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datasai 2023 vol. 2

overview & computational basics

aditya nair

CHEN INSTITUTE TIANQIAO & CHRISSY

course organizers

Helen O'Connor

Programs Coordinator

Mary Sikora

Executive Director, Tianqiao and Chrissy Chen Institute for Neuroscience

Ralph Adolphs

Bren Professor of Psychology, Neuroscience, and Biology

David J. Anderson

Seymour Benzer Professor of Biology; Tianqiao and Chrissy Chen Institute for Neuroscience Leadership Chair; Investigator, Howard Hughes Medical Institute; Director, Tianqiao and Chrissy Chen Institute for Neuroscience; Interim Director, T&C Chen Center for Systems Neuroscience

Adi Nair

Graduate Student

Daniel Wagenaar

Research Professor of Biology and Biological Engineering

external faculty

Maryam Shanechi

Professor and Viterbi Early Career Chair in Electrical and Computer Engineering, Computer Science, and Biomedical Engineering, University of Southern California

Chethan Pandarinath

Assistant Professor in the Wallace H. Coulter Department of Biomedical Engineering at Georgia Tech and Emory University

Liam Paninski

Professor of Statistics and Neuroscience, Columbia University

external speakers & TAs

Gabriel Rojas-Bowe
Grad Student, Churchland Lab, UCLA

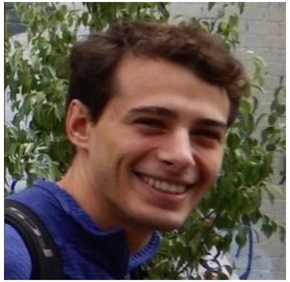
Maxwell Mellin
Grad Student, Churchland Lab, UCLA

Matthew Whiteaway
Postdoc, Paninski Lab, Columbia

Iman Wahle
Grad Student, Princeton

Omid Sani
Postdoc, Shanechi Lab, USC

Domenick Mifsud
Research Specialist, Emory



Frank Lanfranchi
Grad Student, Tsao Lab, UC Berkeley

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internal speakers & faculty

Prof Frederick Eberhardt
Professor of Philosophy

James Gornot
Grad Student, Thompson Lab

Tara Chari
Grad Student, Pachter Lab

Tarun Sharma
Grad Student, Dickinson Lab

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course schedule

foundations & essential tools (10th - 14th)

- July 10th:

ethics, replication and generalizability of neural data analysis
Ralph Adolphs, Caltech

- July 11th:

machine learning basics and dynamical systems.
Adi Nair, James Gornet, Caltech

- July 12th:

encoding models in neuroscience
Maxwell Melin, Gabriel Rojas-Bowe, Churchland lab, UCLA

- July 13th:

adapting Your recordings for big data techniques
Daniel Wagenaar, Caltech

- July 14th:

dimensionality reduction & hypothesis testing
Tara Chari, Caltech

✦ computational & machine learning basics

✦ dynamical systems

✦ encoding & decoding

✦ pre-processing

✦ dimensionality reduction & statistics

course schedule

the frontier & deep learning (18th - 21st)

- July 17th:

state space models in neuroscience
Liam Paninski & Matt Whiteway, Columbia

- July 18th:

understanding behavior & bring your own data day!
Tarun Sharma, Caltech, Frank Lanfranchi, UC Berkeley

- July 19th:

latent variable dynamical models in neuroscience
Maryam Shanechi, USC

- July 20th:

causal modelling from observational data
Frederick Eberhardt, Caltech

- July 21th:

transformers in neuroscience
Chethan Pandarinath & Domenick Mifsud, Emory

✦ state-space models

✦ behavior & pose estimation

✦ recurrent neural networks

✦ causal learning

✦ transformers

daily schedule

- 8:30AM - 9:30AM: **breakfast**
- 9:45AM - 10:45AM: **introductory lecture**
- 10:45AM - 11:00AM: **bio break**
- 11:00AM - 12:00PM: **philosophy and general questions**
- 12:15PM - 1:15PM: **lunch**
- 1:30PM - 2:30PM: **methods lecture**
- 2:30PM - 6:00PM: **hands-on session**

on BYOD (18th)

