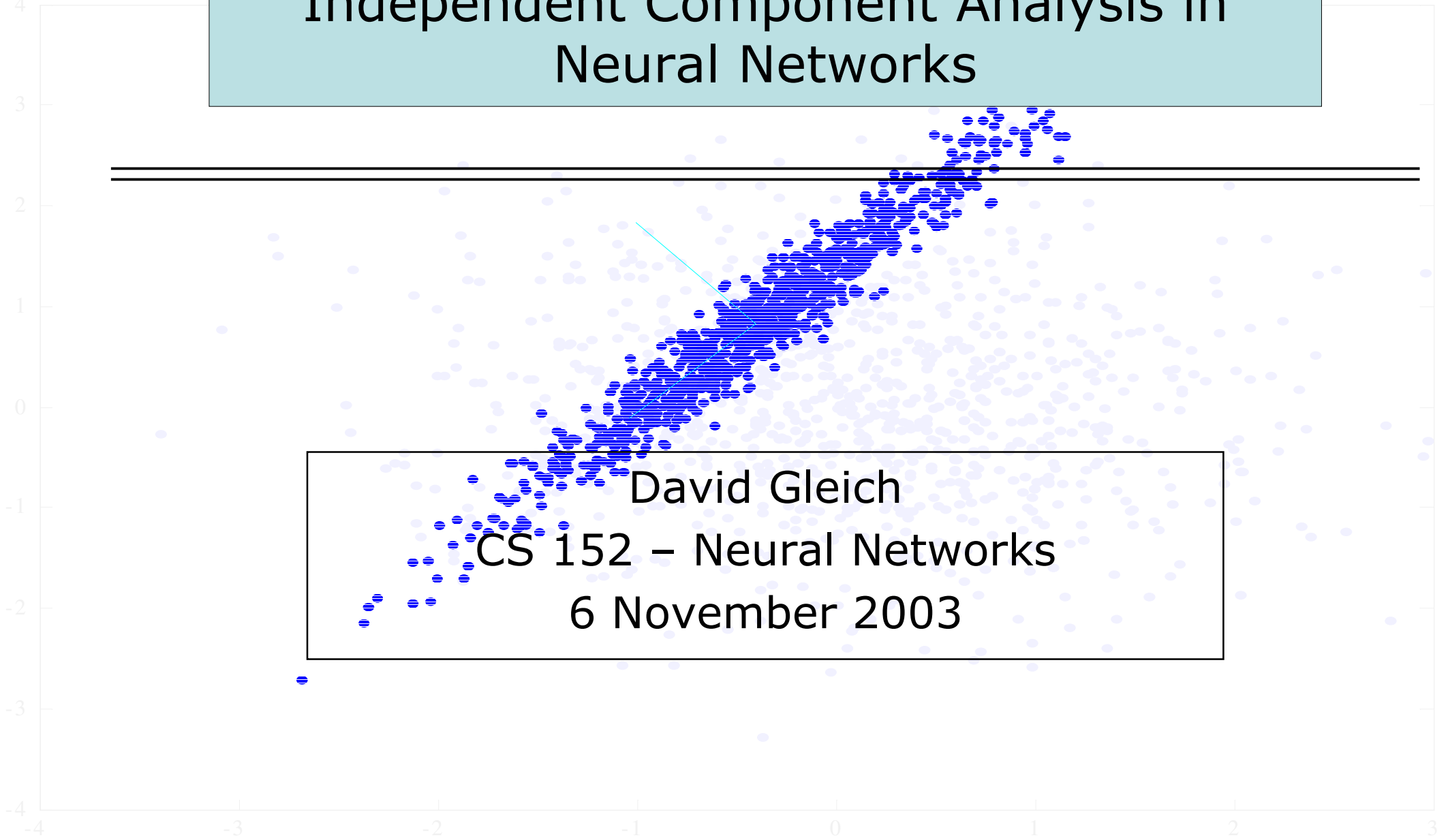


Principal Component Analysis and Independent Component Analysis in Neural Networks



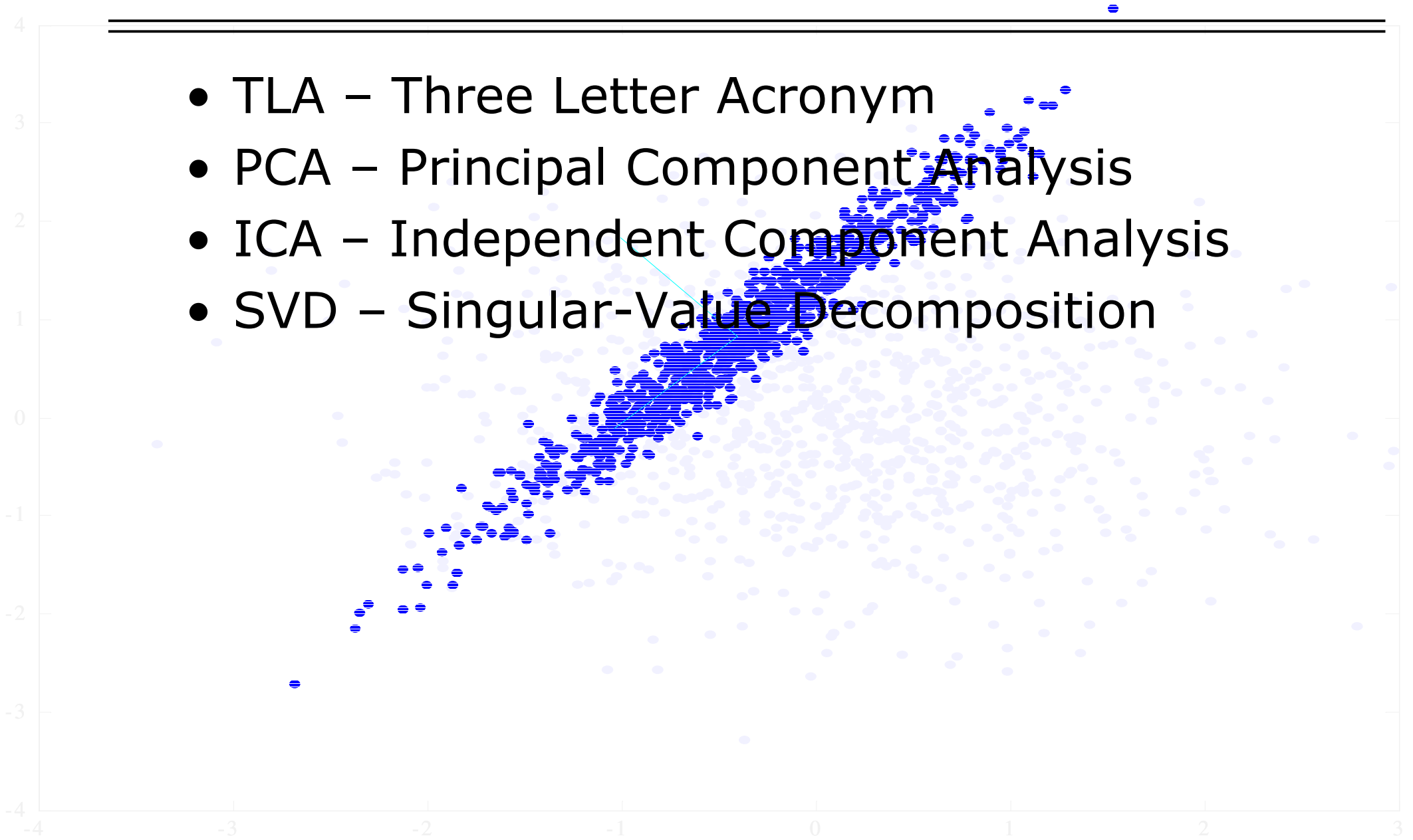
David Gleich

CS 152 – Neural Networks

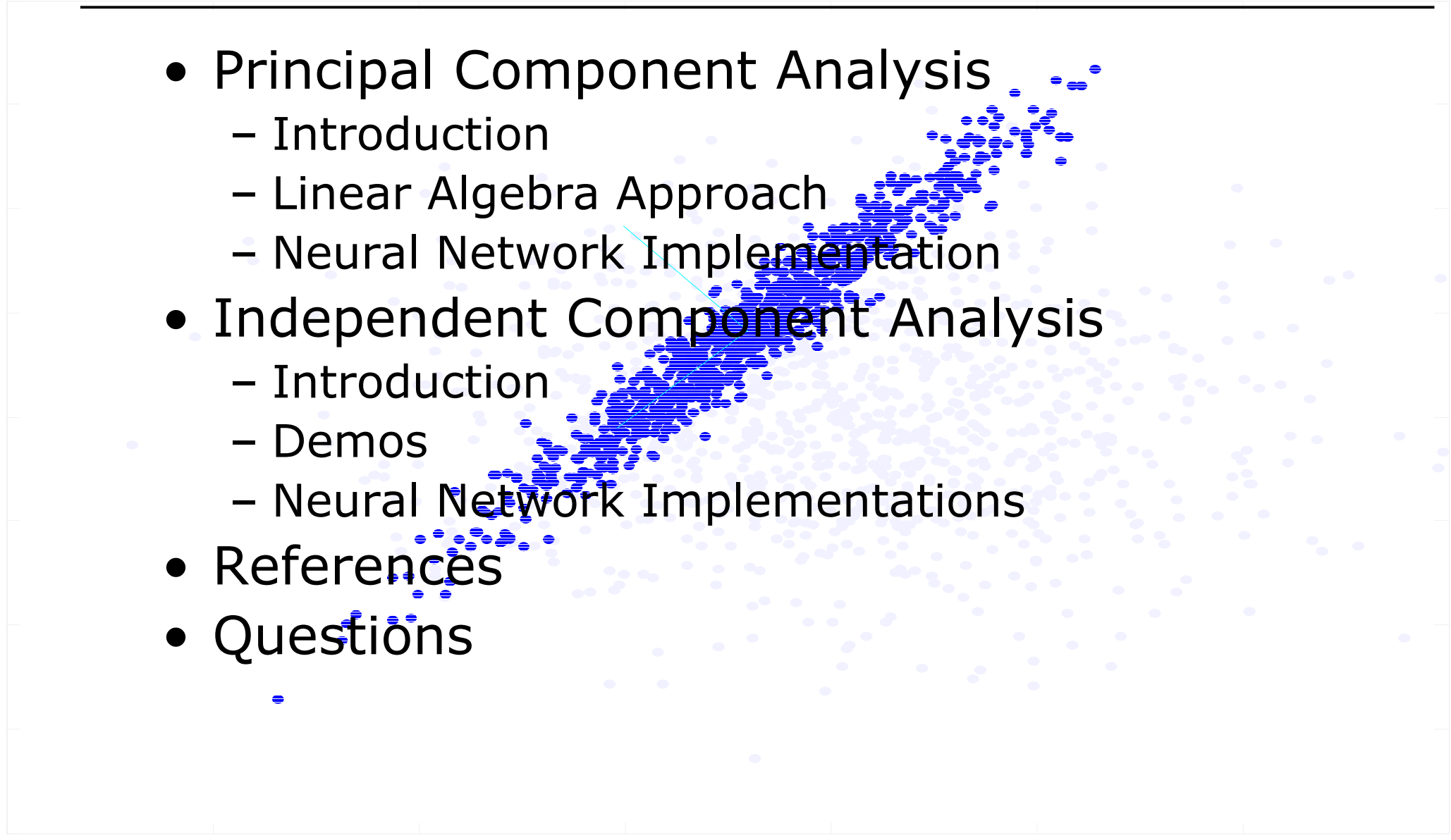
6 November 2003

TLAs

- TLA – Three Letter Acronym
- PCA – Principal Component Analysis
- ICA – Independent Component Analysis
- SVD – Singular-Value Decomposition

