\overleftrightarrow{W}\,\overrightarrow{v} = \overrightarrow{u}$$

The matrix *W* transforms *v* into *u* – maps *v* onto *u.* Resulting vector can be a rotated and scaled version of *v*.

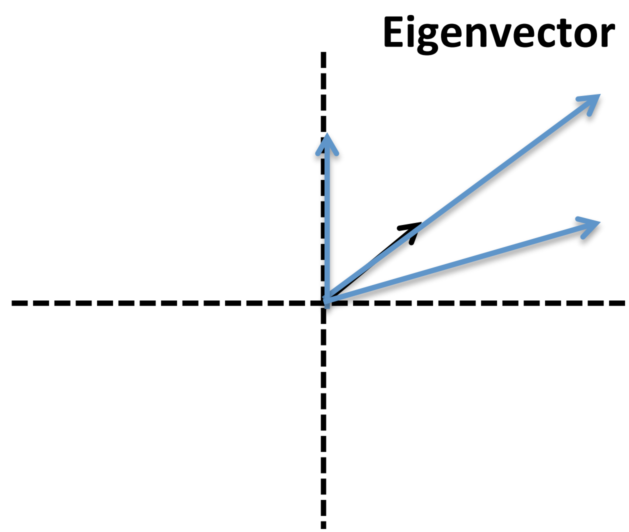
But it doesn't have to be rotated…

The special vectors for which the direction is preserved but the length changes: ***EIGENVECTOR***

An example:

$$\begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 1 \begin{bmatrix} 0 \\ 2 \end{bmatrix} + 1 \begin{bmatrix} 3 \\ 1 \end{bmatrix}$$

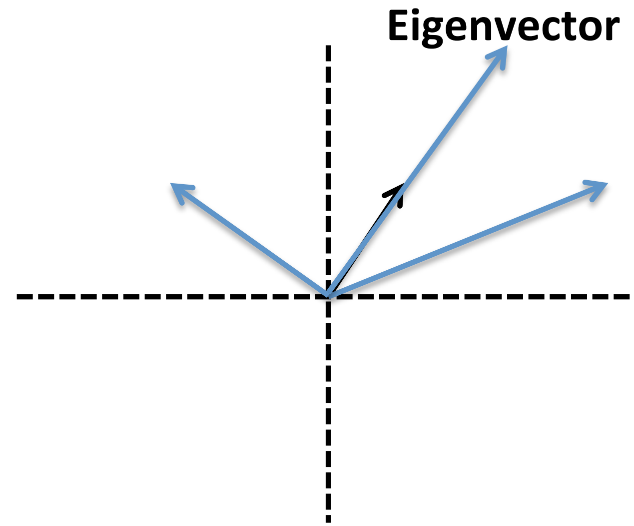
$$= \begin{bmatrix} 3 \\ 3 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



Eigenvalues and eigenvectors

$$\begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\overleftrightarrow{W} \underbrace{\overrightarrow{v}}_{\text{Eigenvector}} = \underbrace{\lambda}_{\text{Eigenvalue}} \overrightarrow{v}$$



For an eigenvector, multiplication by the matrix is the same as multiplying the vector by a scalar. This scalar is called an eigenvalue.

How many eigenvectors can a matrix have???

→ An *n* x *n* matrix (the only type we will consider here) can have <u>up to</u> *n* distinct eigenvalues and *n* eigenvectors

→ The set of eigenvectors, with distinct eigenvalues, are linearly independent. For symmetric matrices: they are orthogonal, or their dot product is 0.

Illustration of eigenvector and eigenvalues

Population dynamics of rabbits

$$x = \begin{bmatrix} \text{\# of rabbits b/w 0 and 1 year old} \\ \text{\# of rabbits b/w 1 and 2 years old} \\ \text{\# of rabbits b/w 2 and 3 years old} \end{bmatrix} \begin{bmatrix} 10 \\ 10 \\ 10 \end{bmatrix}$$

A = age transition matrix – probability that a member of the i^{th} age class will become a member of the $(i+1)^{th}$ age class

$$\begin{bmatrix} 0 & 6 & 8 \\ 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \end{bmatrix}$$

Population growth/loss: $Ax_t = x_{t+1}$

$$\begin{bmatrix} 0 & 6 & 8 \\ 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \end{bmatrix} \begin{bmatrix} 10 \\ 10 \\ 10 \end{bmatrix} = \begin{bmatrix} 140 \\ 5 \\ 5 \end{bmatrix}$$

In this case, an eigenvector of matrix A represents a 'stable' population distribution

$$Ax_t = \lambda x_{t+1} \qquad x_t = x_{t+1}$$

If $\lambda = 1$, then there is a solution for which the population doesn't change every year.

If $\lambda < 1$, then the population is shrinking

If $\lambda > 1$, then the population is growing

If the population starts on an eigenvector, it will stay on the eigenvector

This will be revisited in a few classes!

http://homepage.ntu.edu.tw/~jryanwang/course/Mathematics%20for%20Management%20(undergraduate%20level)/Applications%20in%20Ch7.pdf

Side-note on eigenvectors

Previous example

$$\overleftrightarrow{W}\overrightarrow{v} = \lambda \overrightarrow{v}$$

discusses RIGHT eigenvectors – the eigenvector is on the RIGHT side of the matrix.

Does this matter? Yes, maybe. If a matrix is symmetric, the right and left eigenvectors are the same.

Left eigenvectors can be found by solving this equation:

$$\overrightarrow{v}^T \overleftrightarrow{W} = \lambda \overrightarrow{v}$$

Note: This eigenvector is a row vector

Most of the time, left eigenvectors aren't that useful. But it's good to know that they exist.

