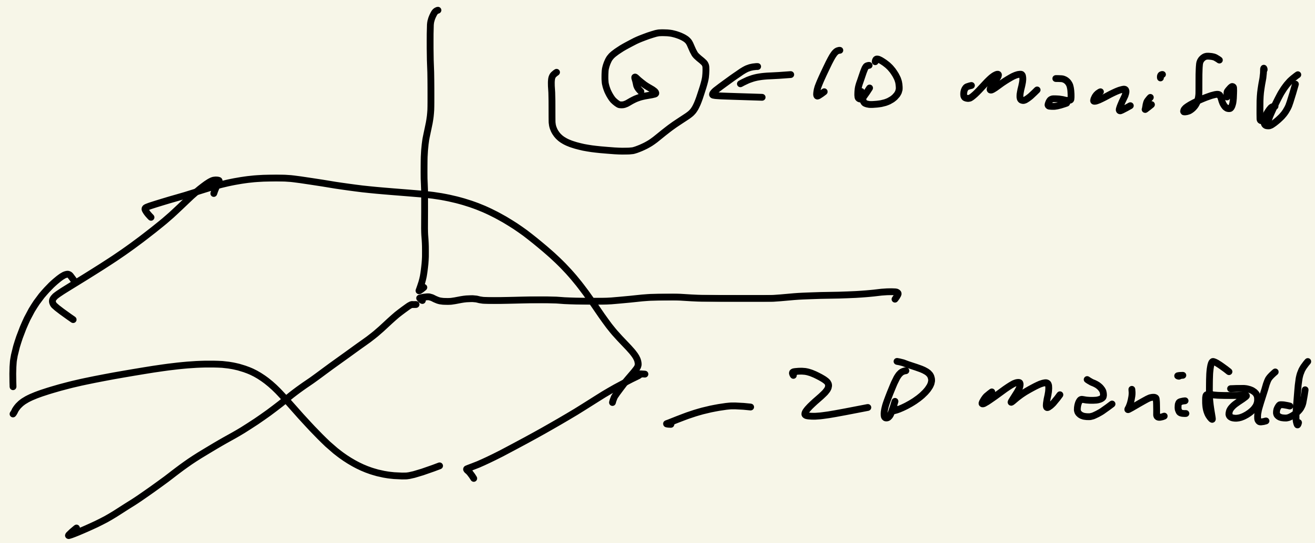
Dimensional Reduction

Idea: data in high-D space

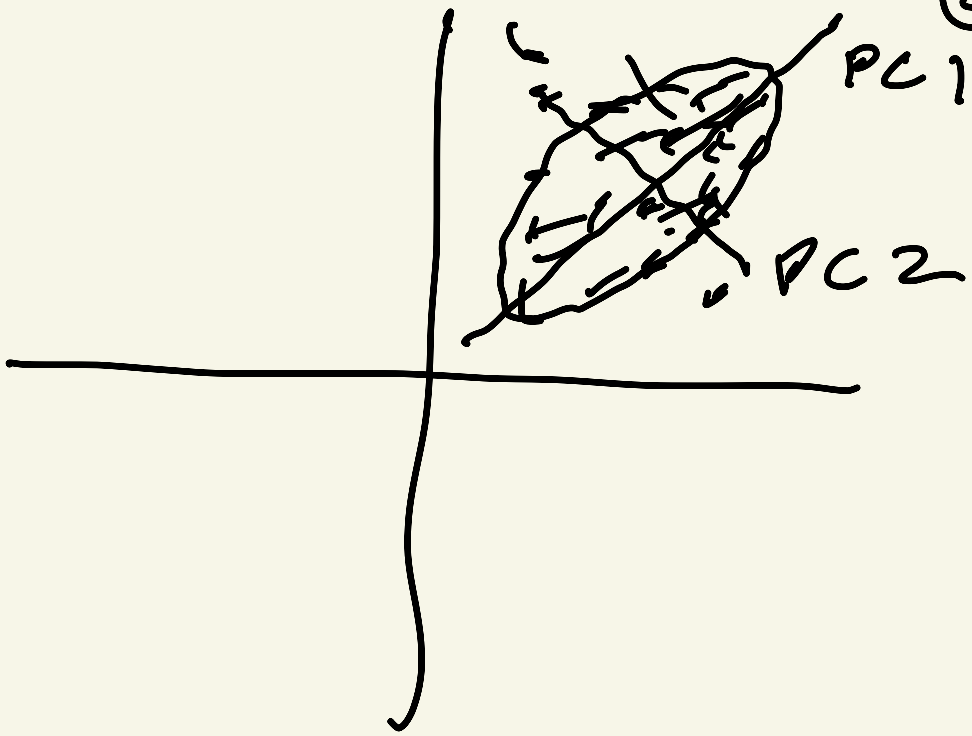
400 neurons $\Rightarrow$ 400D