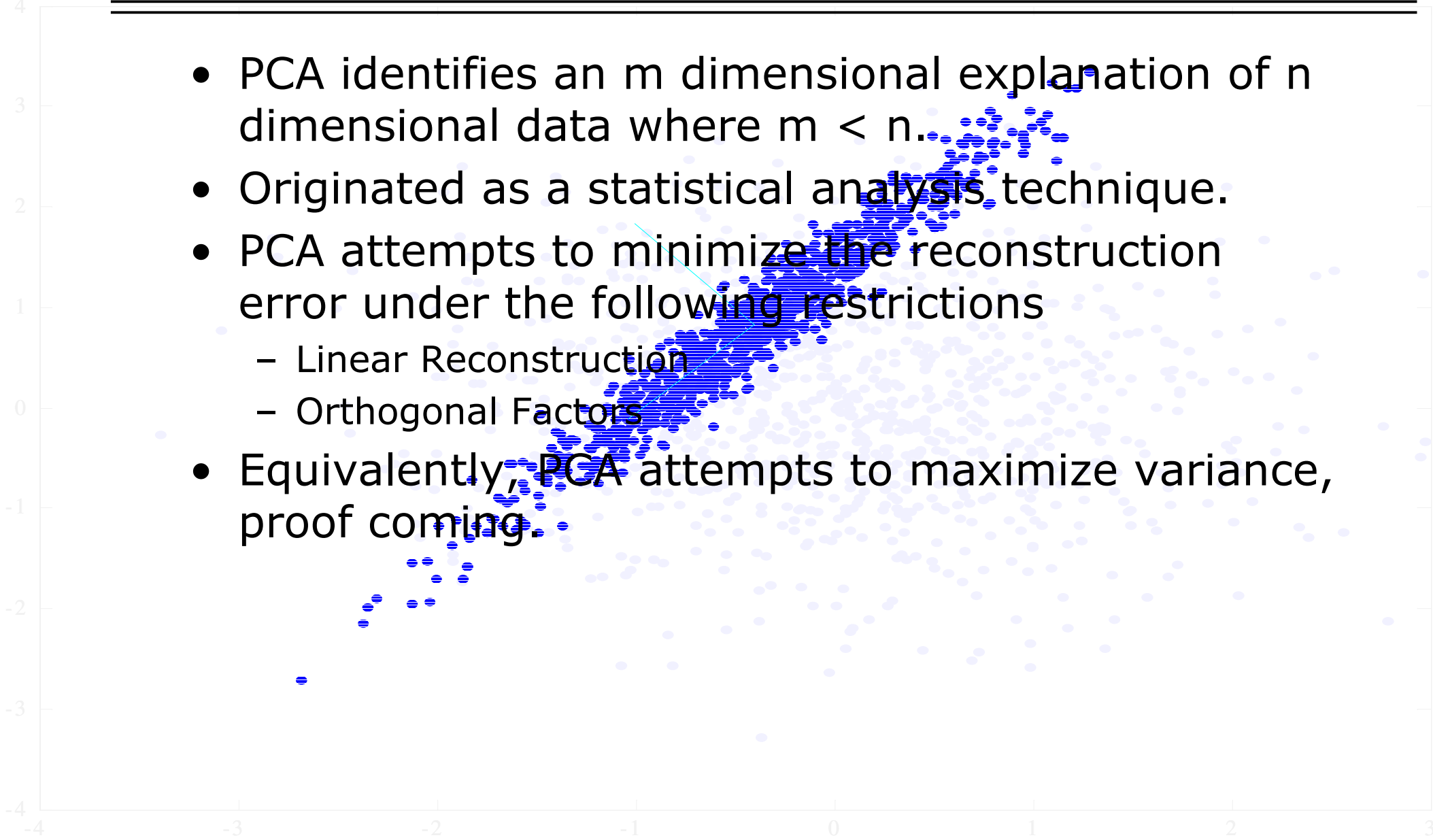


Outline

- Principal Component Analysis
 - Introduction
 - Linear Algebra Approach
 - Neural Network Implementation
 - Independent Component Analysis
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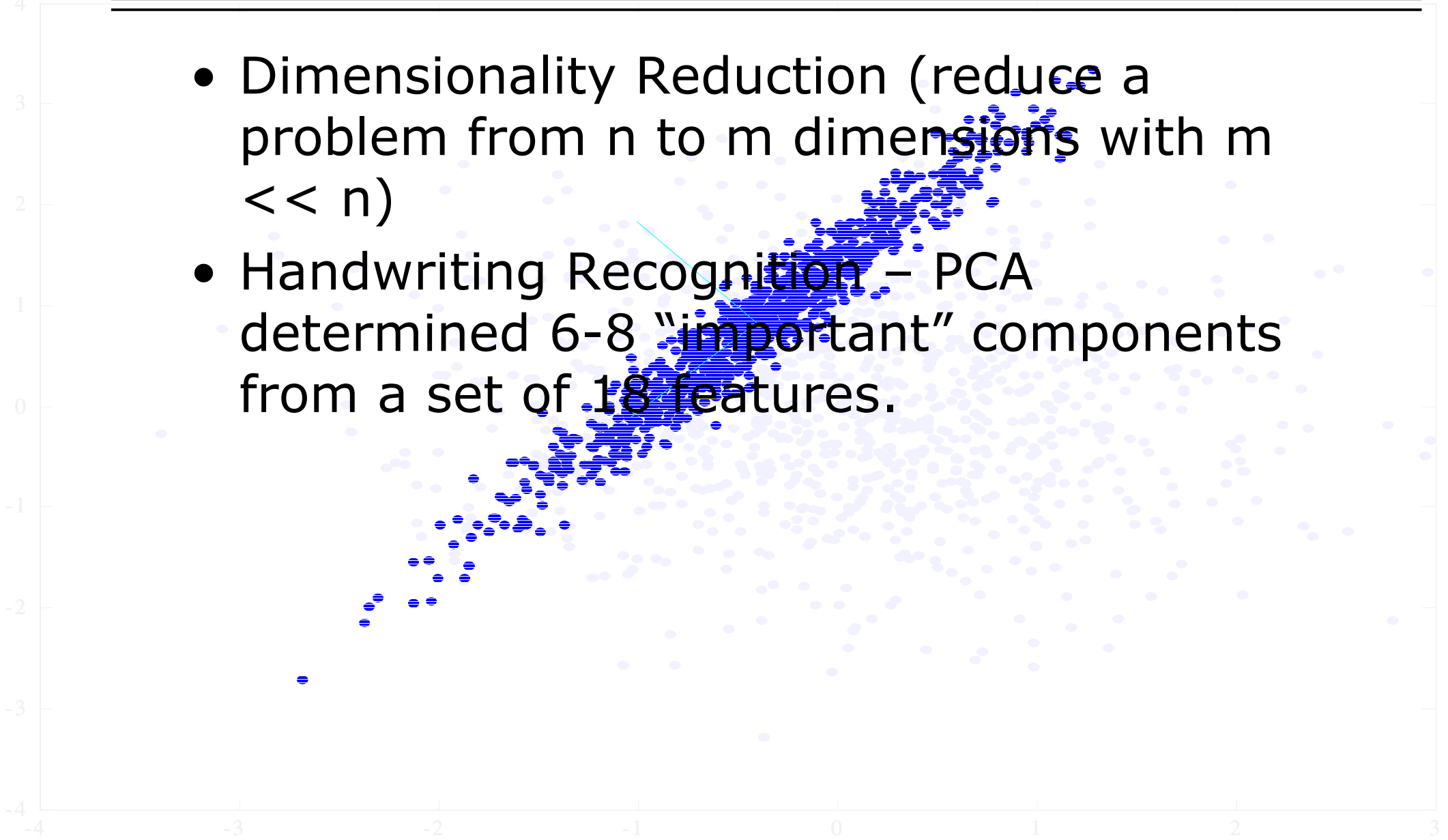
Principal Component Analysis

- PCA identifies an m dimensional explanation of n dimensional data where $m < n$.
- Originated as a statistical analysis technique.
- PCA attempts to minimize the reconstruction error under the following restrictions
 - Linear Reconstruction
 - Orthogonal Factors
- Equivalently, PCA attempts to maximize variance, proof coming.