How to find eigenvalues and eigenvectors

Real life and easiest way: Using MATLAB's eig command

[V,D] = eig(W) will return a matrix V, where each column is an eigenvector, and a diagonal matrix D with the corresponding eigenvalues along the diagonal

MATLAB output:

```
[V,D] = eig(W)

V =
   -0.8321   -0.7071
    0.5547   -0.7071

D =
    -2     0
     0     3
```

W = $\begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix}$

Eigenvectors are defined only up to a scale factor, and so they are typically scaled such that the norm of the vector is 1

Eigenvalue is 3, like we found before!

The set of eigenvalues is called the *spectrum* of a matrix

How to find eigenvalues and eigenvectors

The math way:

Eigenvector-eigenvalue equation: $\overleftrightarrow{W}\overrightarrow{v} = \lambda\overrightarrow{v}$

$$\overleftrightarrow{W}\overrightarrow{v} - \lambda\overrightarrow{v} = 0$$

$$(\overleftrightarrow{W} - \lambda I)\overrightarrow{v} = 0$$

(WHITEBOARD) Assume that *v* is not 0, this equation only has a solution if:

$$det(\overleftrightarrow{W} - \lambda I) = 0$$

If $\overleftrightarrow{W} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ then $\overleftrightarrow{W} - \lambda I = \begin{bmatrix} a-\lambda & b \\ c & d-\lambda \end{bmatrix}$

$$\begin{aligned} det(\overleftrightarrow{W} - \lambda I) &= (a-\lambda)(d-\lambda) - bc \\ &= \lambda^2 - \lambda(a+d) + ad - bc \\ &= \lambda^2 - \lambda\mathrm{Trace} + \mathrm{Det} \end{aligned}$$

$$\lambda = \frac{\mathrm{Trace} \pm \sqrt{\mathrm{Trace}^2 - 4\mathrm{Det}}}{2}$$

Practice

Find eigenvectors and eigenvalues of this matrix:

$$W = \begin{bmatrix} 4 & -1 \\ 2 & 1 \end{bmatrix}$$

Some fun facts that actually come in handy

$$W = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

Determinant of a matrix is equal to the product of eigenvalues

$$ad - bd = \lambda_1 \lambda_2$$

Trace of a matrix is equal to the sum of eigenvalues

$$a + d = \lambda_1 + \lambda_2$$

Eigenvalues of a triangular matrix can be read off the diagonal:

$$\begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \qquad \lambda_1 = 3 \quad \lambda_2 = 2$$

When are eigenvectors/eigenvalues useful?

1. **Gives you a way to ‘decompose a matrix’**
2. Allows some easy shortcuts in computation
3. Give you a sense of what kind of ‘matrix’ or dynamics you are dealing with
4. Allows for a convenient change of basis
5. Frequently used in both modeling and data analysis

Eigen-decomposition (matrix diagonalization)

Eigen-decomposition, or the decomposition of a matrix into eigenvalues and eigenvectors, can be thought of as similar to prime factorization

Example with primes: 12 = 2*2*3

Example with matrices: $W = VDV^{-1}$

V is a matrix of eigenvectors, and D is a diagonal matrix of eigenvalues (WB)

Note: only works for NxN matrices with N linearly independent eigenvectors

Eigenvectors of a matrix form an orthogonal basis for the matrix – any other vector in the column space of the matrix can be re-written with eigenvectors:

General example:

$$\overrightarrow{v} = c_1\overrightarrow{v_1} + c_2\overrightarrow{v_2}$$

$$\overrightarrow{u} = W\overrightarrow{v}$$

$$\overrightarrow{u} = W(c_1\overrightarrow{v_1} + c_2\overrightarrow{v_2})$$

$$\overrightarrow{u} = c_1W\overrightarrow{v_1} + c_2W\overrightarrow{v_2} \qquad W\overrightarrow{v_1} = \lambda_1\overrightarrow{v_1}$$

Don't even need the matrix!

$$\overrightarrow{u} = c_1\lambda_1\overrightarrow{v_1} + c_2\lambda_2\overrightarrow{v_2}$$

When are eigenvectors/eigenvalues useful?

Eigenvalues can reveal the preferred inputs to a system

$$\overrightarrow{u} = W\overrightarrow{v} \qquad \overrightarrow{v} = c_1\overrightarrow{v_1} + c_2\overrightarrow{v_2} \qquad \overrightarrow{u} = c_1\lambda_1\overrightarrow{v_1} + c_2\lambda_2\overrightarrow{v_2}$$