- 8:30AM - 9:30AM: **breakfast**
- 9:45AM - 10:45AM: **introductory lecture**
- 10:45AM - 11:00AM: **bio break**
- 11:00AM - 12:00PM: **hands-on session**
- 12:15PM - 1:15PM: **lunch**
- 1:30PM - 2:30PM: **lecture on behavior**
- 2:30PM - 6:00PM: **hands-on session**

Ask a lot of questions,
feel free to interrupt!

resources:

course website:
https://neuroscience.caltech.edu/about/research-centers/chen-center-for-datasai/2023-data-science-and-ai-for-neuroscience-summer-school

github repo:
https://github.com/cheninstitutecaltech/Caltech_DATASAI_Neuroscience_23

resources:

google colab pro+:
https://colab.research.google.com/signup

slack channel:
https://join.slack.com/t/cheninstitute-9181373/shared_invite
/zt-1b54fb5gi-fuAhn51vD_qorBqTbXoKcQ

bring your own data day (BYOD) - 18th

google colab pro+:

first go to: https://www.prepaidgiftbalance.com/

register your card with the following address:
1200 E California Blvd
MSC 2-59
Pasadena, CA - 91125

then go to: https://colab.research.google.com/signup

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computational mindset

you will see many course concepts 2-3 times across multiple days, at different levels of depth.

- architectures
- mathematical functions
- code

- applying a method
- implementing a method
- practicing the math behind the method

you are meant to struggle through this

don’t be afraid to ‘break’ things while you code

your recourse when you don’t know what to do is:

- ✦ google → stack overflow, …
- ✦ ask your neighbor. debug problems together!
- ✦ Ask the TAs for help if neither you nor any of your neighbors can figure it out.
- ✦ as a last resort you can check out the solution code also in the notebook!

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resources beyond this course

`datasai` teaches concepts,covers a broad overview of tools and provides practical training on using tools

!! <u>does not</u> go into in-depth mathematical treatments of methods

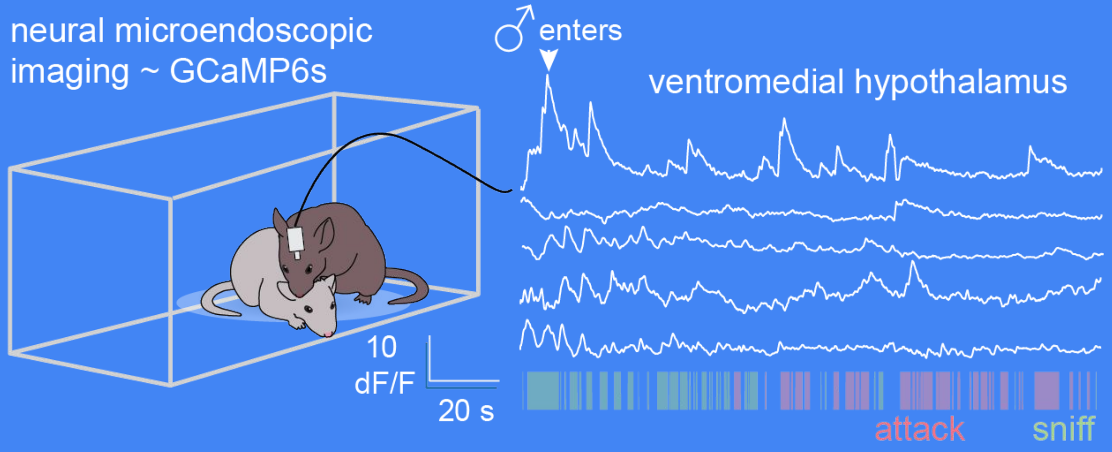
ML courses at Caltech:

`CS156: Learning from data`
`Yaser Abu-Mostafa`

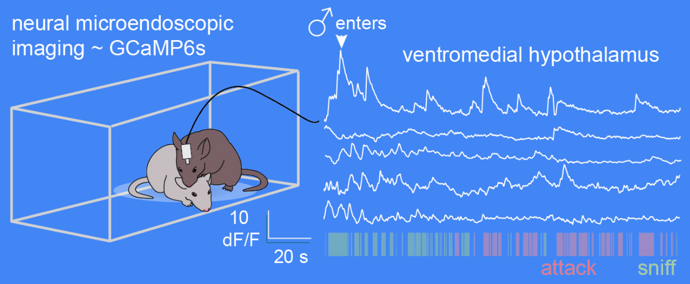
`CS155: Machine Learning & Data Mining`
`Yisong Yue`