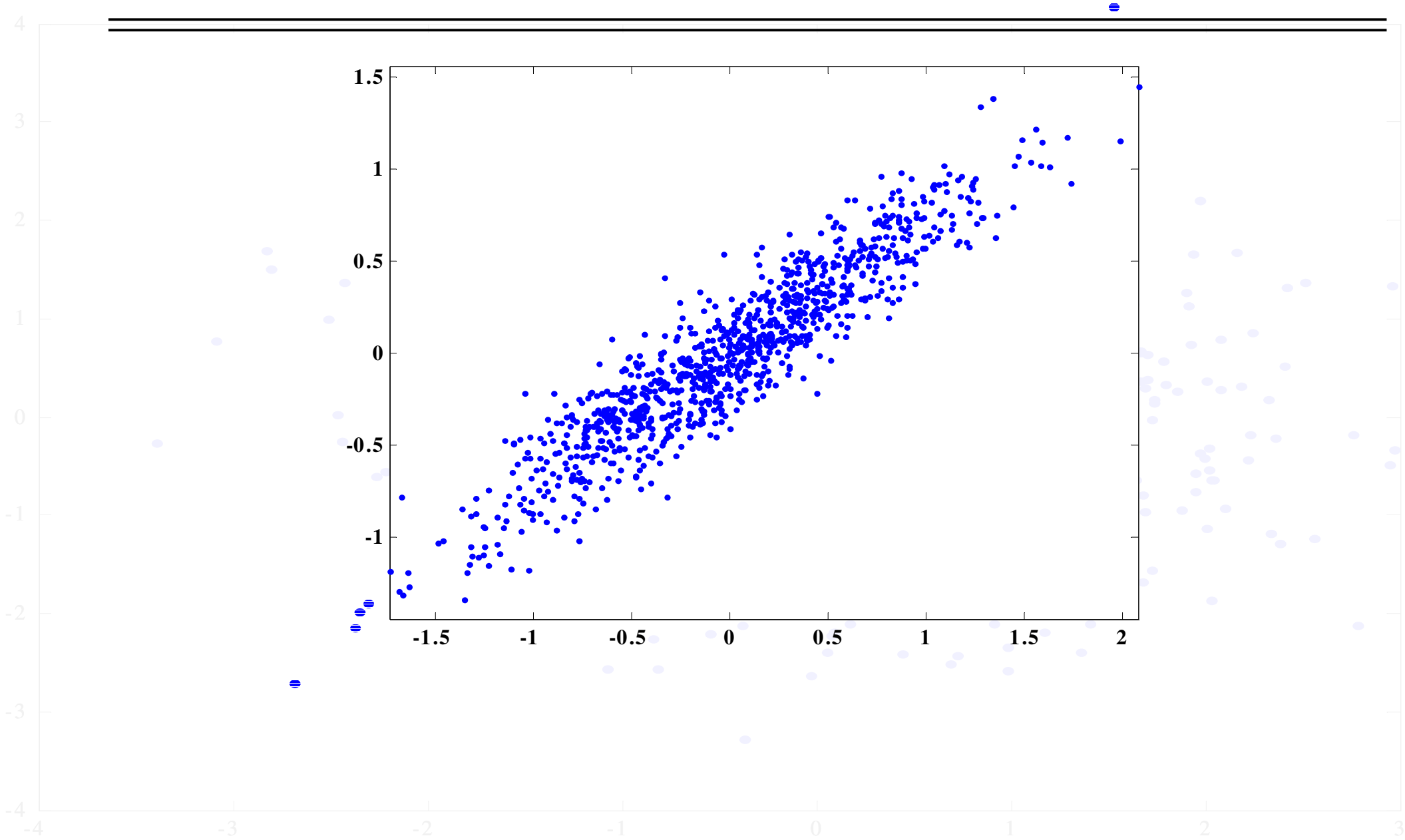


PCA Applications

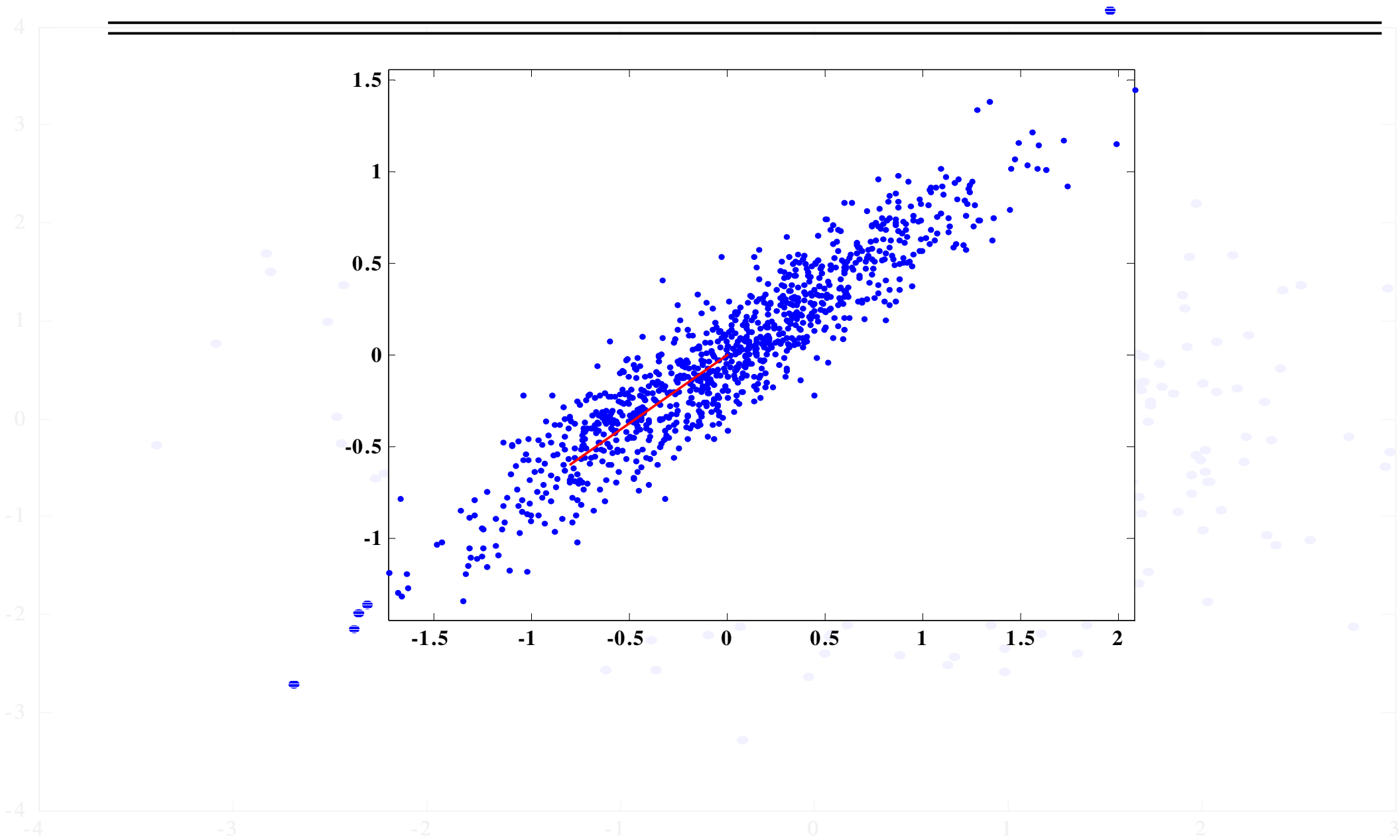
- Dimensionality Reduction (reduce a problem from n to m dimensions with $m \ll n$)
- Handwriting Recognition – PCA determined 6-8 “important” components from a set of 18 features.



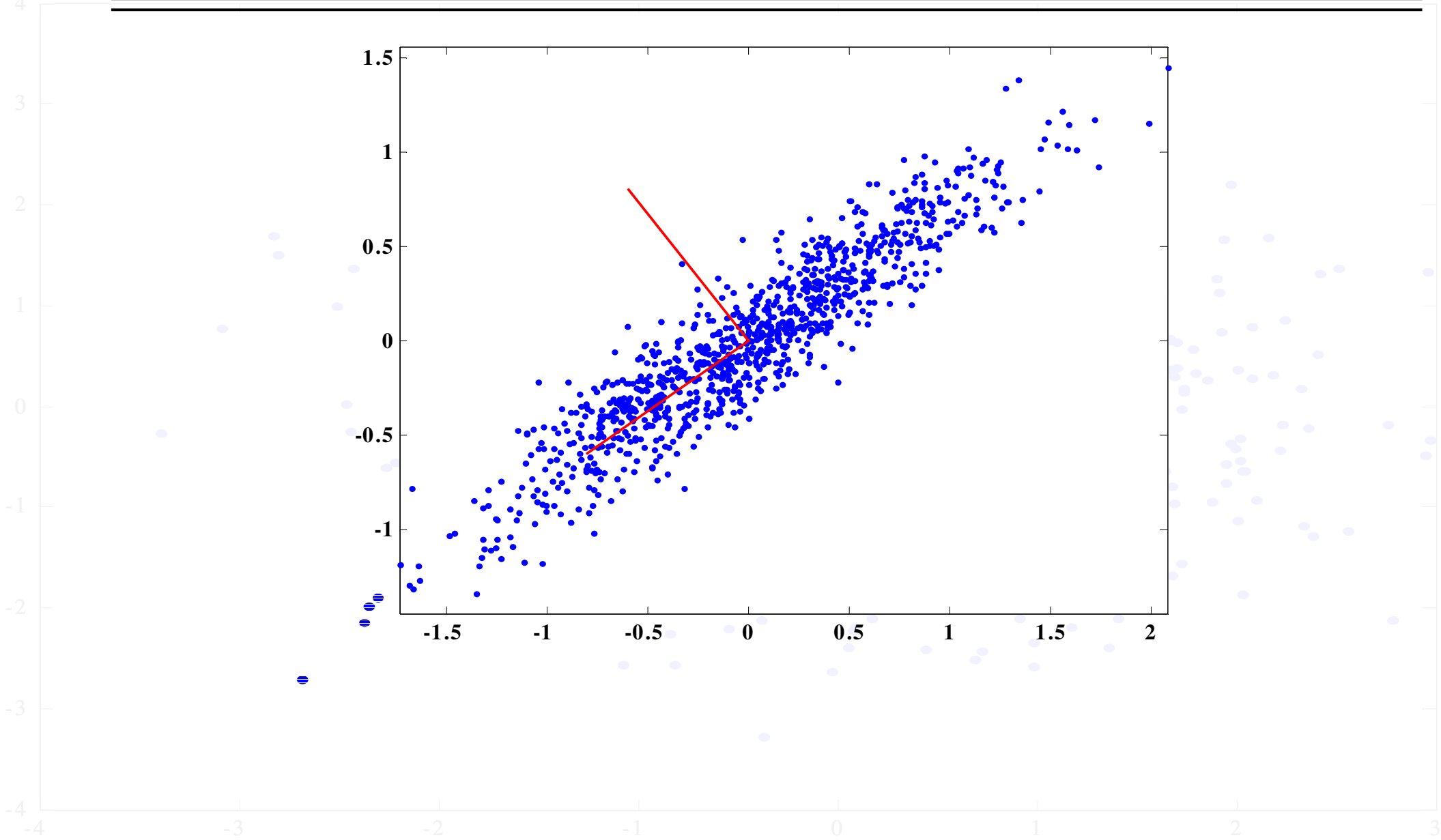
PCA Example



PCA Example



PCA Example



Minimum Reconstruction Error) Maximum Variance

Proof from Diamantaras and Kung

Take a random vector $x = [x_1, x_2, \dots, x_n]^T$ with $E\{x\} = 0$, i.e. zero mean.

Make the covariance matrix $R_x = E\{xx^T\}$.

Let $y = Wx$ be a orthogonal, linear transformation of the data.

$$WW^T = I$$

Reconstruct the data through W^T .

$$\hat{x} = W^T y = W^T W x$$

Minimize the error.