Lives on low-D manifold

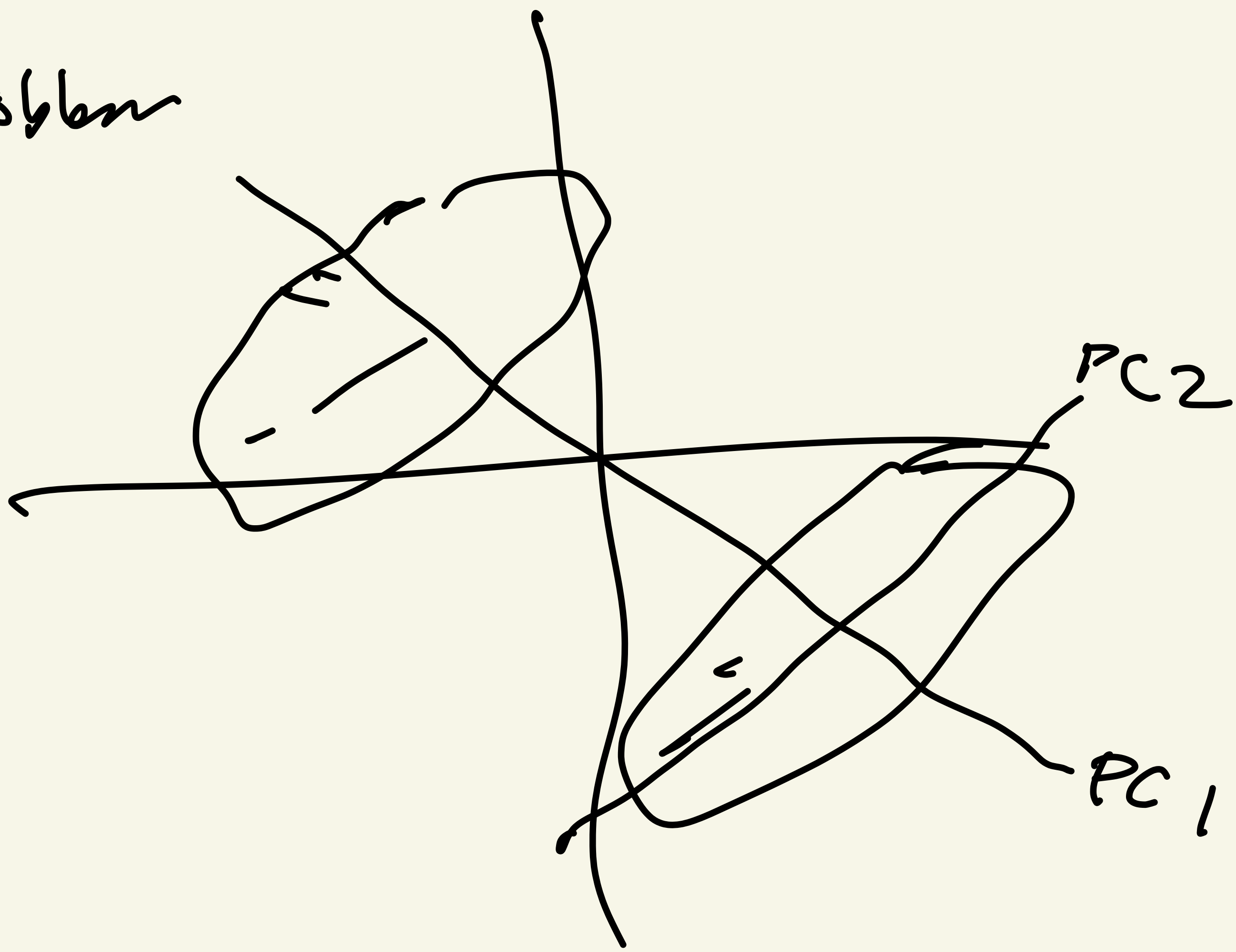


Idea: $\exists$ latent factors (small #)
that drive the data (activity)