WAINT

why am I not talking

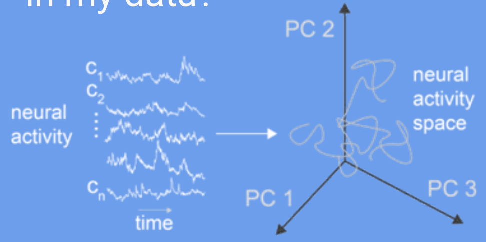


so you have some data.....



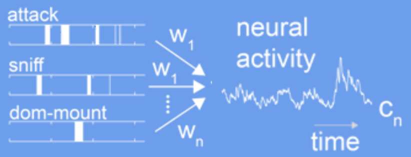
discovering brain-behavior relationships

what are the major signals in my data?



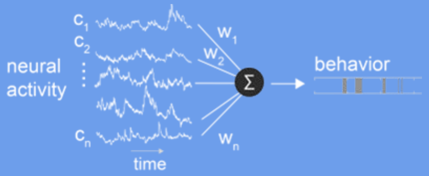
dimensionality reduction

what are single neurons tuned to?



linear encoding models

is information about behavior present in my data?



linear decoding models

we'll cover these methods in week 1

foundations & essential tools

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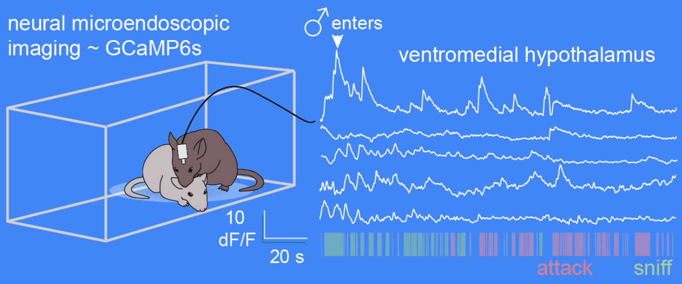
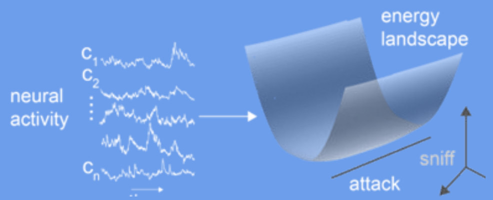


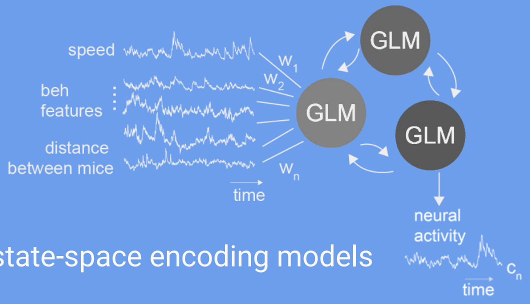
discovering brain-behavior relationships

can I discover computations in data in an unsupervised manner?



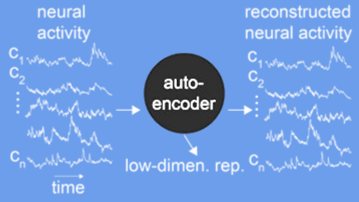
dynamical systems

what if the encoding of behavior in single neurons is dynamic?



state-space encoding models

How much non-linearly encoded behavior information is available?



autoencoders & transformers models

we’ll cover these methods in week 2

the ‘frontier’ & deep learning

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today we're going to cover: computational basics

part 1

dimensionality reduction via PCA

data visualization and familiarity with python

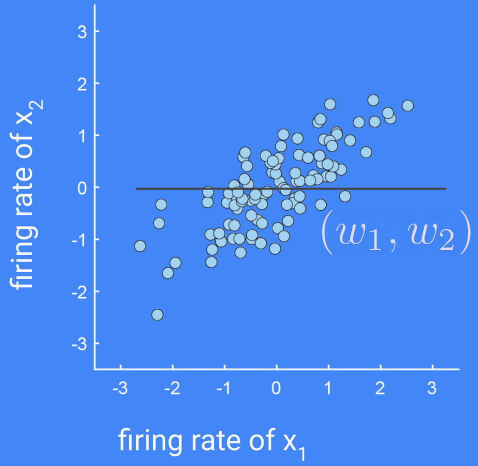
part 2

decode behavior using regression

overfitting & regularization

let's consider a system of two neurons

how can we best summarize this data?