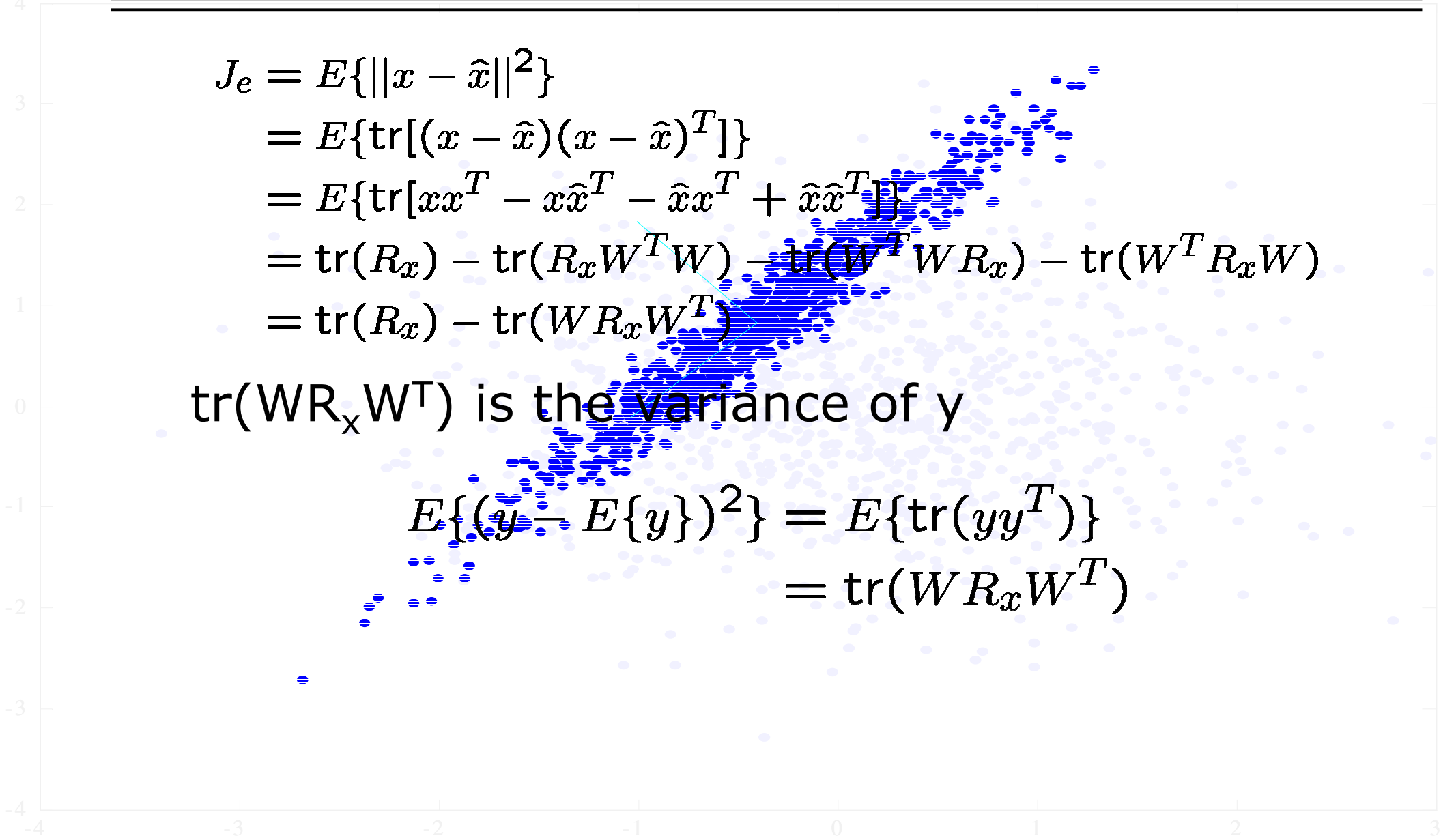
$$E\{\|x - \hat{x}\|^2\}$$

Minimum Reconstruction Error) Maximum Variance

$$\begin{aligned}
 J_e &= E\{\|x - \hat{x}\|^2\} \\
 &= E\{\text{tr}[(x - \hat{x})(x - \hat{x})^T]\} \\
 &= E\{\text{tr}[xx^T - x\hat{x}^T - \hat{x}x^T + \hat{x}\hat{x}^T]\} \\
 &= \text{tr}(R_x) - \text{tr}(R_x W^T W) - \text{tr}(W^T W R_x) - \text{tr}(W^T R_x W) \\
 &= \text{tr}(R_x) - \text{tr}(W R_x W^T)
 \end{aligned}$$

$\text{tr}(W R_x W^T)$ is the variance of y

$$\begin{aligned}
 E\{(y - E\{y\})^2\} &= E\{\text{tr}(yy^T)\} \\
 &= \text{tr}(W R_x W^T)
 \end{aligned}$$



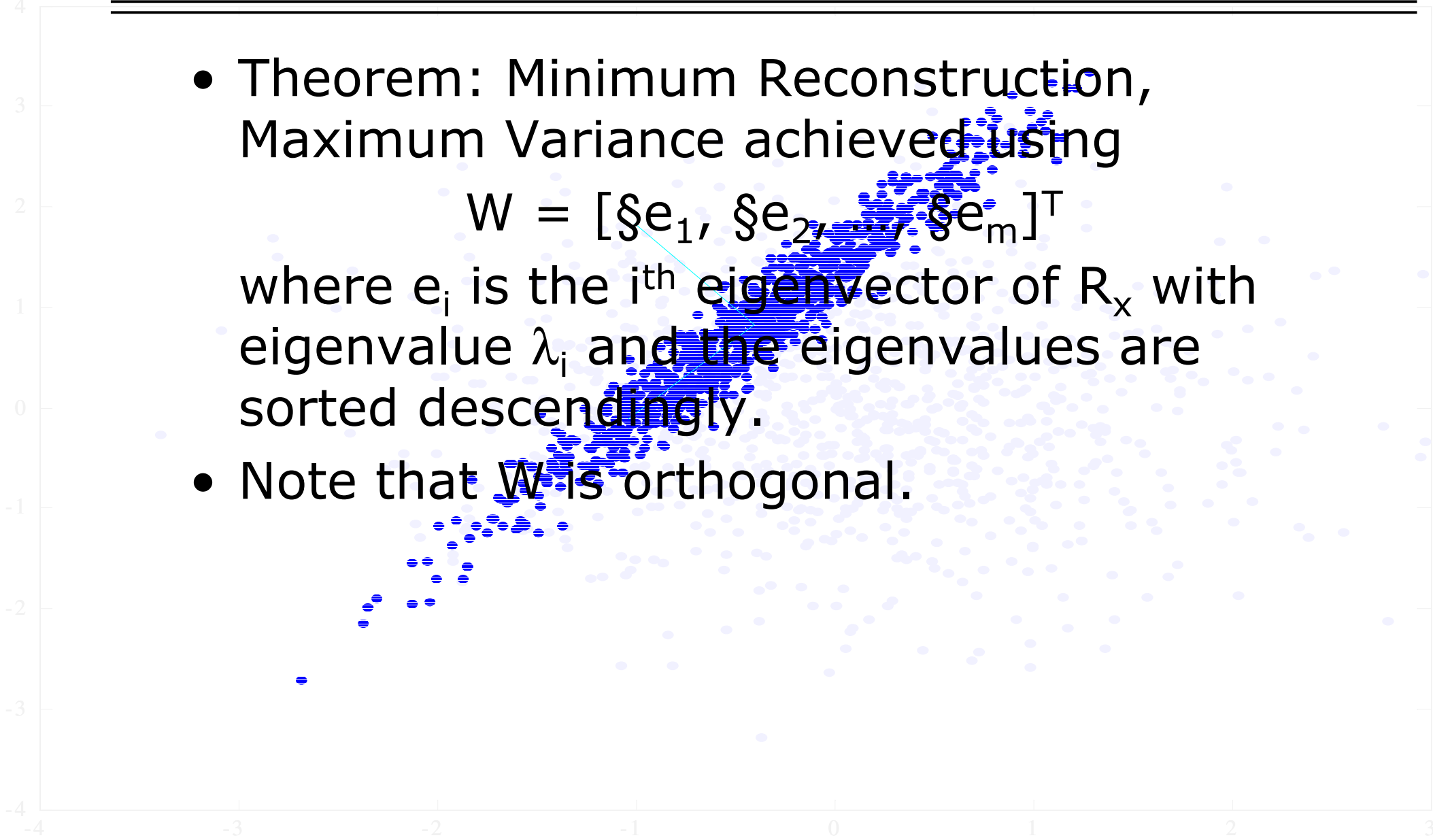
PCA: Linear Algebra

- Theorem: Minimum Reconstruction, Maximum Variance achieved using

$$W = [\xi e_1, \xi e_2, \dots, \xi e_m]^T$$

where e_i is the i^{th} eigenvector of R_x with eigenvalue λ_i and the eigenvalues are sorted descendingly.

- Note that W is orthogonal.



PCA with Linear Algebra

Given m signals of length n , construct the data matrix

$$X = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix}.$$

Then subtract the mean from each signal and compute the covariance matrix

$$C = XX^T.$$

PCA with Linear Algebra

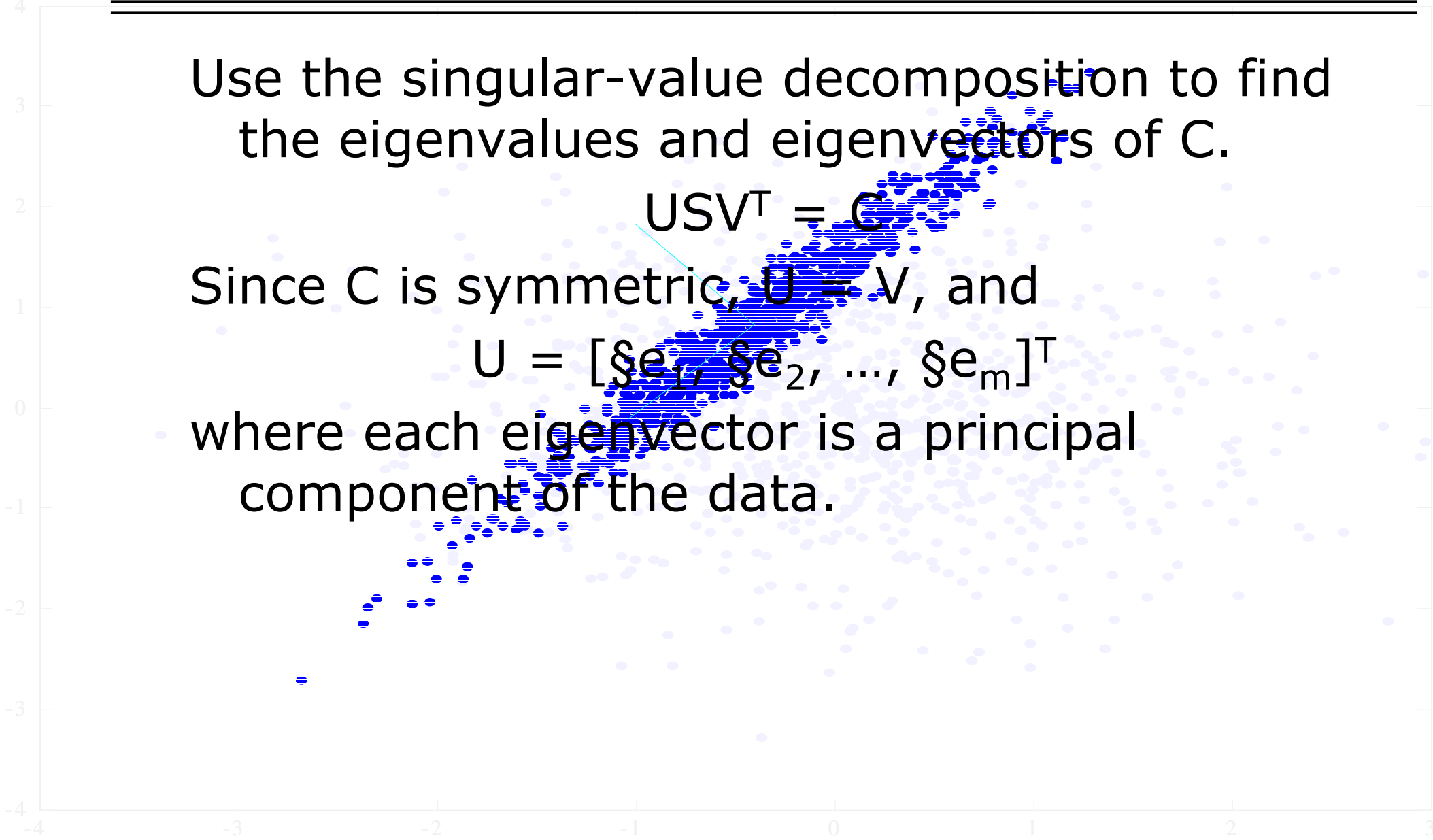
Use the singular-value decomposition to find the eigenvalues and eigenvectors of C .

$$USV^T = C$$

Since C is symmetric, $U = V$, and

$$U = [\xi e_1, \xi e_2, \dots, \xi e_m]^T$$

where each eigenvector is a principal component of the data.