PCA: General idea: model data as coming from high-D Gaussian



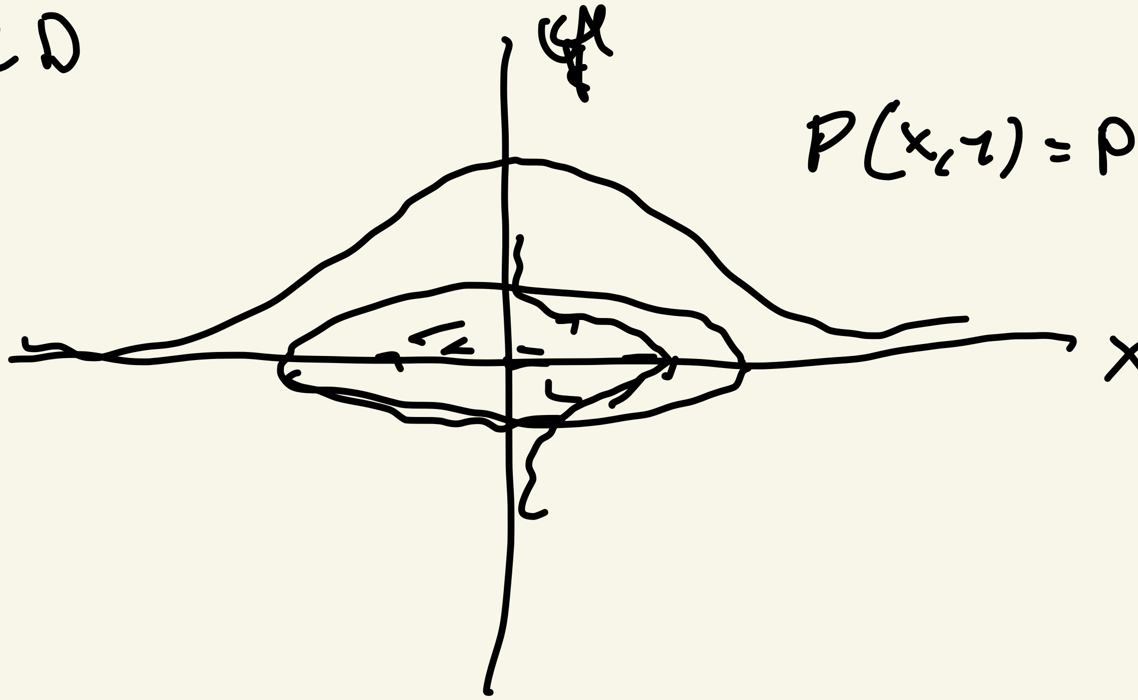
Problem



1D: $P(x) = \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{(x-x_m)^2}{2\sigma_x^2}}$ x_m: mean
σ_x: stdev

take mean = 0

2D



$P(x,y) = P(x)P(y)$

ND: $P(x_1, x_2, \ldots, x_N) = P(x_1)P(x_2)\ldots P(x_N)$

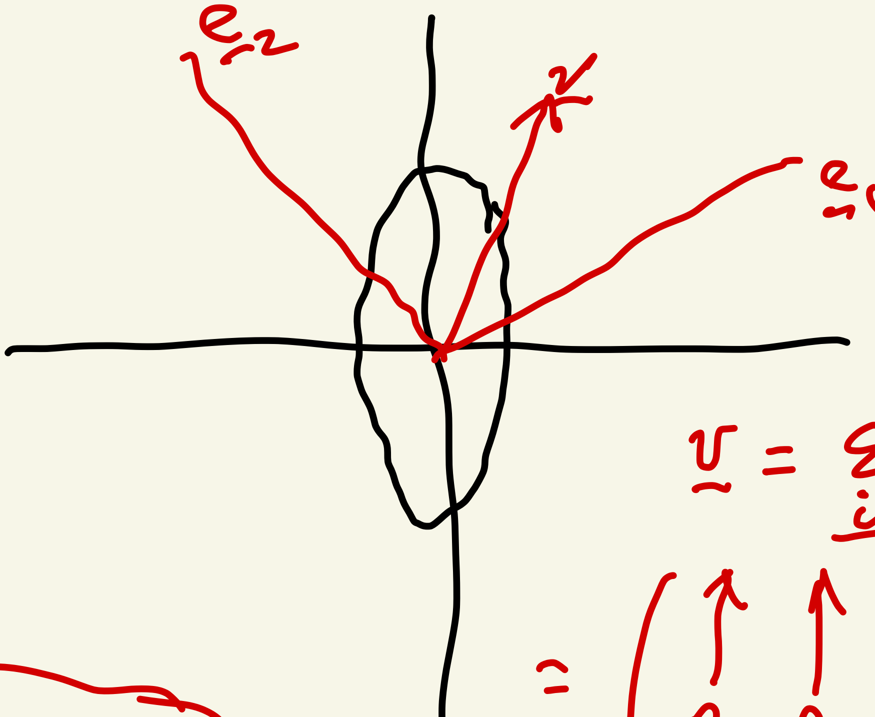
$$= \underbrace{\frac{1}{(2\pi)^{N/2}\sigma_1\sigma_2\ldots\sigma_N}}_{k} \underline{e^{-\sum_i \frac{x_i^2}{2\sigma_i^2}}}$$