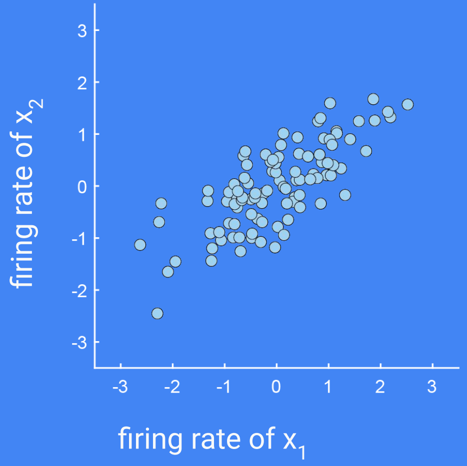


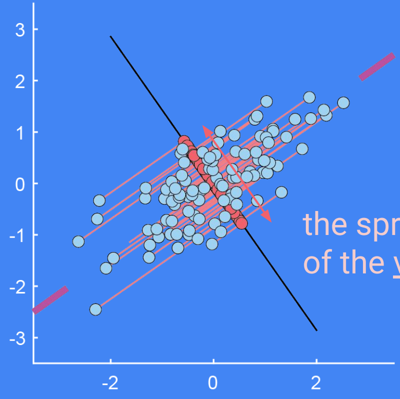
make a 1-D 'projection', i.e a weighted combination of activities of neurons

$$s_1(t) = w_1 x_1(t) + w_2 x_2(t)$$

let's consider a system of two neurons

how can we best summarize this data?





the sum of the pink lines tells us how well s reconstructs the data

the spread of the projection of x onto s tell us of the variance captured by s

an example projection

$$s_1(t) = w_1 x_1(t) + w_2 x_2(t)$$

one way to summarize the data is maximize variance or minimize reconstruction → PCA

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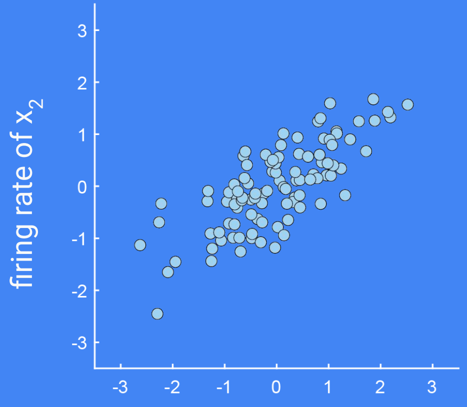
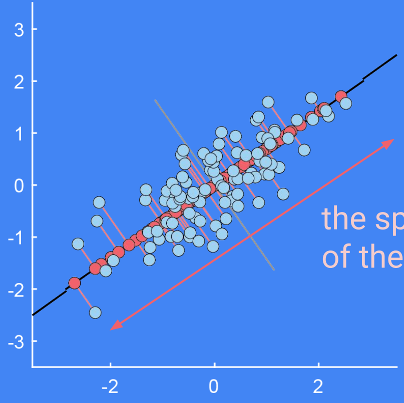
let's consider a system of two neurons

how can we best summarize this data?





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an example projection

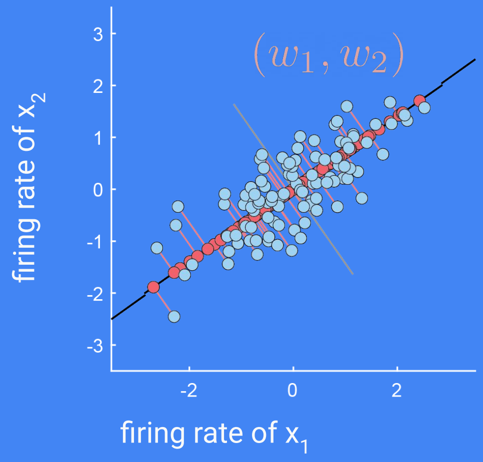
$$s_1(t) = w_1 x_1(t) + w_2 x_2(t)$$

PCA maximizes variance or minimize reconstruction

how do we find the right projections?