PCA with Neural Networks

- Most PCA Neural Networks use some form of Hebbian learning.

“Adjust the strength of the connection between units A and B in proportion to the product of their simultaneous activations.”

$$w_{k+1} = w_k + \beta_k (y_k x_k)$$

- Applied directly, this equation is unstable.

$$\|w_k\|^2 \rightarrow \infty \text{ as } k \rightarrow \infty$$

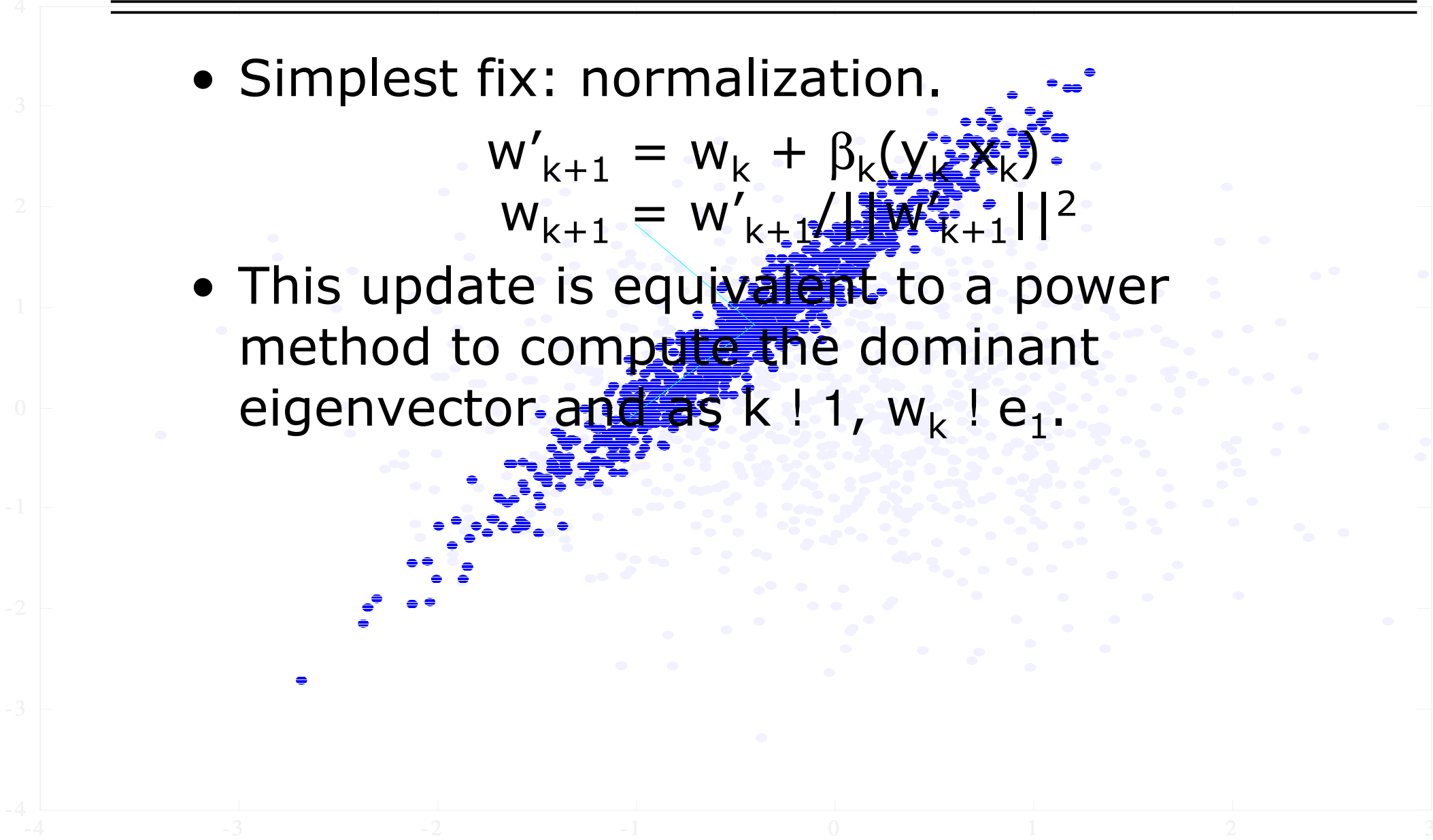
- Important Note: neural PCA algorithms are unsupervised.

PCA with Neural Networks

- Simplest fix: normalization.

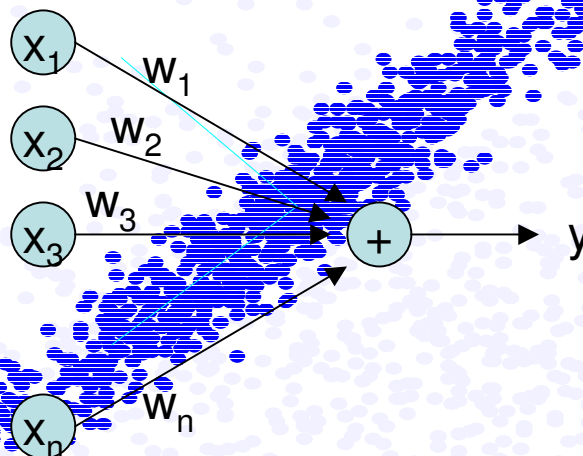
$$w'_{k+1} = w_k + \beta_k (y_k x_k)$$
$$w_{k+1} = w'_{k+1} / \|w'_{k+1}\|^2$$

- This update is equivalent to a power method to compute the dominant eigenvector and as $k \rightarrow 1$, $w_k \rightarrow e_1$.



PCA with Neural Networks

- Another fix: Oja's rule.
- Proposed in 1982 by Oja and Karhunen.

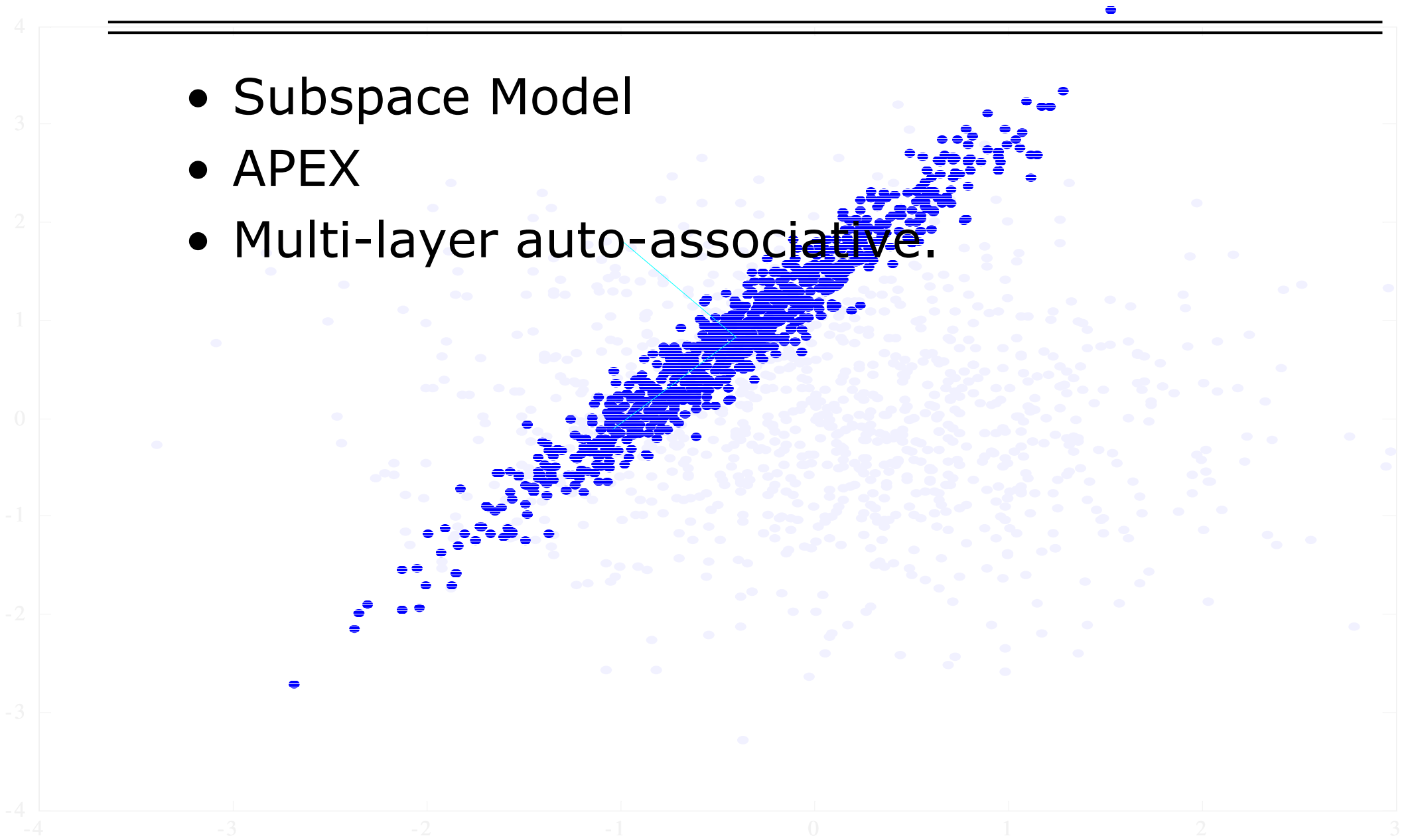


$$w_{k+1} = w_k + \beta_k (y_k x_k - y_k^2 w_k)$$

- This is a linearized version of the normalized Hebbian rule.
- Convergence, as $k \rightarrow \infty$, $w_k \rightarrow e_1$.

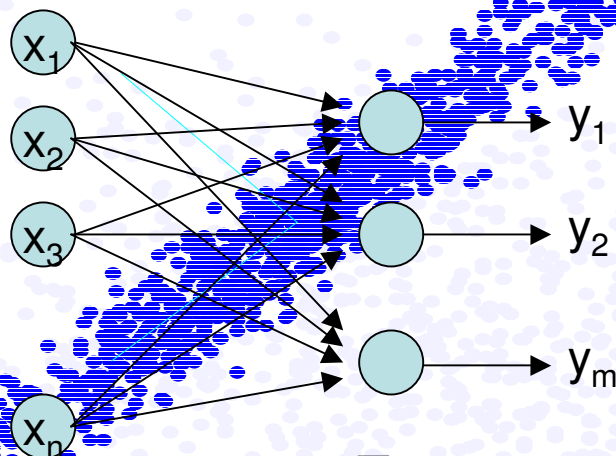
PCA with Neural Networks

- Subspace Model
- APEX
- Multi-layer auto-associative.



PCA with Neural Networks

- Subspace Model: a multi-component extension of Oja's rule.