$$\underline{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \qquad C = \begin{pmatrix} \sigma_1^2 & & & 0 \\ & \sigma_2^2 & & \\ & & \ddots & \\ 0 & & & \sigma_N^2 \end{pmatrix}$$

$$= k e^{-\frac{1}{2}\underline{x}^T C^{-1} \underline{x}}$$

$$\underline{x}^T C^{-1} \underline{x} = (x_1 \cdots x_N) \begin{pmatrix} \frac{1}{\sigma_1^2} & & \\ & \ddots & \\ & & \frac{1}{\sigma_N^2} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix}$$

$$= \sum_i \frac{x_i^2}{\sigma_i^2} \qquad k\, e^{-\frac{1}{2}\underline{x}^T C^{-1} \underline{x}}$$



$$\underset{\sim}{v} = \underbrace{\sum_i \tilde{v}_i \underset{\sim}{e}_i}$$

$$= \begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ \underline{e}_1 & \underline{e}_2 & \cdots & \underline{e}_N \\ \downarrow & \downarrow & & \downarrow \end{pmatrix} \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_2 \\ \vdots \\ \tilde{v}_N \end{pmatrix}$$

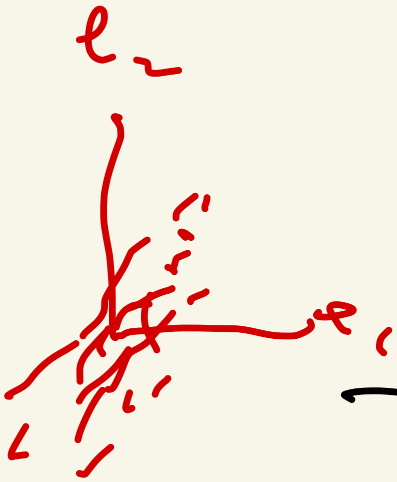
$$= \underline{E}\, \underset{\sim}{\tilde{v}}$$