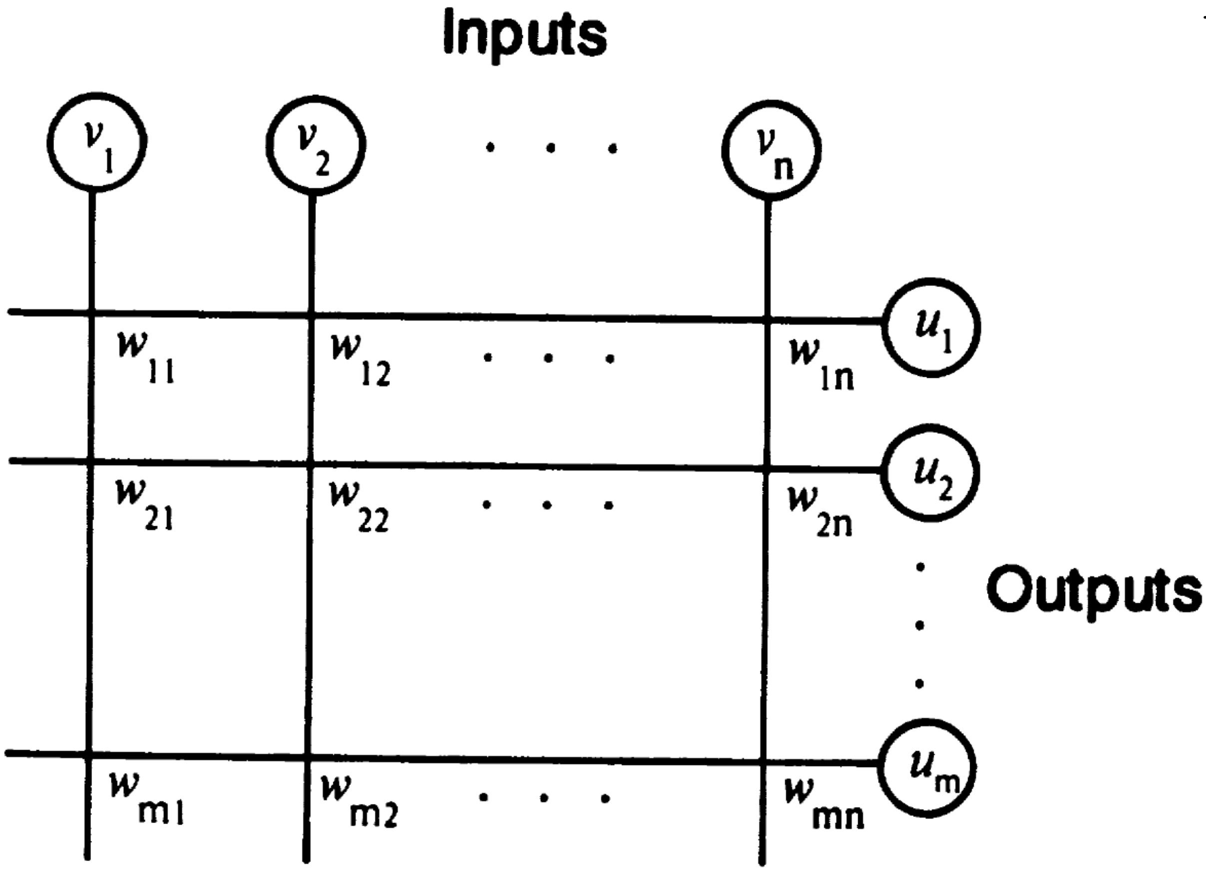
Assume that all *v*'s are of unit length, so the length of *u* depends on the *c*'s and λ's

If a vector v points in the direction of eigenvector v_1, then c_1 will be large (or at least positive)

If λ_1 is also large, then multiplication by *W* effectively lengthens the vector along this direction

More generally – the eigenvectors with the large eigenvalues can tell you which input vectors (*v*) the matrix "prefers", or will give a large response to

Connect this back to Neuroscience



$$\overrightarrow{u} = W\overrightarrow{v}$$

$$\overrightarrow{u} = c_1\lambda_1\overrightarrow{v_1} + c_2\lambda_2\overrightarrow{v_2}$$

Each output value u is computed by an inner product with the input vector *v* and the weight matrix row, *w*

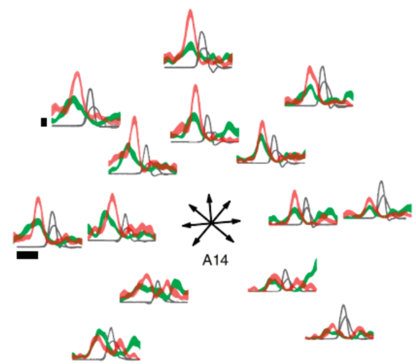
Large activation happens when the input vector closely matches eigenvectors with large eigenvalues

Also: Given *v* and *u,* you can compute the matrix *W* (well-defined if *u* is long enough)

Utility of eigenvectors/eigenvalues: PCA

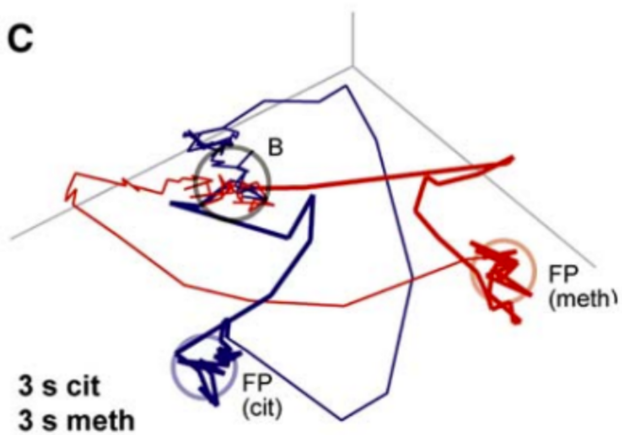
What is PCA?