principal components analysis

through the lens of eigendecomposition



for a matrix X of size (t x n), where t: time and n: neurons

the projection that maximises variance in X is the first eigenvector of the covariance matrix C of mean-centered X

$$C = X^T X$$

$$CV = \lambda V$$ — eigendecomposition

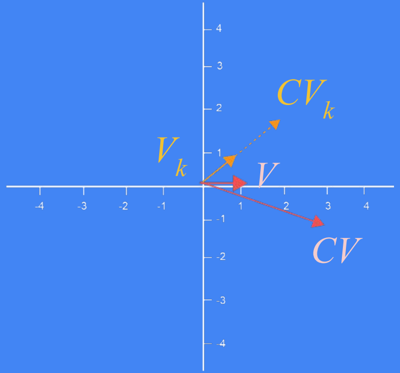
V and λ are eigenvectors and eigenvalues of C resp.

the foundation for dimensionality reduction & dynamical systems

Christodoulou & Vogel (2022), the eigenvalue in neuroscience

principal components analysis

building intuition about eigendecomposition



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the projection that maximises variance in X is the first eigenvector of the covariance matrix C of mean-centered X

$$C = X^T X$$

$$CV = \lambda V$$

V and λ are eigenvectors and eigenvalues of C resp.

eigenvectors are <u>special vectors</u> s.t multiplying them by C is the same as multiplying them by a scalar value

let $C = \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix}$ let's try $V = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ then $CV = \begin{bmatrix} 3 \\ -1 \end{bmatrix}$ not an eigenvector, why?

let's try $V_k = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ then $CV_k = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$ same as $2*V$, where λ = 2
an eigenvector!

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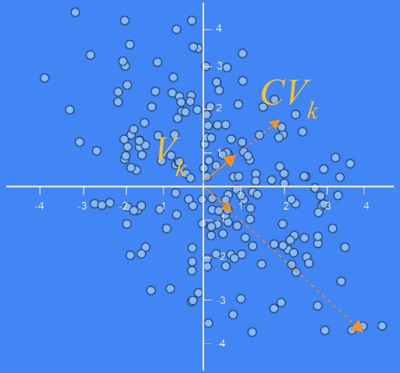
principal components analysis

building intuition about eigendecomposition



for a matrix X of size $(t \times n)$, where t: time and n: neurons

the projection that maximises variance in X is the first eigenvector of the covariance matrix C of mean-centered X

$$C = X^T X$$

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V and λ are eigenvectors and eigenvalues of C resp.

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let $C = \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix}$

let's try $V_k = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

then $CV_k = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$

same as $2*V$, where λ = 2
an eigenvector!

what's the remaining eigenvector?

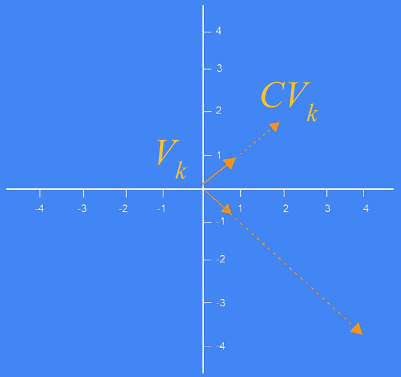
let's try $V_m = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

then $CV_m = \begin{bmatrix} 4 \\ -4 \end{bmatrix}$

What's the relationship between the eigenvectors?

principal components analysis

building intuition about eigendecomposition



for a matrix X of size $(t \; x \; n)$, where t: time and n: neurons

the projection that maximises variance in X is the first eigenvector of the covariance matrix C of mean-centered X

$$C = X^T X$$

$$CV = \lambda V$$

V and λ are eigenvectors and eigenvalues of C resp.

eigenvectors are special vectors s.t multiplying them by C is the same as multiplying them by a scalar value

to summarize: we can find V, s.t different eigenvectors are orthogonal and define a basis that maximizes variance in your data

in practice, we rarely derive V & λ, we instead use singular value decomposition as eigendecomp. is computationally less efficient

principal components analysis

through the lens of singular value decomposition (SVD)

for a matrix X of size (t x n), where t: time and n: neurons

in eigendecomposition

$$C = X^T X$$

$$CV = \lambda V$$

V and λ are eigenvectors and eigenvalues of C resp.