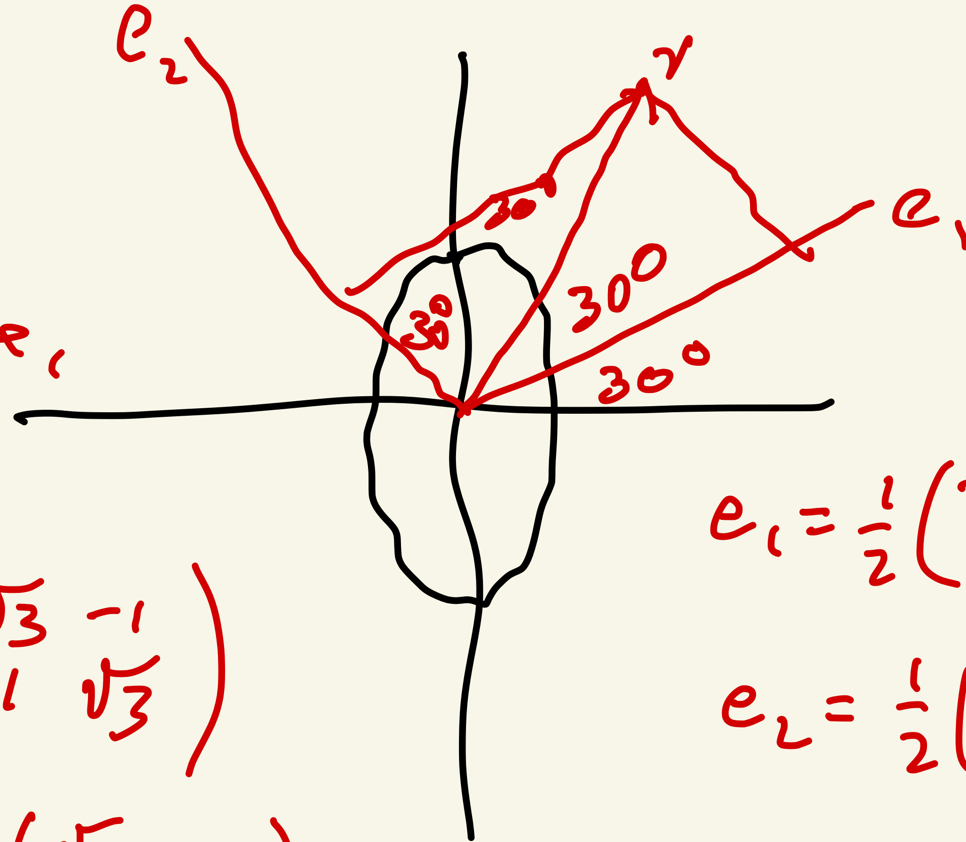
$\underline{v} = E\, \underset{\sim}{\tilde{v}}$

$\underline{\tilde{v}} = E^{-1} \underline{v}$

$\underline{e}_i \cdot \underline{e}_j = \delta_{ij}$

$\Rightarrow E^{-1} = E^T = \underbrace{\begin{pmatrix} \leftarrow e_1^T \rightarrow \\ \leftarrow e_2^T \rightarrow \\ \vdots \\ \leftarrow e_N^T \rightarrow \end{pmatrix}}$





$$e_1 = \frac{1}{2}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix}$$

$$E = \frac{1}{2}\begin{pmatrix}\sqrt{3} & -1\\ 1 & \sqrt{3}\end{pmatrix}$$

$$e_2 = \frac{1}{2}\begin{pmatrix}-1\\ \sqrt{3}\end{pmatrix}$$

$$E^{-1} = \frac{1}{2}\begin{pmatrix}\sqrt{3} & 1\\ -1 & \sqrt{3}\end{pmatrix}$$

$$\underline{v = \frac{1}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix}}$$

$$E^{-1}\underline{v} = \frac{1}{4}\begin{pmatrix}\sqrt{3} & 1\\ -1 & \sqrt{3}\end{pmatrix}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix}$$

$$\underline{\tilde{v}} = E^{-1}\underline{v}$$

$$M\underline{v} \to E^{-1}M\underline{v} = \tilde{M}\underline{\tilde{v}} \qquad = \frac{1}{4}\begin{pmatrix}2\sqrt{3}\\ 2\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \underline{\tilde{v}}$$

$$= \underbrace{E^{-1}ME}_{\tilde{M}}\underbrace{E^{-1}\underline{v}}_{\tilde{v}}$$

$$\underline{\tilde{v}} = \underset{\text{old}\to\text{new}}{E^{-1}}\underline{v}$$

$$\underline{v} = \underset{\text{new}\to\text{old}}{E}\underline{\tilde{v}}$$

$$\underset{\text{new}}{\tilde{M}} = \underset{\text{old}\to\text{new}}{E^{-1}}\ \underset{\text{old}}{M}\ \underset{\text{new}\to\text{old}}{E}$$

$\underset{\sim}{e}_i \cdot \underset{\sim}{e}_j = \delta_{ij}$ $\quad E$ orthogonal

$E^{-1} = E^T \quad EE^T = E^T E = \mathbb{1}$

Back to Gaussian

map to $\underset{\sim}{e}_i$

$$P(\underline{x}) = k\, e^{-\frac{1}{2}\underset{\sim}{x}^T C^{-1} \underline{x}}$$

$$O = \begin{pmatrix} | & & | \\ e_1 & \cdots & e_n \\ | & & | \end{pmatrix}$$

$$C \to O^{-1} C O$$

$$C^{-1} \to O^{-1} C^{-1} O$$

$$\underline{x} \to O^{-1}\underline{x} = O^T \underline{x}$$

$$\underline{x}^T \to (O^{-1}\underline{x})^T = (O^T \underline{x})^T = \underline{x}^T O$$