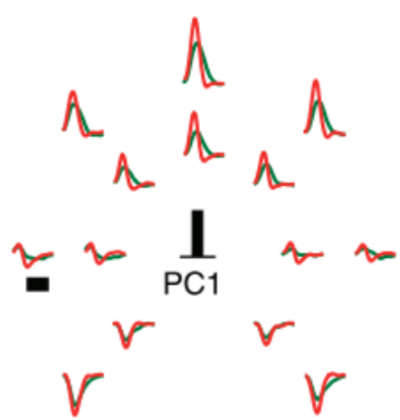
- Dimensionality reduction method (that keeps as much variation as possible)
- Pull structure out of seemingly complicated datasets
- De-noising technique
- Useful when # of variables that you record may be 'excessive'



Neural data

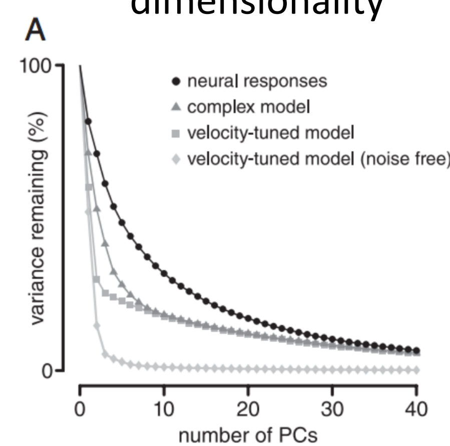
800 PN responding to 2 separate odors





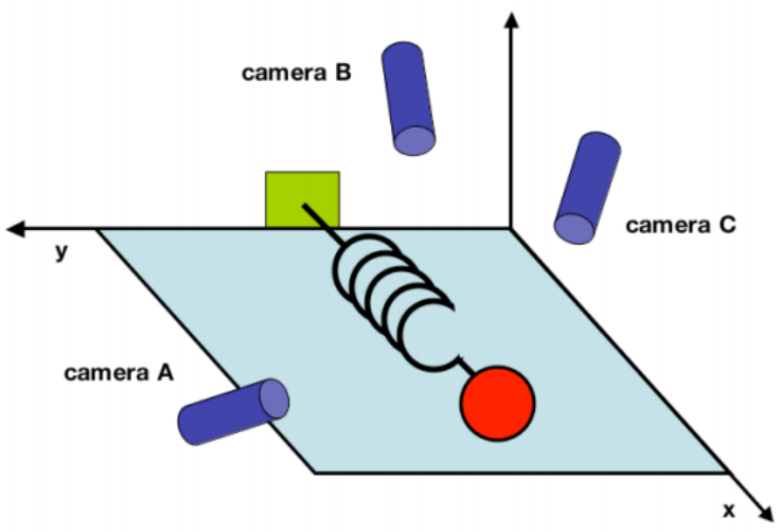
PC1

Analyze dimensionality



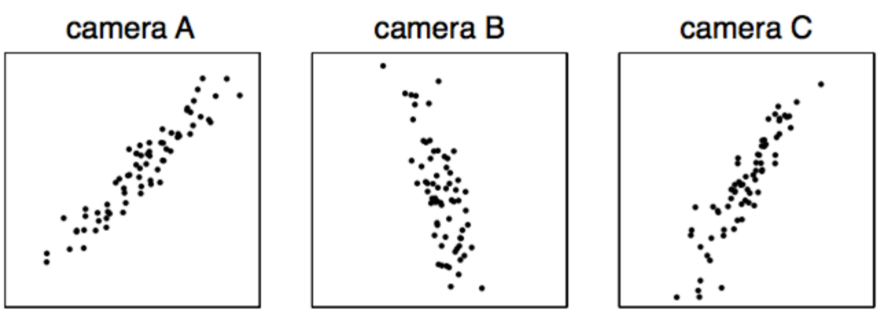
PCA: a motivating example

We do an experiment: we record a spring (with a mass attached at the end) oscillate in one dimension:



BUT, we don't know this – don't know which measurements best reflect the dynamics of our system

Record in 3 dimensions

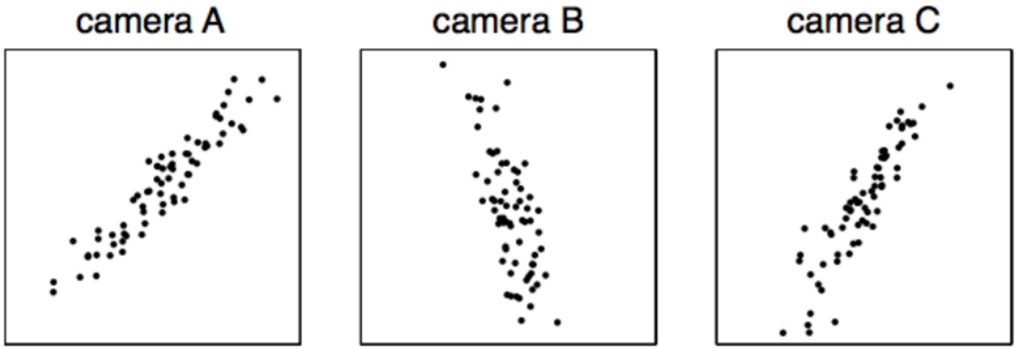


Each black dot – position of ball at each time frame

Can we determine the dimension along which the dynamics occur? Want to uncover that the dynamics are truly 1-dimensional

http://arxiv.org/pdf/1404.1100v1.pdf

PCA: a motivating example



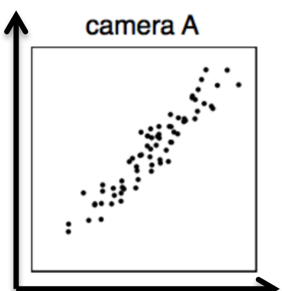
Data vector for 1 time point:

$$\vec{X} = \begin{bmatrix} x_A \\ y_A \\ x_B \\ y_B \\ x_C \\ y_C \end{bmatrix}$$

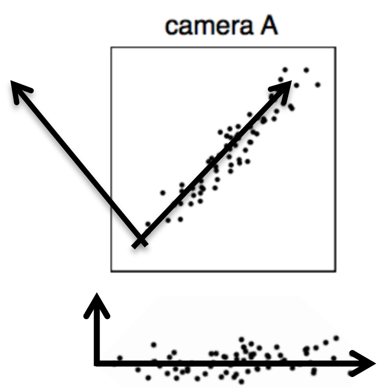
Together, data points form some cloud in a 6-dimensional space

6-d space has too many dimensions to visualize, and the data might not be truly 6-dimensional anyway

Is there a better way to represent this data?