in SVD, we decompose X directly

$$X = USV^T$$

U is the left singular vector, S are singular values and V consists of right singular vectors

what's the relationship?

$$X^T XV = VS^2$$

$$CV = VS^2$$

singular values (S) are the square root of eigenvalues and the right singular vectors (V) are eigenvectors

we'll try both these methods and look at their equivalence in the hands-on session!

principal components analysis

through the lens of singular value decomposition (SVD)

for a matrix X of size (t x n), where t: time and n: neurons

in eigendecomposition

$$C = X^T X$$

$$CV = \lambda V$$

V and λ are eigenvectors and eigenvalues of C resp.

in SVD, we decompose X directly

$$X = USV^T$$

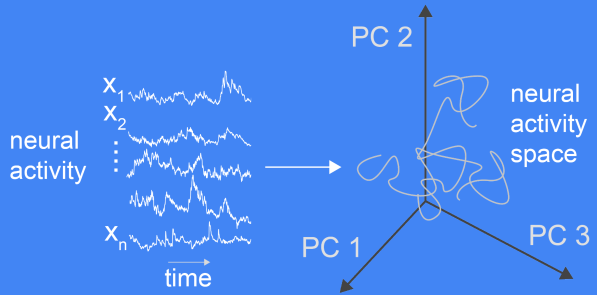
U is the left singular vector, S are singular values and V consists of right singular vectors

what's the relationship?

if $X = USV^T$, then $X^T X = VSU^T USV^T = VS^2 V^T$

if we multiply V on both sides, we obtain, $X^T XV = VS^2$, or $CV = VS^2$

I.e singular values (S) are the square root of eigenvalues and the right singular vectors (V) are eigenvectors



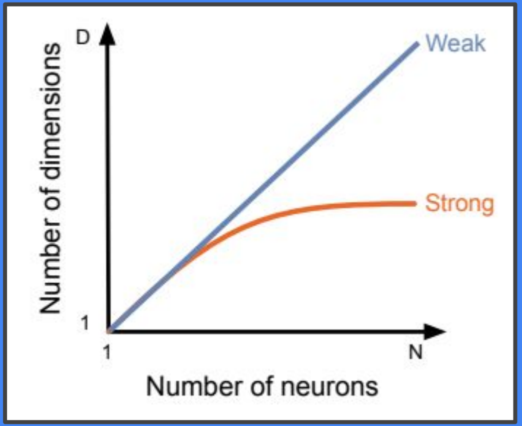
why perform dimensionality reduction?

principal components analysis

weak principle :
dimensionality reduction is a convenient tool for making sense of complex data

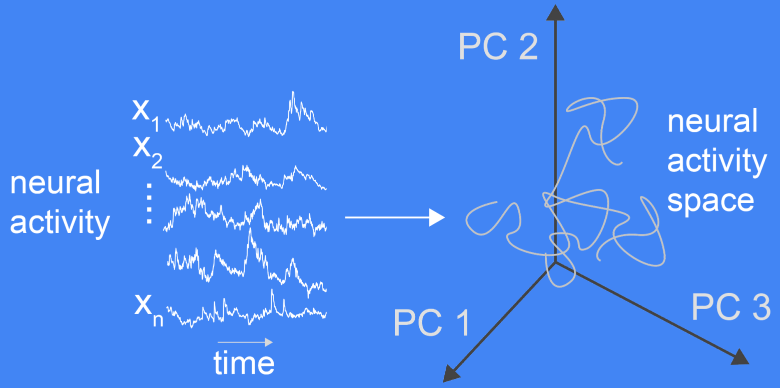
strong principle :
dimensionality reduction is a hypothesis for how neural circuits compute

we'll talk about this tomorrow



From Mark Humphries (2020), Strong and weak principles of dimensionality reduction

hands-on session part 1
dimensionality reduction via PCA



- learn to use a pre-made Principal Component Analysis (PCA) library.
- implement PCA with our own matrix operations.
- use Singular Value Decomposition (SVD) to build PCA.