$$x^T C^{-1} \underline{x} = \underbrace{x^T O}_{\underline{\tilde{x}}^T} \underbrace{O^T C^{-1} O}_{\tilde{C}} \underbrace{O^T \underline{x}}_{\underset{\sim}{\tilde{x}}}$$

$$= k\, e^{-\frac{1}{2}\underline{\tilde{x}}\, \tilde{C}^{-1} \underline{\tilde{x}}}$$

$$C_{ij} = \langle x_i x_j \rangle = \delta_{ij} \sigma_i^2$$

$$C = \langle \underline{x}\, \underline{x}^T \rangle$$

$$\tilde{C} = O^{-1} C O = O^{-1} \langle \underline{x}\, \underline{x}^T \rangle O$$

$$= \langle O^{-1} \underline{x}\, \underline{x}^T O \rangle$$

$$= \langle \underline{\tilde{x}}\, \underline{\tilde{x}}^T \rangle$$

Conclusion: Gaussian distribution in arbitrary orthog basis

if $k e^{-\underline{x}^T C^{-1} \underline{x}} = P(\underline{x})$ $\quad \underline{x} \to \underline{x} - \underline{x}_m$

where $C = \langle \underline{x}\, \underline{x}^T \rangle$

But: there's a special basis in which C is diagonal

- eigenvector basis of C

& in that basis $\langle x_i x_j \rangle = \delta_{ij} \sigma_i^2$

so diag entries of C are variances

& C is symmetric $\quad (XX^T)^T = XX^T$

$\Rightarrow$ always has a complete orthonormal basis of eigenvec's w/ real eigenvalues

Recall: Gaussian is the max entropy distribution w/ given mean & variance on $(-\infty, \infty)$

1D Max entropy constraining $\langle f_1(x)\rangle, \langle f_2(x)\rangle, \ldots$

$$L(P(x)) = -\int dx\, \underline{P(x)} \ln \underline{P(x)}$$
$$+ \lambda_0 \left(\int dx\, P(x) - 1 \right)$$
$$\longrightarrow \quad + \lambda_1 \left(\int dx\, P(x) f_1(x) - \langle f_1(x)\rangle \right)$$
$$+ \lambda_2 \left(\int dx\, P(x) f_2(x) - \langle f_2(x)\rangle \right)$$
$$+ \ldots$$

$$\frac{\delta L}{\delta P} = -\ln P(x) - 1 + \lambda_0 + \lambda_1 f_1(x) + \lambda_2 f_2(x) + \ldots$$
$$= 0$$

$$P(x) = e^{\underline{\lambda_0 - 1}}\, e^{\underline{\lambda_1} f_1(x) + \underline{\lambda_2} f_2(x) + \ldots}$$

$$f_1(x) = x \qquad f_2(x) = (x - \langle x\rangle)^2$$

$$e^{(\lambda_2 (x - \cancel{x})^2 + \lambda_1 x^2)}$$

$$\Rightarrow e^{-\frac{(x - x_{m})^2}{2\sigma^2}}$$

PCA: mean & cov

$\Rightarrow$ principal axes = eig vec's of cov

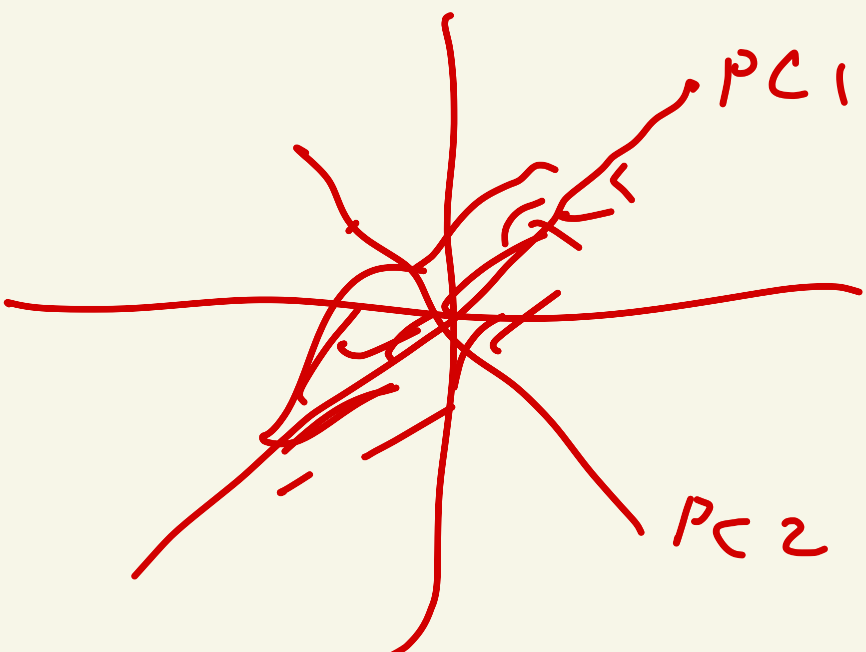
(1) zero-mean data $\rightarrow \underline{x}$