Naïve basis for each camera: {(0,1), (1,0)}



Could choose a different basis that makes more sense for this data

Assumption/limit of PCA: new basis will be a linear combination of the old basis

PCA: into the details

Define the relevant matrices:

Data matrix: $\mathbf{X} = \begin{bmatrix} \overrightarrow{X_1} & \overrightarrow{X_2} & \cdots & \overrightarrow{X_T} \end{bmatrix}$

Each vector: $\overrightarrow{X} = \begin{bmatrix} x_A \\ y_A \\ x_B \\ y_B \\ x_C \\ y_C \end{bmatrix}$

If we record for 10 mins at 120 Hz, X has 6 rows and
10*60*120 = 72000 columns

To project the data into a more sensible basis: $\mathbf{PX} = \mathbf{Y}$

Projection matrix	Data matrix	New data matrix
6 x 6	6 x 72000	6 x 72000

P transforms **X** into **Y** through a rotation and scaling

The *rows* of **P** are the basis vectors for expressing the *columns* of **X** – they are the principal components!

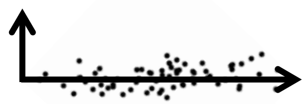
$$\mathbf{PX} = \begin{bmatrix} \overrightarrow{p_1} \\ \overrightarrow{p_2} \\ \vdots \\ \overrightarrow{p_m} \end{bmatrix} \begin{bmatrix} \overrightarrow{X_1} & \overrightarrow{X_2} & \cdots & \overrightarrow{X_T} \end{bmatrix} \qquad \mathbf{Y} = \begin{bmatrix} \overrightarrow{p_1} \cdot \overrightarrow{X_1} & \cdots & \overrightarrow{p_1} \cdot \overrightarrow{X_T} \\ \vdots & \ddots & \vdots \\ \overrightarrow{p_m} \cdot \overrightarrow{X_1} & \cdots & \overrightarrow{p_m} \cdot \overrightarrow{X_T} \end{bmatrix}$$

PCA: into the details

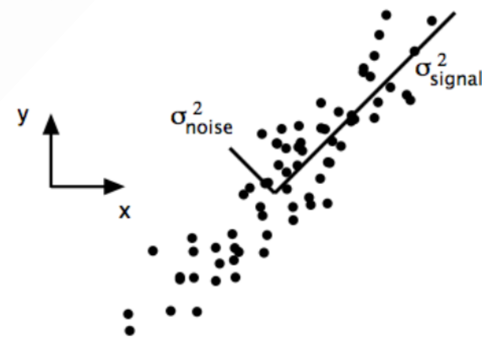
$$\mathbf{PX} = \mathbf{Y}$$

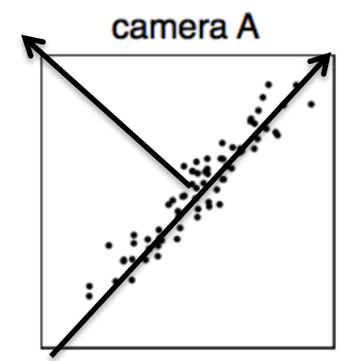
$$\mathbf{Y} = \begin{bmatrix} \overrightarrow{p_1} \cdot \overrightarrow{X_1} & \cdots & \overrightarrow{p_1} \cdot \overrightarrow{X_T} \\ \vdots & \ddots & \vdots \\ \overrightarrow{p_m} \cdot \overrightarrow{X_1} & \cdots & \overrightarrow{p_m} \cdot \overrightarrow{X_T} \end{bmatrix}$$

Okay… so how do we choose P?
What do we want?



Assume that the direction with the largest variance comes from real dynamics





Look for directions that capture redundancy – might allow us to reduce the dimensions

Want **Y** to have low redundancy

PCA: into the details

Can quantify these goals through the covariance matrix!

For two vectors:

Variance: $\sigma_A^2 = \frac{1}{n}\sum_i a_i^2$ $\quad \sigma_B^2 = \frac{1}{n}\sum_i b_i^2$ (assume the data is mean-subtracted)

Covariance: $\sigma_{AB}^2 = \frac{1}{n}\sum_i a_i b_i$ Rewriting using vector notation:

$$a = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

$$b = \begin{bmatrix} b_1 & b_2 & \cdots & b_n \end{bmatrix}$$

$$\sigma_{AB}^2 = \frac{1}{n} a b^T$$

For lotsa vectors:

$$Z = \begin{bmatrix} \overrightarrow{z_1} \\ \overrightarrow{z_2} \\ \vdots \\ \overrightarrow{z_n} \end{bmatrix}$$

Each row corresponds to measurements of a certain type (from one camera)

$$C_Z = \frac{1}{n} Z Z^T$$

Diagonal elements correspond to variance and off-diagonal elements correspond to covariance between measurement types