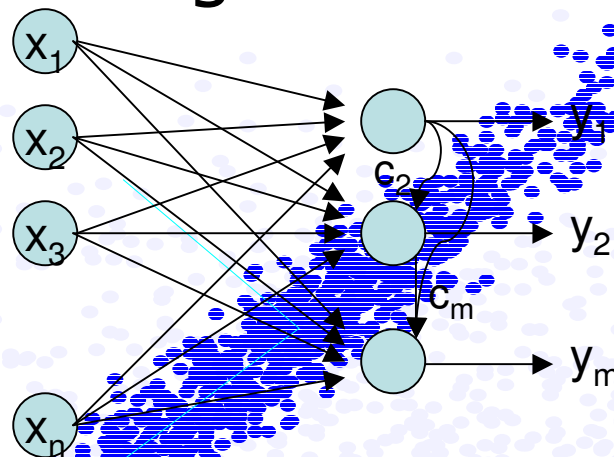


$$\Delta W_k = \beta_k (y_k x_k^T - y_k y_k^T W_k)$$

Eventually W spans the same subspace as the top m principal eigenvectors. This method does not extract the exact eigenvectors.

PCA with Neural Networks

- APEX Model: Kung and Diamantaras



$$y = Wx - Cy, \quad y = (I + C)^{-1}Wx \quad \text{or} \quad (I - C)Wx$$

$$C = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ c_{21} & 0 & 0 & \dots & 0 \\ c_{31} & c_{32} & 0 & \dots & 0 \\ \vdots & & \ddots & & \vdots \\ c_{m-1,1} & \dots & c_{m-1,m-2} & 0 & 0 \\ c_{m,1} & \dots & \dots & c_{m,m-1} & 0 \end{bmatrix}$$

PCA with Neural Networks

- APEX Learning

$$\Delta w_{i,j,k} = \beta_k (y_{ik} x_{jk} - y_{ik}^2 w_{i,j,k})$$

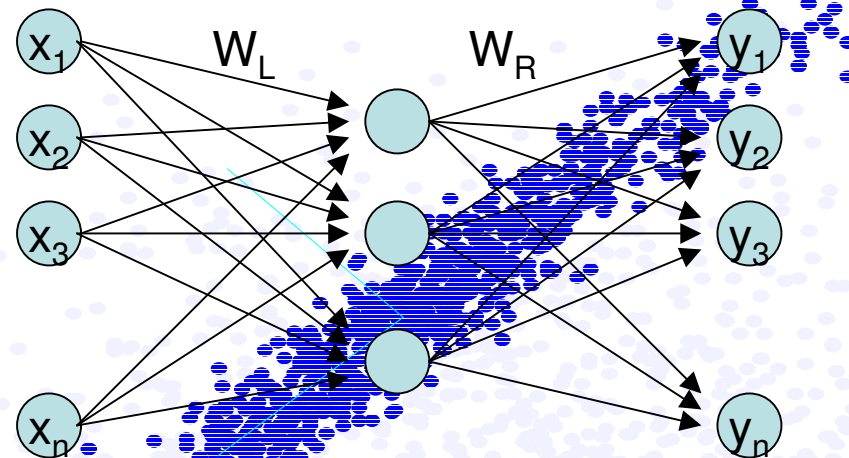
$$\Delta c_{i,j,k} = \beta_k (y_{ik} y_{jk} - y_{ik}^2 c_{i,j,k})$$

- Properties of APEX model:

- Exact principal components
- Local updates, Δw_{ab} only depends on x_a, x_b, w_{ab}
- “-Cy” acts as an orthogonalization term

PCA with Neural Networks

- Multi-layer networks: bottlenecks

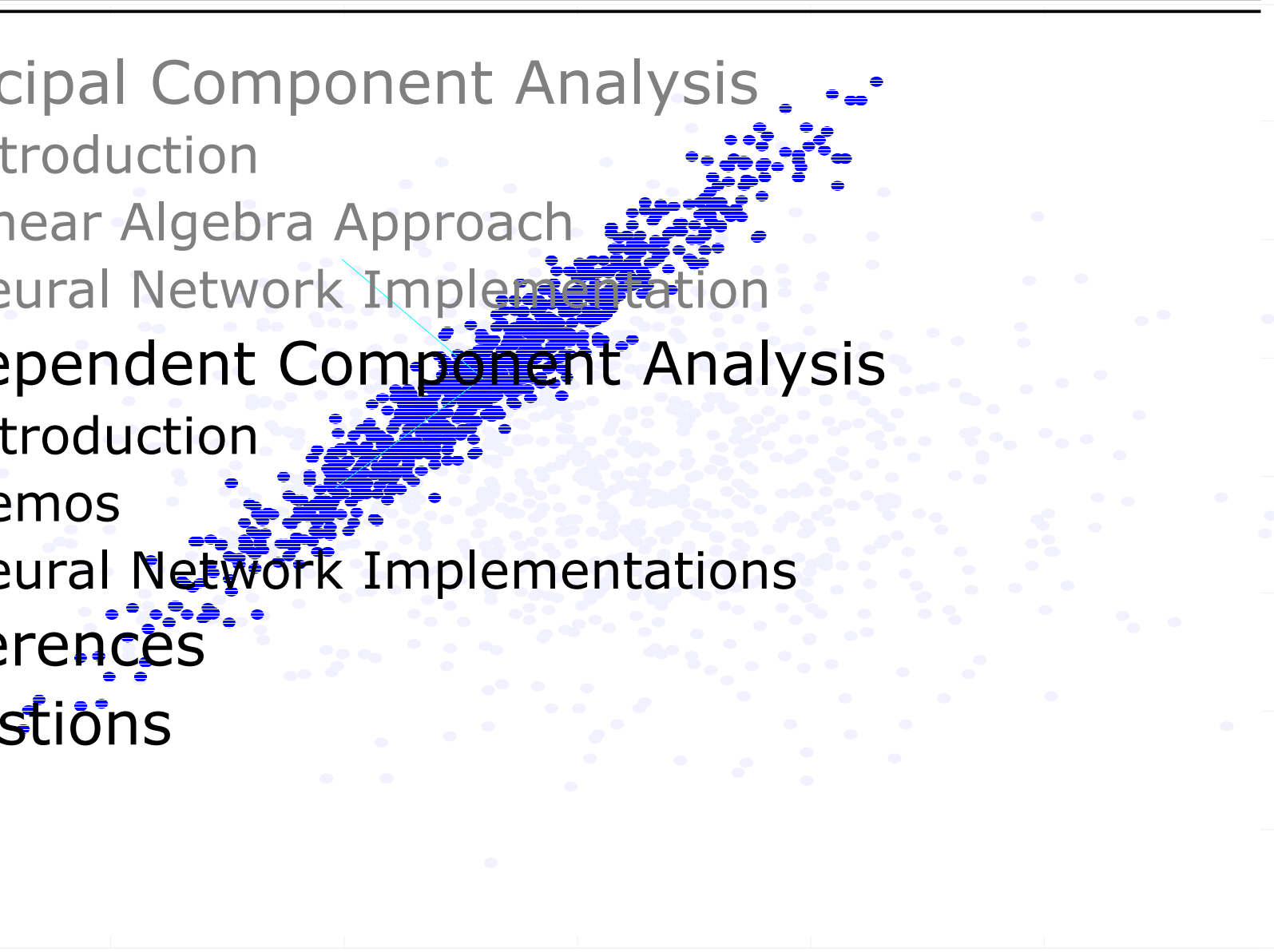


- Train using auto-associative output.

$$e = x - y$$

- W_L spans the subspace of the first m principal eigenvectors.

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Independent Component Analysis

- Also known as Blind Source Separation.
- Proposed for neuromimetic hardware in 1983 by Herault and Jutten.
- ICA seeks components that are independent in the statistical sense.

Two variables x, y are *statistically independent* iff $P(x \wedge y) = P(x)P(y)$.

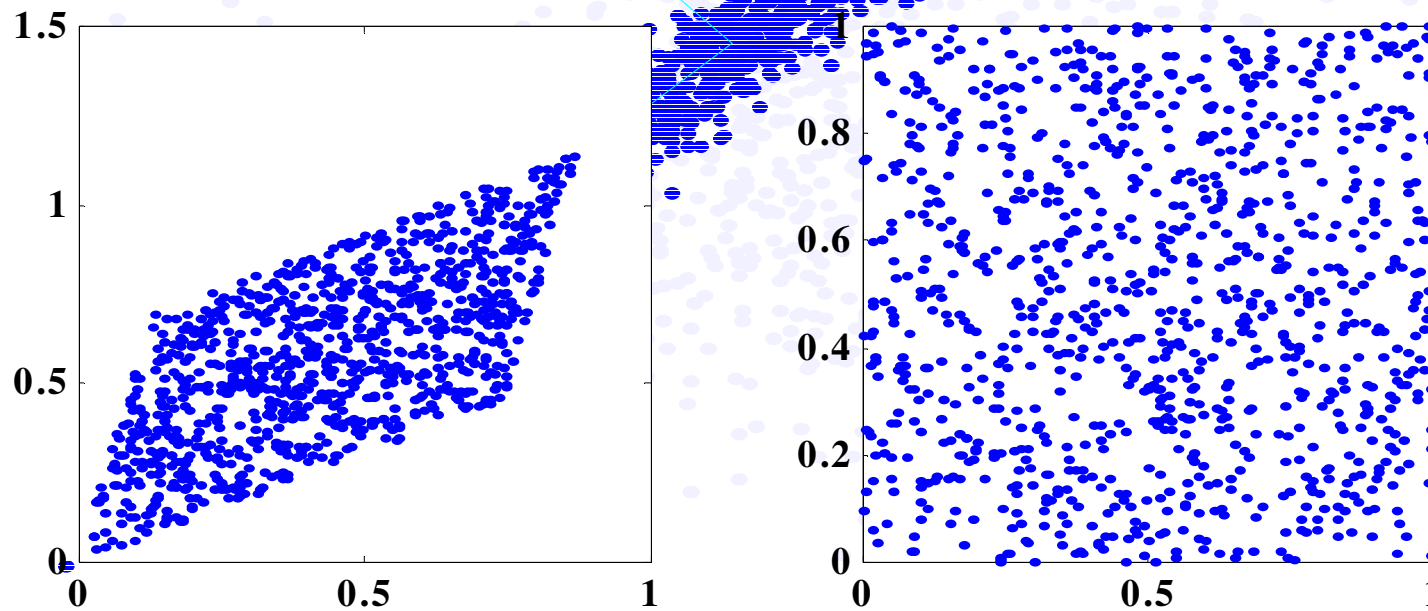
Equivalently,

$$E\{g(x)h(y)\} - E\{g(x)\}E\{h(y)\} = 0$$

where g and h are any functions.