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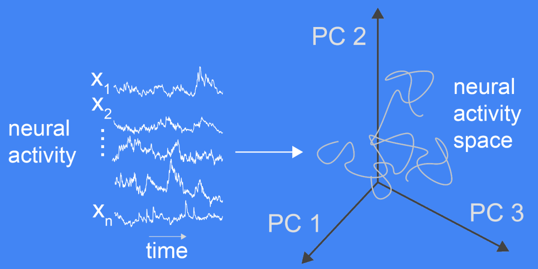
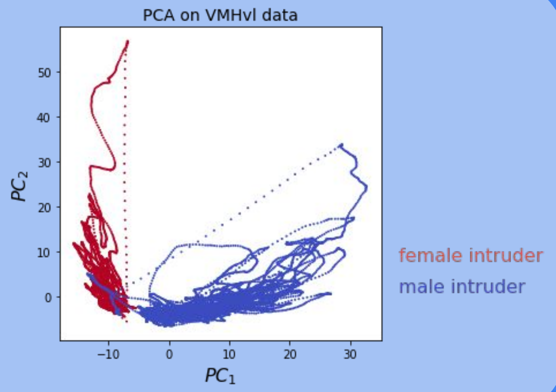
let’s code!

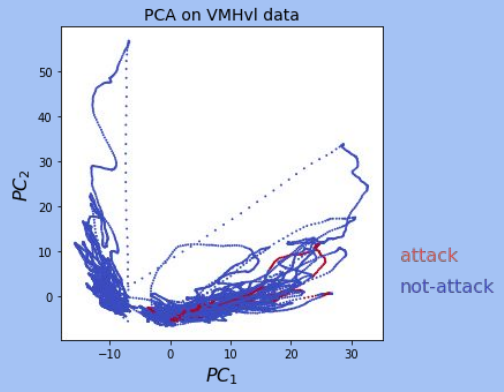
github repo:
https://github.com/cheninstitutecaltech/Caltech_DATASAI_Neuroscience_23/tree/main/07_10_23_day1_ethics_regression/code/diy_notebooks

use the notebook ‘dimensionality_reduction.ipynb’

PCA preserves information about neural activity but not necessarily behavior







how can we predict behavior from neural activity?

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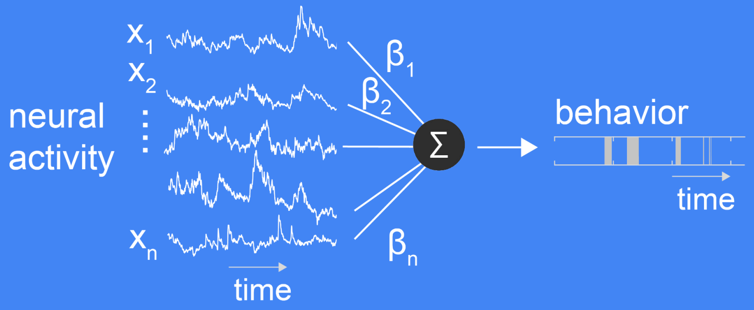
hands-on session part 2
overfitting & regularization

how can we predict behavior from neural activity?



details of regression will be covered in day 3 & 5

- we'll fit a simple linear model (aka linear regression)
- learn how to identify overfitting
- combat overfitting using regularization and shuffling techniques
- implement linear regression from scratch.
- learn about methods that combine dimensionality reduction with regression.

let’s code!

github repo:
https://github.com/cheninstitutecaltech/Caltech_DATASAI_Neuroscience_23/tree/main/07_10_23_day1_ethics_regression/code/diy_notebooks

use the notebook ‘overfitting_regularization.ipynb’

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reminder

welcome social starts at 6 PM in the breezeway tomorrow morning:

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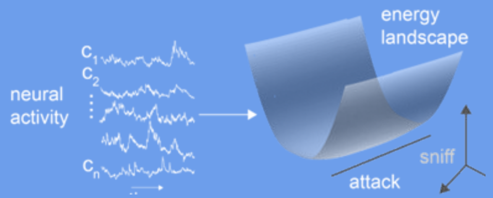
can I discover computations in data in an unsupervised manner?



dynamical systems

dynamical systems
& neural population dynamics

stay tuned!

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