PCA: into the details

$$C_Z = \frac{1}{n} Z Z^T$$

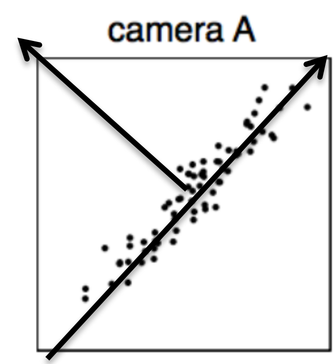
Diagonal elements correspond to variance within measurement types and off-diagonal elements correspond to covariance between measurement types

Want the covariance matrix for our projected data (***Y***) to have large values along the diagonal (large variance for the signal) and small values everywhere else (low covariance – low redundancy)

Technical term for this: diagonalize $\boldsymbol{C_Y}$

One algorithm that accomplishes this:

1. Select a normalized direction in *m*-dimensional space along which the variance is maximized. This is p_1.
2. Find an orthogonal direction along which remaining variance is maximized. This is p_2.
3. Repeat until *m* vectors are chosen.



PCA: eigenvector-based solution

Goal: Find some orthonormal matrix ***P*** for ***Y*** = ***PX*** such that $\boldsymbol{C_Y}$ = (1\n)$\boldsymbol{YY^T}$ is a diagonal matrix

$$C_Y = \frac{1}{n}YY^T$$
$$= \frac{1}{n}(PX)(PX)^T$$
$$= \frac{1}{n}PXX^TP^T \qquad C_x = \frac{1}{n}XX^T$$
$$= PC_XP^T$$

$\boldsymbol{C_X}$ is symmetric, so we can decompose it into the following: $C_X = EDE^T$

E is a matrix of eigenvectors and *D* is a diagonal matrix with eigenvalues along the diagonal

$$C_Y = P(EDE^T)P^T$$

What if we choose P = E^T?

$$C_Y = P(P^TDP)P^T$$

Because P is a matrix of orthogonal eigenvectors, $P^T = P^{-1}$

$$C_Y = (PP^{-1})D(PP^{-1})$$
$$C_Y = D$$

Our choice of P diagonalized C_Y!

PCA: summary and utility

What just happened:

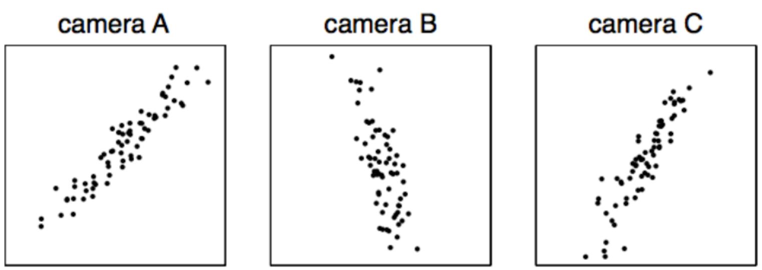
If we choose P to be the matrix of eigenvectors of the covariance matrix of X, then Y = PX returns a Y matrix whose covariance matrix is diagonalized.

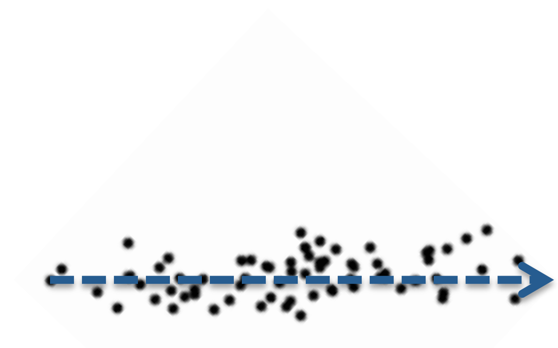
→ The principal components (or 'axes') are the eigenvectors of the covariance matrix of the data matrix X

Now what???

People usually use PCA to do 2 things:

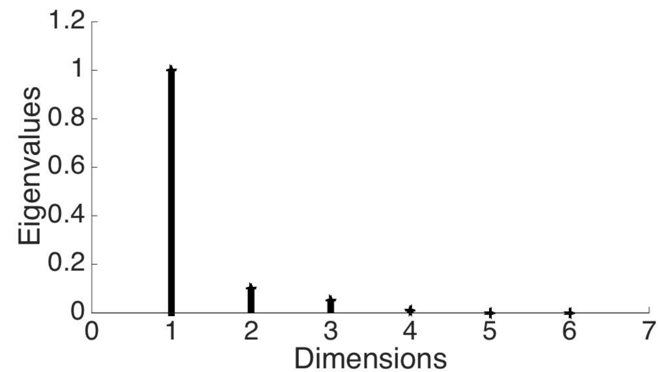
1. Replot the data using Y





2. Look at the spectrum (the eigenvalues)

Can tell you the 'dimensionality of your data'