(2) Find $C = \langle \underline{x}\,\underline{x}^T \rangle$

(3) PC1 = Eigvec of C w/ most var

PC2 = " " " w/ 2nd most var

etc.

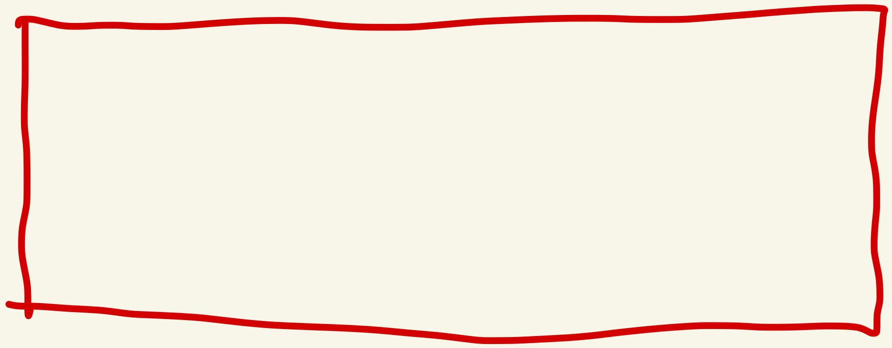


$\rightarrow$ Pick # that have X% of variance

OR

Relationship to SVD

neurons
N



Time
T

$M: N \times T$

MM^T: $N \times N$ covariance — neuron neuron cov

$$\langle a_i a_j \rangle = \frac{1}{T} MM^T_{ij}$$

M^TM: $T \times T$ time-time covariance

SVD

$$M = \underset{N\times N}{U}\ \underset{\substack{\text{diag} \\ N\times T}}{S}\ \underset{T\times T}{V^T}$$

$UU^T = \mathbb{1}$

$VV^T = \mathbb{1}$

$$MM^T = U \underset{N\times T}{S} \underbrace{V^T V}_{\mathbb{1}} \underset{T\times N}{S^T} U^T$$

$$= \underbrace{U}\, \underset{N\times N}{S^2}\, \underline{U^T \begin{pmatrix} \uparrow \\ u_3 \\ \downarrow \end{pmatrix}}$$

$Mv = \sum_i v_i m_i$

eigenvectors = columns of U

eigenvalues = s_i^2

$$M = USV^T$$

$$M^T M = \underbrace{V}_{T\times T}\,\underbrace{S^T}_{T\times N}\,\underbrace{U^T U}_{I}\,\underbrace{S}_{N\times T}\,\underbrace{V^T}_{T\times T}$$