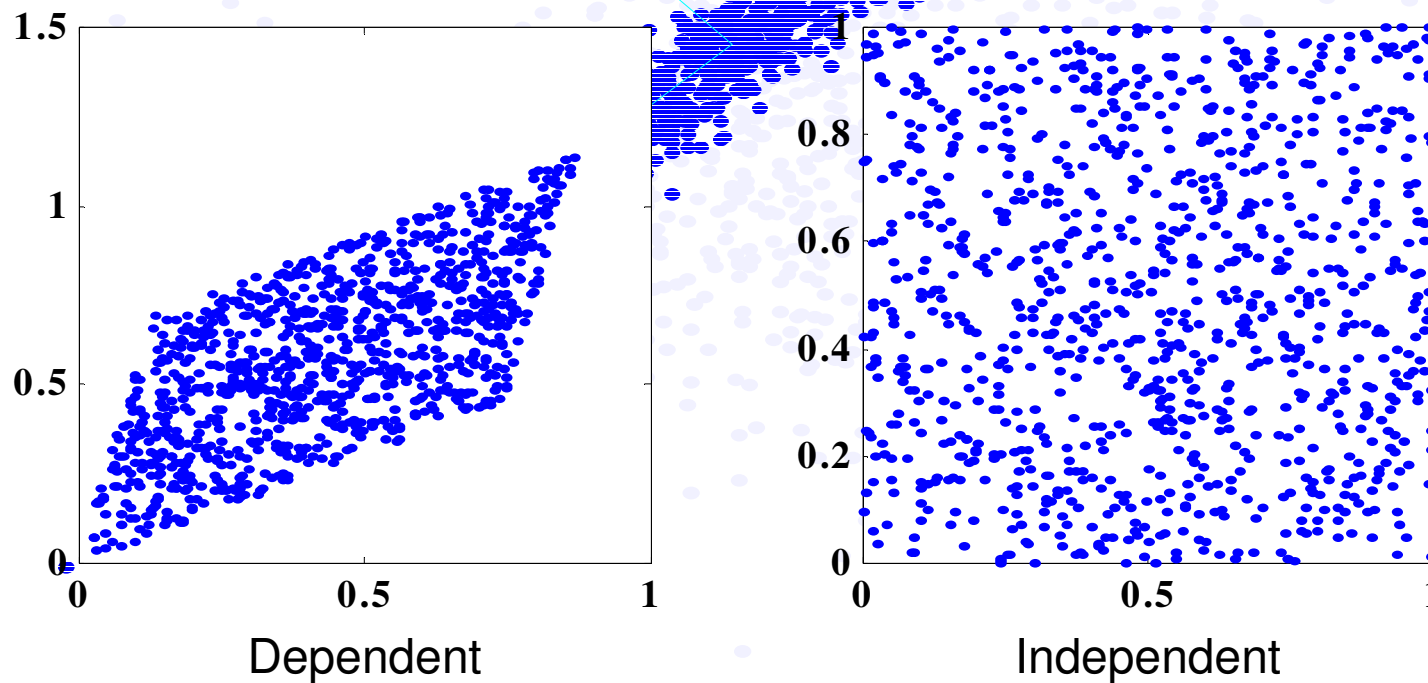
Statistical Independence

- In other words, if we know something about x , that should tell us *nothing* about y .



Statistical Independence

- In other words, if we know something about x , that should tell us *nothing* about y .



Independent Component Analysis

Given m signals of length n , construct the data matrix

$$X = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix}.$$

We assume that X consists of m sources such that

$$X = AS$$

where A is an unknown m by m mixing matrix and S is m independent sources.

Independent Component Analysis

ICA seeks to determine a matrix W such that

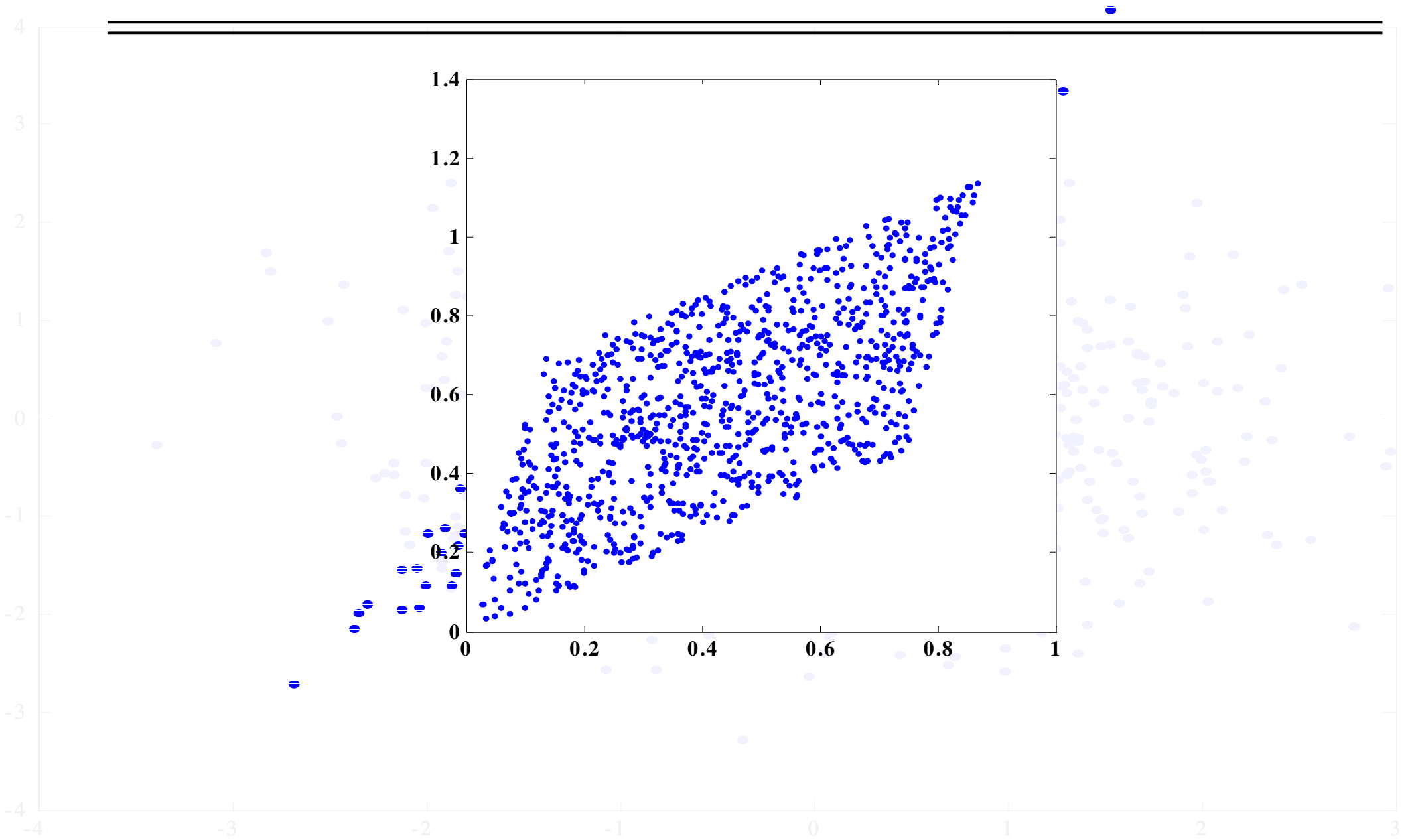
$$Y = WX$$

where W is an m by m matrix and Y is the set of independent source signals, i.e. the independent components.

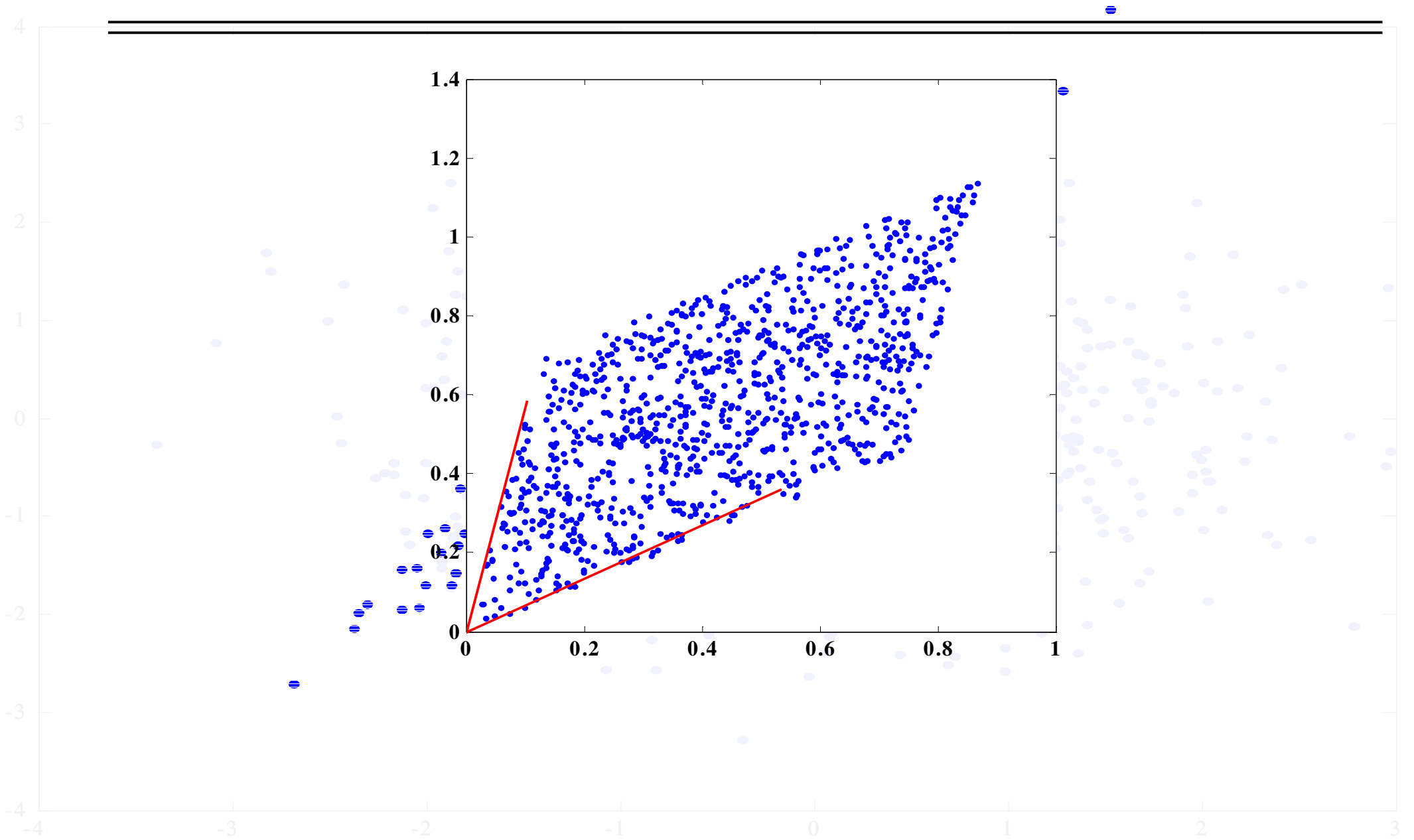
$$W = A^{-1} \Rightarrow Y = A^{-1}AX = X$$

- Note that the components need not be orthogonal, but that the reconstruction is still linear.