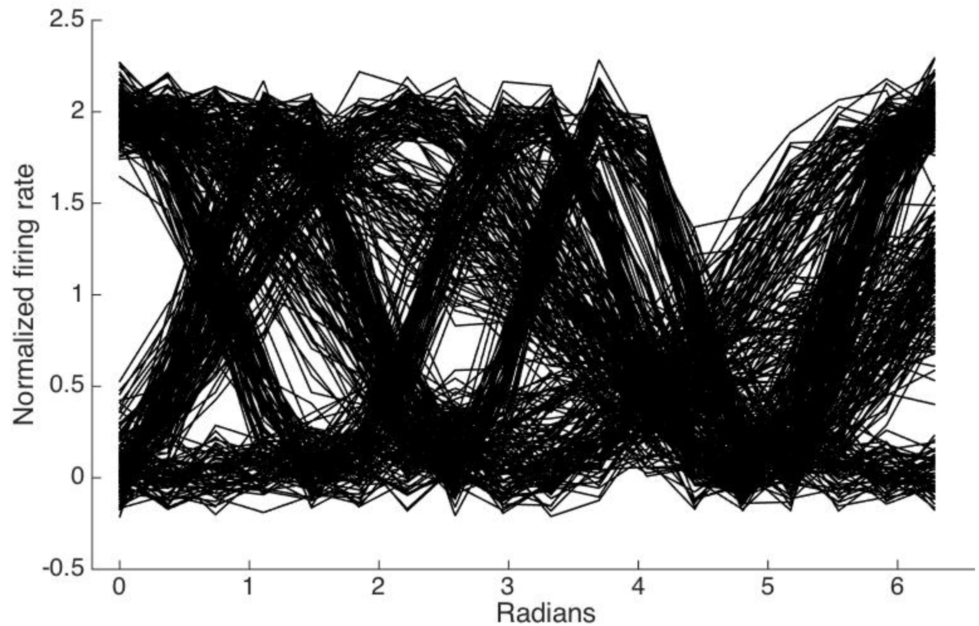


PCA: how to do this in the real world

Step 0. Explicitly define what the data matrix X is.

Let's say we have a bunch (360) of head direction tuning curves.

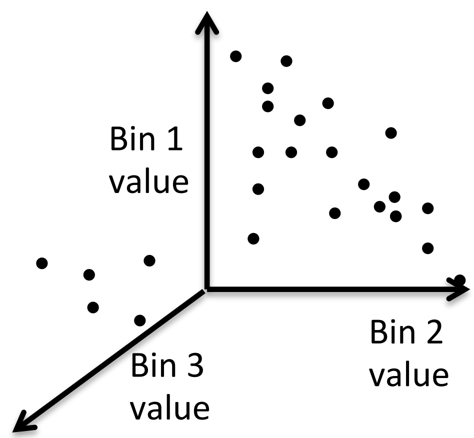
We can tell there are a couple different types… but can we say this quantitatively?



Bin each tuning curve into 18 bins

Each tuning curve is then a point in an 18-dimensional space

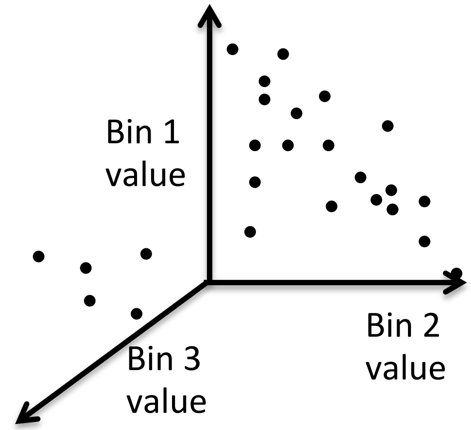
X = [TC1 TC2 … TC360]
X is a 18 x 360 matrix



PCA: how to do this in the real world

Step 1. Center the data

- Compute and subtract off the mean
- Compute and divide by standard deviation




```
MATLAB:
[~,N] = size(X);
mn = mean(X,2);
X= X-mn*ones(1,N);
stdX = std(X,[],2);
X= X./(stdX*ones(1,N));
```

Otherwise, the first component will capture how far away from the origin the data is

Step 2. Compute covariance matrix

```
MATLAB:
covariance = 1/(N-1)*X*X'; (or: covariance = cov(X');)
```

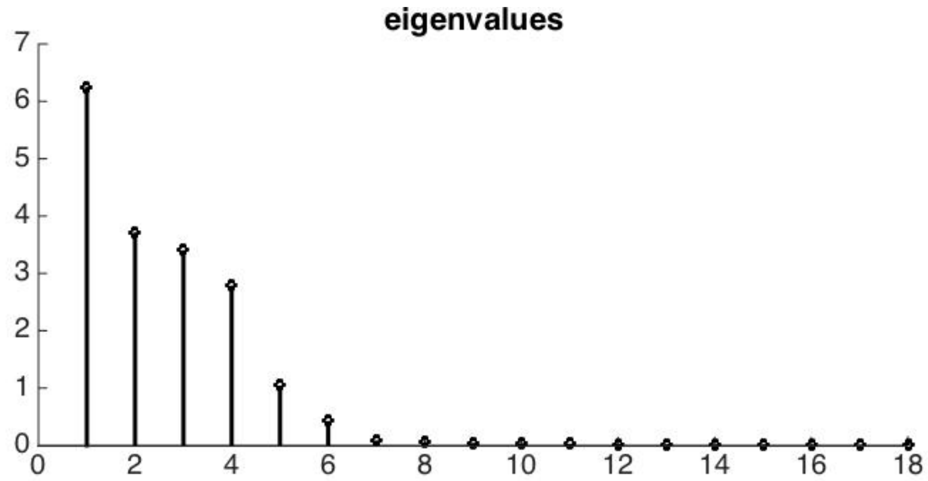
Step 3. Compute and sort eigenvectors and eigenvalues of covariance matrix