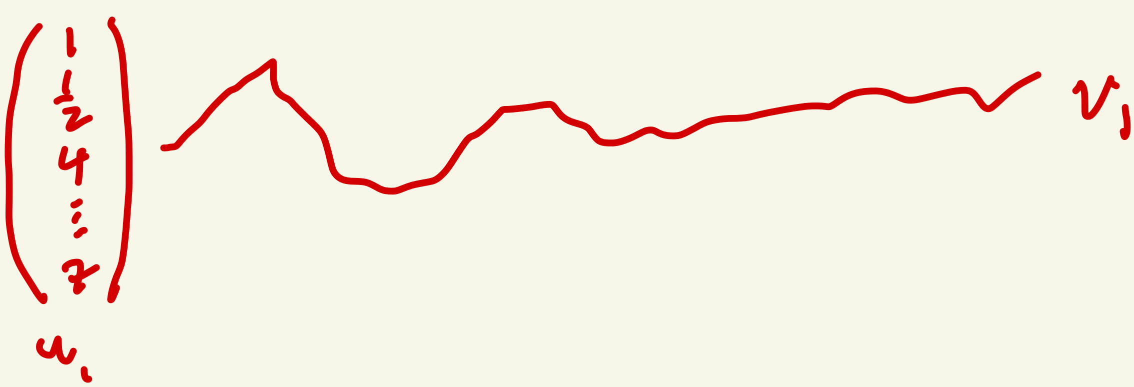
$$= V S^2 V^T$$

eigenvectors are columns of V
w/ eigenvalues s_i^2

Neuron PCA = eigenvectors of MM^T
of U

Time PCA = " " $M^T M$
of V

$$M = \sum_i s_i^2 \underbrace{\underline{u}_i \underline{v}_i^T}$$



$$M = N \times (\#\text{trials} \times \#\text{stim} \times \#\text{time})$$

Variants on PCA

Demixed PCA (dPCA)

Kobak, ...
& Machens
2016

Find components w/ most variance __about__ some aspect of data

Data: neurons × time × stimuli × decisions × trials
N t s d k

$N \times (TSDK)$

$\underline{x}_{tsdk}$

$\underline{x}_{tsd} = \langle \underline{x}_{tsdk} \rangle_k$

$$x_{tsd} = \langle x_{tsdk} \rangle_k$$

$$
\begin{array}{c}
\Sigma \\
= \underline{x}_{tsdk}
\end{array}
\left\{
\begin{aligned}
\bar{\underline{x}} &= \langle x_{tsd} \rangle_{tsd} \\
\bar{\underline{x}}_t &= \langle \underline{x}_{tsd} - \bar{\underline{x}} \rangle_{sd} \\
\bar{\underline{x}}_s &= \langle \underline{x}_{tsd} - \bar{\underline{x}} \rangle_{td} \\
\bar{\underline{x}}_d &= \langle \underline{x}_{tsd} - \bar{\underline{x}} \rangle_{st} \\
\bar{\underline{x}}_{ts} &= \langle \underline{x}_{tsd} - \bar{\underline{x}} - \bar{\underline{x}}_t - \bar{\underline{x}}_s - \bar{\underline{x}}_d \rangle_d \\
\bar{\underline{x}}_{td} &= \langle \qquad \rangle_s \\
\bar{\underline{x}}_{sd} &= \langle \qquad \rangle_t \\
\underset{\frown}{\bar{\underline{x}}_{tsd}} &= \underset{\frown}{\underline{x}_{tsd}} - \bar{\underline{x}} - \bar{\underline{x}}_t - \bar{\underline{x}}_s - \bar{\underline{x}}_d - \bar{\underline{x}}_{ts} \\
&\qquad - \bar{\underline{x}}_{td} - x_{sd} \\
\underline{\epsilon}_{tsdk} &= \underline{x}_{tsdk} - \underline{x}_{tsd}
\end{aligned}
\right.
$$

$\bar{\underline{x}}_{ts} \Leftarrow \bar{\underline{x}}_s + \bar{\underline{x}}_{ts}$ "stimulus term"

$\bar{\underline{x}}_{td} \Leftarrow \bar{\underline{x}}_d + \bar{\underline{x}}_{td}$ "decision term"

$\bar{\underline{x}}_{tsd} \Leftarrow \bar{\underline{x}}_{sd} + x_{tsd}$ "stim-dec interaction"

$$\underline{X}_{tsdk} = \bar{\underline{X}} + \bar{\underline{X}}_t + \bar{\underline{X}}_{ts} + \bar{\underline{X}}_{td} + \bar{\underline{X}}_{tsd} + \varepsilon_{tsdk}$$

$$X \Rightarrow \underline{X}_{tsdk} \Leftarrow \underline{x}_{tsdk} - \bar{\underline{X}}$$

X_t $N \times KTSD$

X_{ts} $N \times T$ unique values repeated KSD times

$$X = X_t + X_{ts} + X_{td} + X_{tsd} + X_{noise}$$

$$= \sum_\phi X_\phi + X_{noise}$$

$$\langle X_a X_b^T \rangle = 0 \text{ fn } a \neq b$$

$$\underset{N \times KSTD}{X}\ \underset{KSTD \times N}{X^T} = C_t + C_{ts} + C_{td} + C_{tsd} + C_{noise}$$

$$= \sum_\phi C_\phi + \text{noise}$$