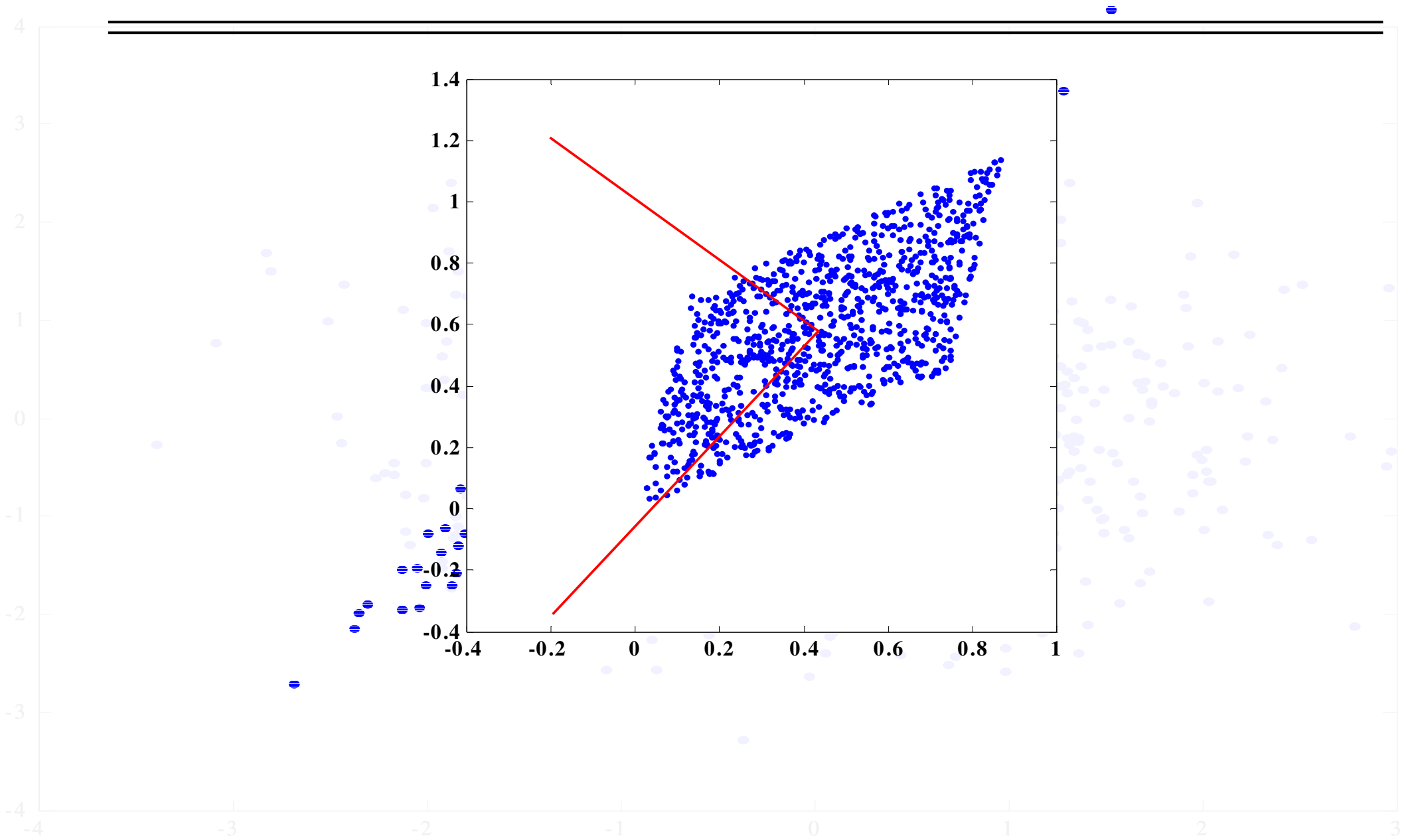
ICA Example



ICA Example

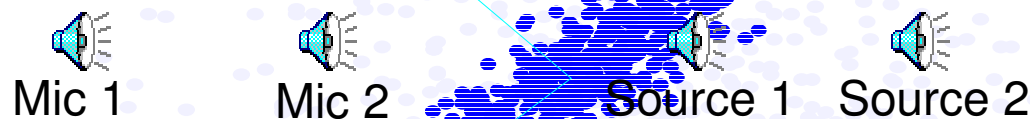


PCA on this data?



Classic ICA Problem

- The “Cocktail” party. How to isolate a single conversation amidst the noisy environment.



http://www.cnl.salk.edu/~tewon/Blind/blind_audio.html

More ICA Examples



More ICA Examples



Notes on ICA

- ICA cannot “perfectly” reconstruct the original signals.

If $X = AS$ then

1) if $AS = (A'M^{-1})(MS')$ then we lose scale

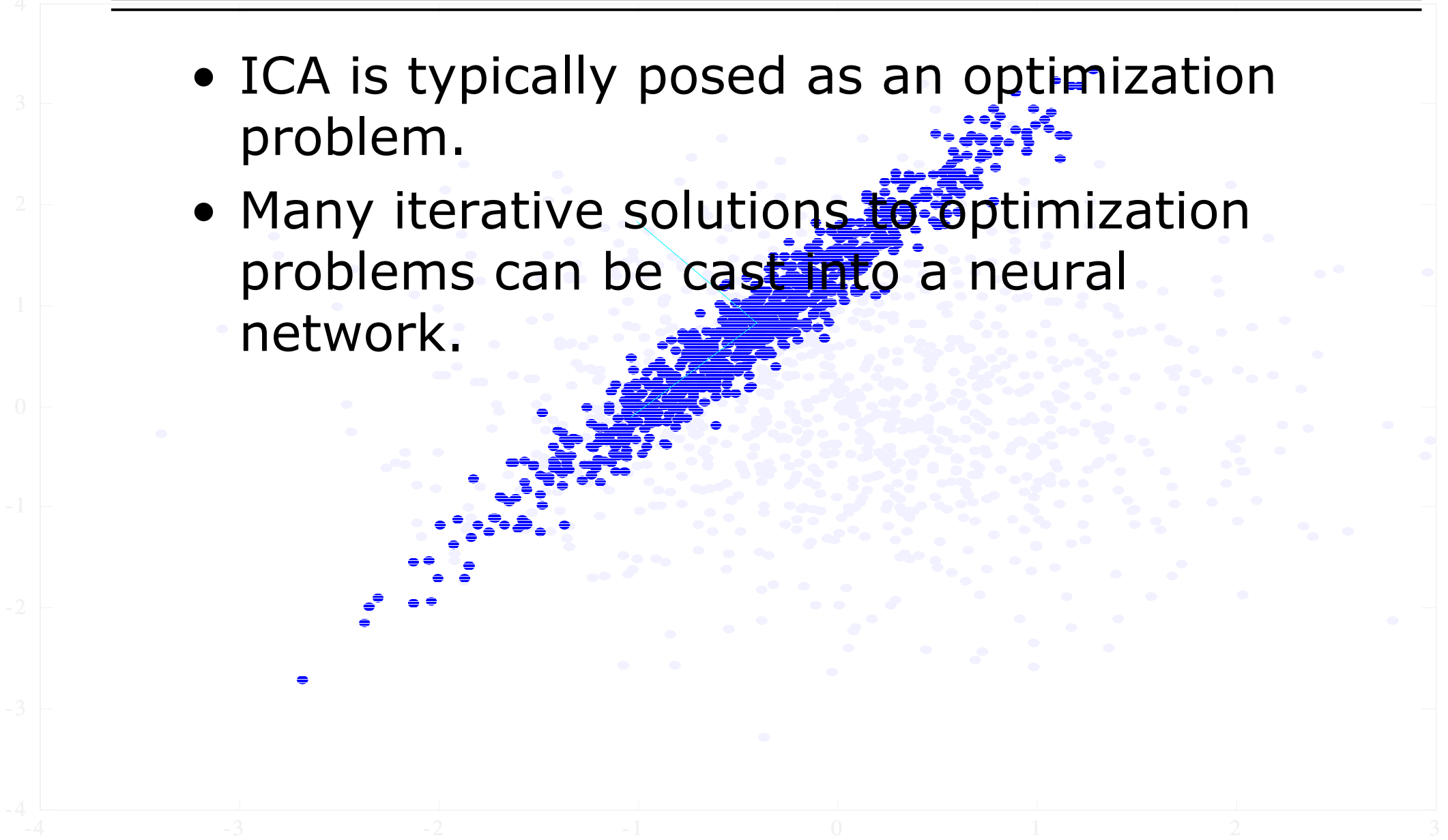
2) if $AS = (A'P^{-1})(PS')$ then we lose order

Thus, we can reconstruct only without scale and order.

- Examples done with FastICA, a non-neural, fixed-point based algorithm.

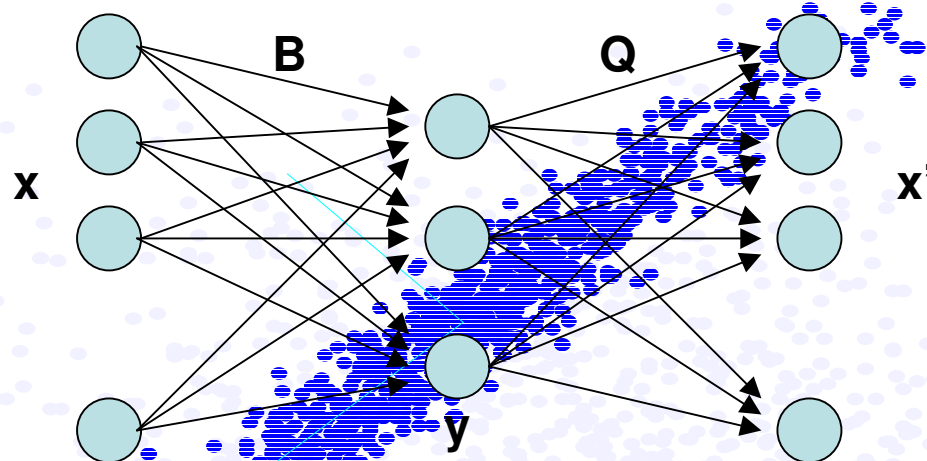
Neural ICA

- ICA is typically posed as an optimization problem.
- Many iterative solutions to optimization problems can be cast into a neural network.



Feed-Forward Neural ICA

General Network Structure



1. Learn B such that $y = Bx$ has independent components.
2. Learn Q which minimizes the mean squared error reconstruction.

Neural ICA

- Herault-Jutten: local updates

$$B = (I+S)^{-1}$$

$$S_{k+1} = S_k + \beta_k g(y_k) h(y_k^T)$$

$g = t, h = t^3$; $g = \text{hardlim}, h = \text{tansig}$

- Bell and Sejnowski: information theory

$$B_{k+1} = B_k + \beta_k [B_k^{-T} + z_k x_k^T]$$

$$z(i) = \partial/\partial u(i) \partial u(i)/\partial y(i)$$

$$u = f(Bx); f = \text{tansig}, \text{ etc.}$$

Recurrent Neural ICA

- Amari: Fully recurrent neural network with self-inhibitory connections.

$$\tau_i \frac{dy_i}{dt} + y_i = x_i(t) - \sum_{j=1}^n \hat{w}_{ij}(t) y_j,$$

$$y(t) = (I + \hat{W}(t))^{-1} x(t),$$

$$y(t) = x(t) - \hat{W}(t) y(t - \tau),$$

$$\frac{d\hat{W}}{dt} = -\mu(t) [I + \hat{W}] [\Lambda - f(y(t)) g^T(y(t))].$$

References

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Questions?