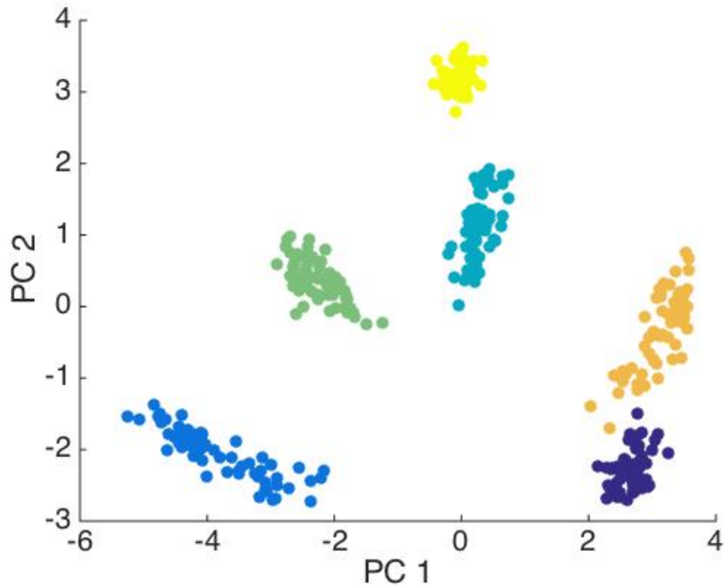
```
MATLAB:
[PC,V]= eig(covariance);
V = diag(V);
[~,ind] = sort(V,'descend');
PC = PC(:,ind); V = V(ind);
```

PCA: how to do this in the real world

Step 4. Transform the data and see what you can see!

```
MATLAB:
    Y = PC'*X;
```





7 types of cells

When PCA fails

The linearity assumption is not a good one

- One fix: kernel PCA, where a nonlinear transformation is applied first

Finding the most decorrelated components isn't what you want

- ICA: independent component analysis: finds the statistically independent components

Interpreting dimensionality in the face of noise can be difficult

- Noise will increase the number of 'dimensions'
- Can be difficult to draw the line between signal and noise

SVD

Recall that for some matrices (symmetric ones), we can decompose them into the following product:

$$X = VDV^{-1}$$

Where V is a matrix of eigenvectors and D is a matrix of eigenvalues along the diagonal

The SVD (singular value decomposition) is similar, but more general – you can do it for all matrices!

$$X = U\Sigma V$$

U is a matrix of eigenvectors for XX' (the principal components!), V is a matrix of eigenvectors for X'X, and Σ is a matrix with singular values along the diagonal. Singular values are the square roots of X'X

→ Columns of U are 'left singular vectors', row of V are 'right singular vectors'

SVD and applications

One great thing about the SVD: it decomposes a matrix into a sum of outer products

$$X = U\Sigma V$$

$$= \begin{pmatrix} | & | & & | \\ \vec{u}^{(1)} & \vec{u}^{(2)} & \cdots & \vec{u}^{(N)} \\ | & | & & | \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 & \cdots & 0 \\ 0 & 0 & \cdots & \lambda_N & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(1)} & - \\ - & \vec{v}^{(2)} & - \\ & \vdots & \\ - & \vec{v}^{(N)} & - \\ & other & \end{pmatrix}$$

$$= \begin{pmatrix} | & | & & | \\ \vec{u}^{(1)} & \vec{u}^{(2)} & \cdots & \vec{u}^{(N)} \\ | & | & & | \end{pmatrix} \begin{pmatrix} - & \lambda_1 \vec{v}^{(1)} & - \\ - & \lambda_2 \vec{v}^{(2)} & - \\ & \vdots & \\ - & \lambda_N \vec{v}^{(N)} & - \end{pmatrix}$$

$$= \lambda_1 \begin{pmatrix} | \\ \vec{u}^{(1)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(1)} & - \end{pmatrix} + \lambda_2 \begin{pmatrix} | \\ \vec{u}^{(2)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(2)} & - \end{pmatrix} + \cdots + \lambda_N \begin{pmatrix} | \\ \vec{u}^{(N)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(N)} & - \end{pmatrix}$$

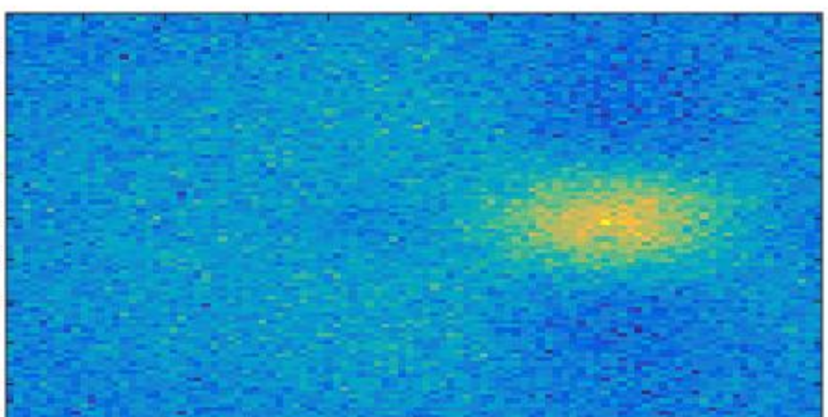
SVD and applications

$$= \underbrace{\lambda_1 \begin{pmatrix} | \\ \vec{u}^{(1)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(1)} & - \end{pmatrix}}_{\text{Each term is a matrix}} + \lambda_2 \begin{pmatrix} | \\ \vec{u}^{(2)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(2)} & - \end{pmatrix} + \cdots + \lambda_N \begin{pmatrix} | \\ \vec{u}^{(N)} \\ | \end{pmatrix} \begin{pmatrix} - & \vec{v}^{(N)} & - \end{pmatrix}$$

Each matrix is ordered in terms of 'importance'
One application: compute low-rank approximations of matrices

```
MATLAB:
[U,S,V] = svd(X,0); % take an svd
X_0 = U(:,1:p)*S(1:p,1:p)*V(:,1:p)';
```

Noisy receptive field:



Low-rank approximation: