Unsupervised Learning: PCA and ICA

KMA Solaiman

Adapted from Chris Ré and Zilinkas

Topics for Today

- We'll discuss Principal Component Analysis (PCA).
- We'll discuss Independent Component Analysis (ICA). *The cocktail party problem.*
- These are less related than their names might suggests!

Outline

Linear Algebra/Math Review

Two Methods of Dimensionality Reduction

- Linear Discriminant Analysis (LDA, LDiscA)
- Principal Component Analysis (PCA)

Covariance

covariance: how (linearly) correlated are variables

Mean of variable *i*

Mean of variable *j*

$$\sigma_{ij} = \frac{1}{N-1}\sum_{k=1}^{N}(x_{ki} - \mu_i)(x_{kj} - \mu_j)$$

covariance of variables *i* and *j*

Value of variable *i* in object k

Value of variable *j* in object k

Covariance

covariance: how (linearly) correlated are variables

Mean of variable *i*

Mean of variable *j*

$$\sigma_{ij} = \frac{1}{N-1}\sum_{k=1}^{N}(x_{ki} - \mu_i)(x_{kj} - \mu_j)$$

covariance of variables *i* and *j*

Value of variable *i* in object k

Value of variable *j* in object k

$$\sigma_{ij} = \sigma_{ji}$$

$$\Sigma = \begin{pmatrix} \sigma_{11} & \cdots & \sigma_{1K} \\ \vdots & \ddots & \vdots \\ \sigma_{K1} & \cdots & \sigma_{KK} \end{pmatrix}$$

Eigenvalues and Eigenvectors

vector

$$Ax = \lambda x$$

matrix scalar

for a given matrix operation (multiplication):

what non-zero vector(s) change linearly?
(by a single multiplication)

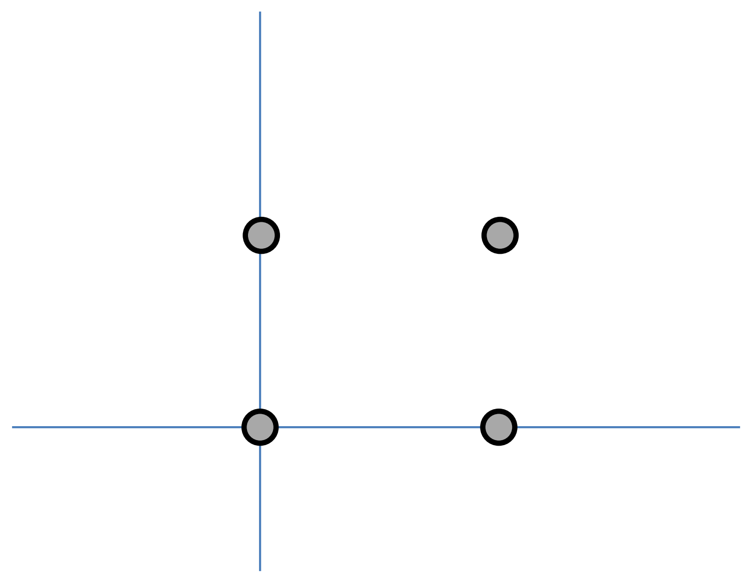
Eigenvalues and Eigenvectors

vector

$$Ax = \lambda x$$

matrix scalar

$$A = \begin{pmatrix} 1 & 5 \\ 0 & 1 \end{pmatrix}$$



Eigenvalues and Eigenvectors

vector

$$Ax = \lambda x$$

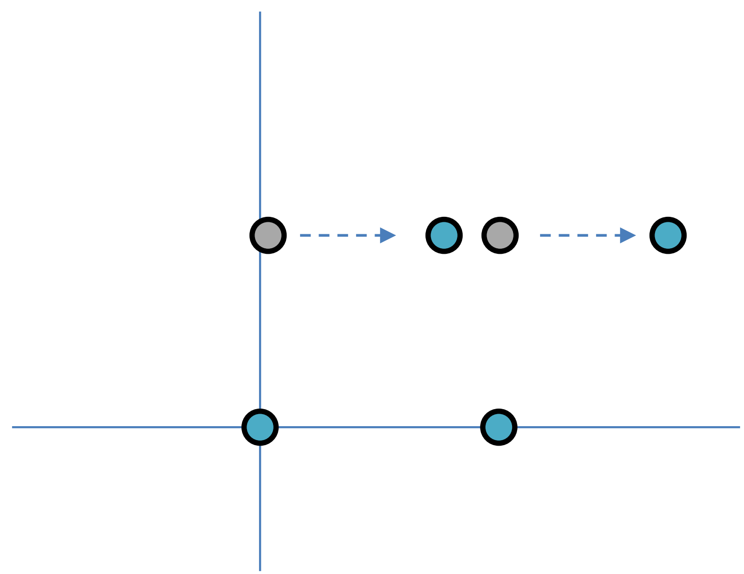
matrix

scalar

$$\begin{pmatrix} x + 5y \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & 5 \\ 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 5 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x + 5y \\ y \end{pmatrix}$$



Eigenvalues and Eigenvectors

vector

$$Ax = \lambda x$$

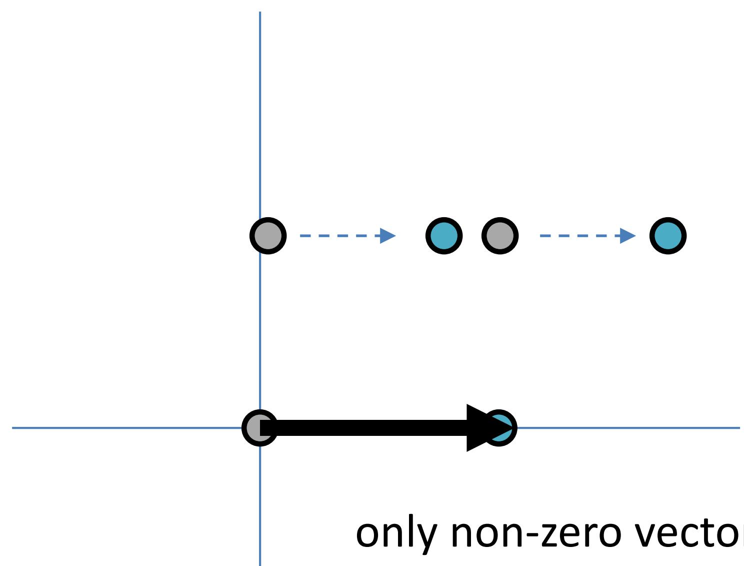
matrix

scalar

$$\begin{pmatrix} x + 5y \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\begin{pmatrix} 1 & 5 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & 5 \\ 0 & 1 \end{pmatrix}$$



only non-zero vector
to scale

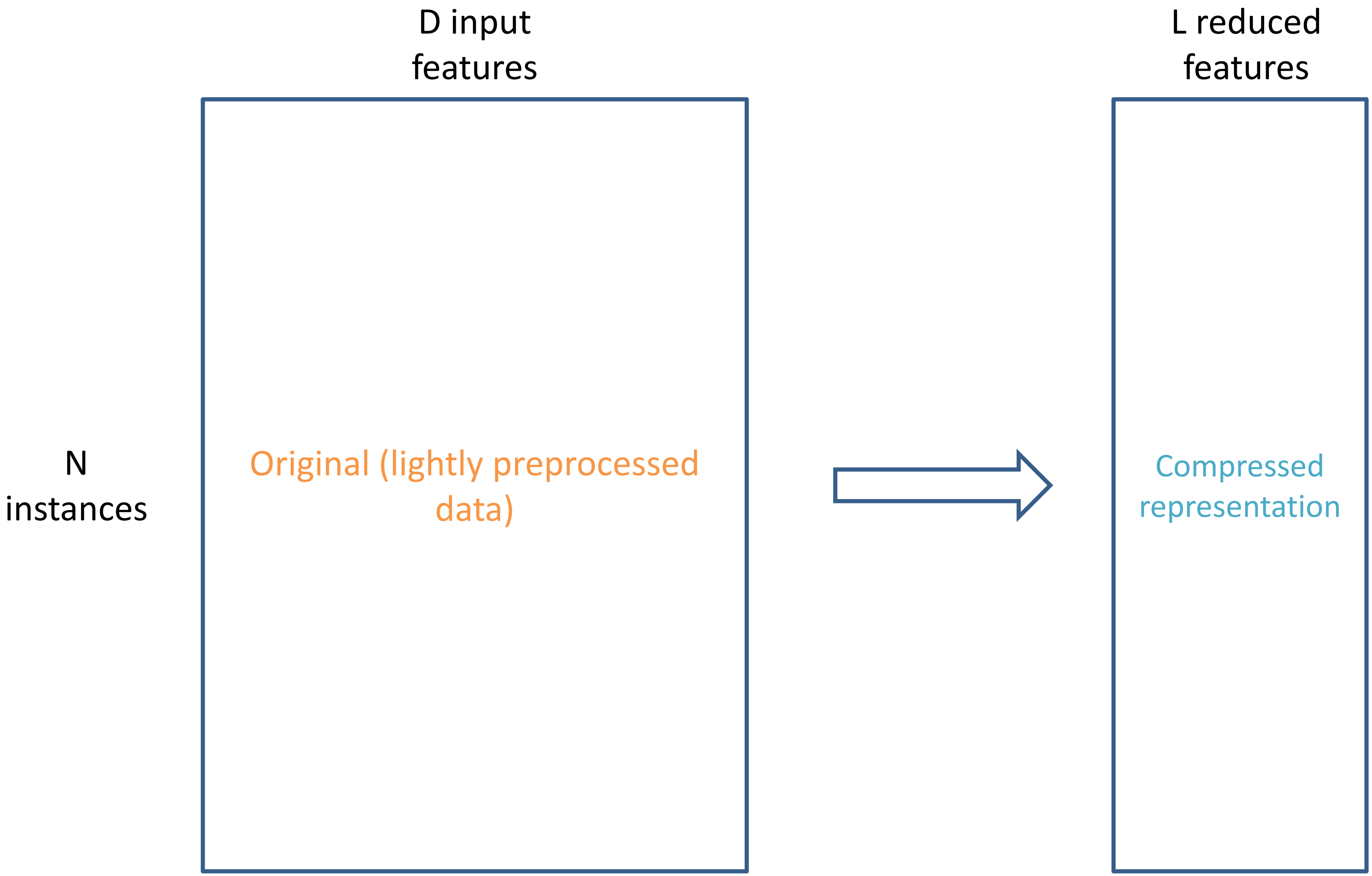
Outline

Linear Algebra/Math Review

Two Methods of Dimensionality Reduction

- Linear Discriminant Analysis (LDA, LDiscA)
- Principal Component Analysis (PCA)

Dimensionality Reduction



Dimensionality Reduction

clarity of representation vs. ease of understanding

oversimplification: loss of important or relevant information

Courtesy Antano Žilinsko

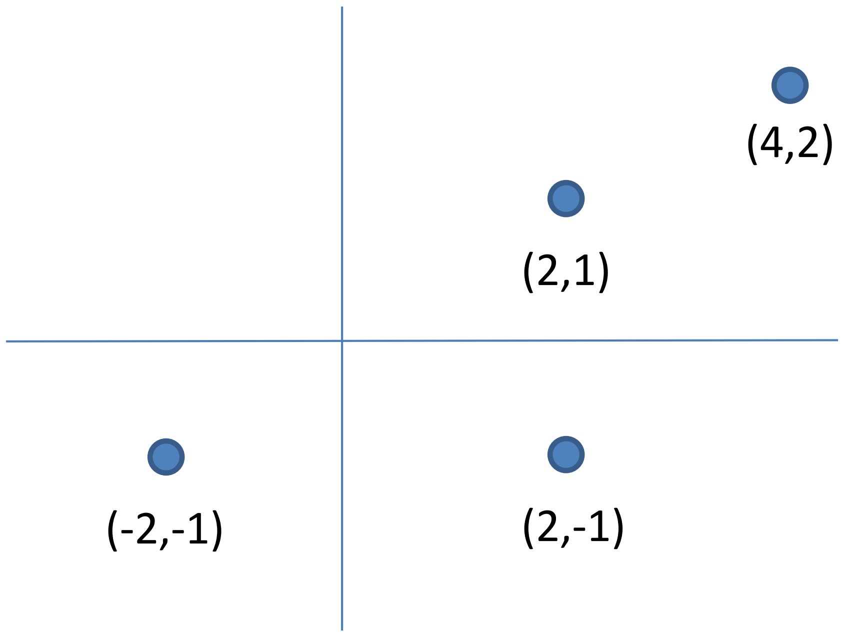
Why “maximize” the variance?

How can we efficiently summarize? We maximize the variance within our summarization

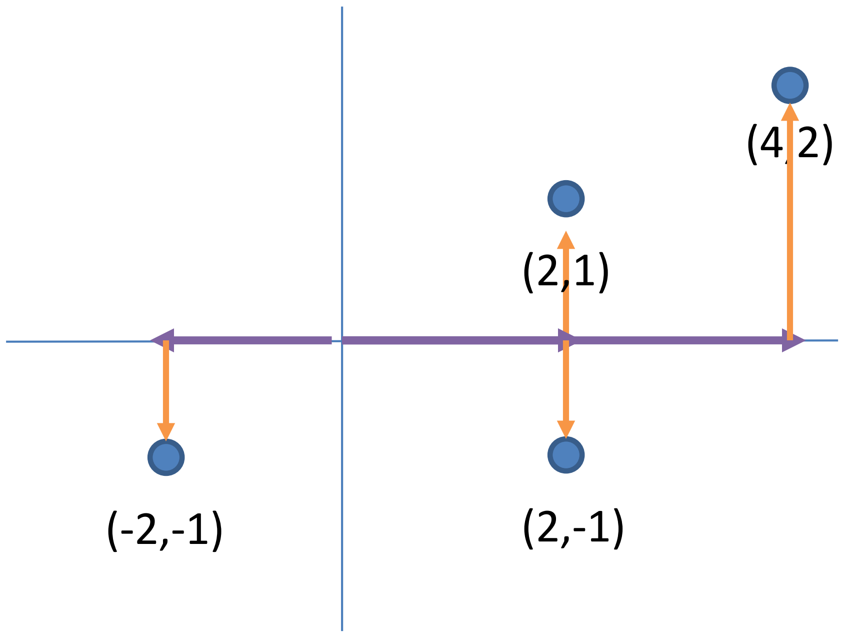
We don’t increase the variance in the dataset

How can we capture the most information with the fewest number of axes?

Summarizing Redundant Information

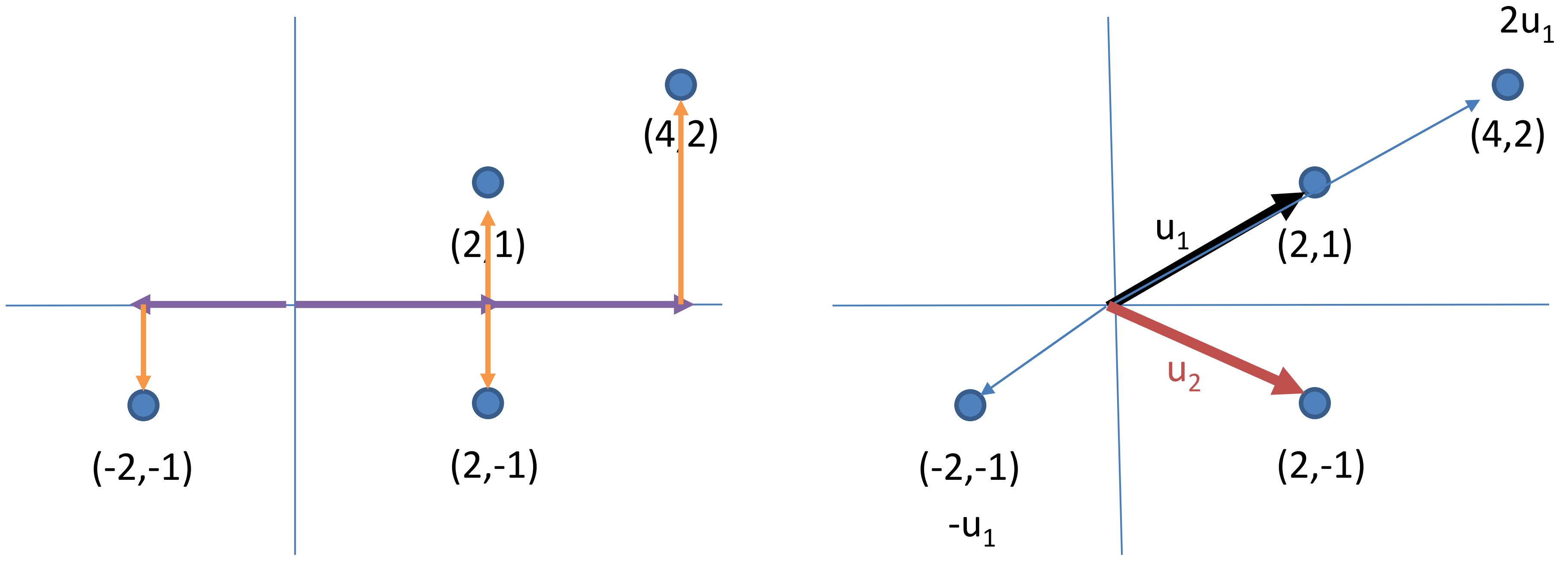


Summarizing Redundant Information



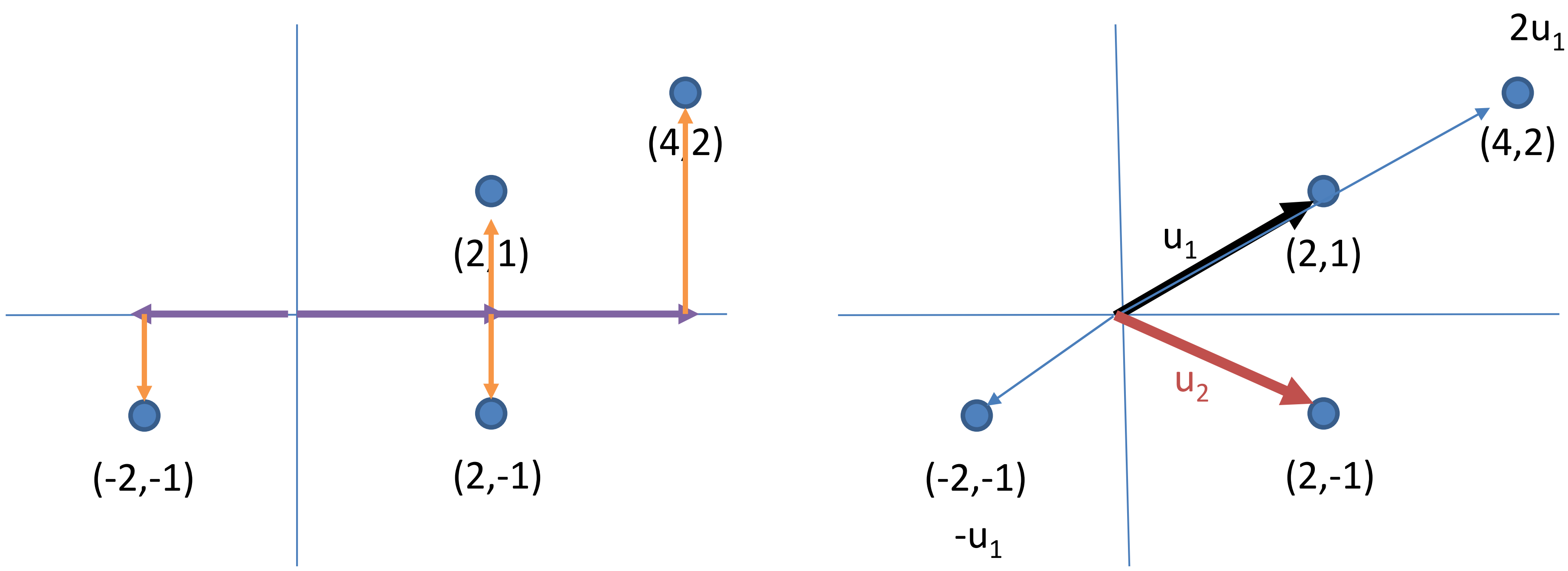
(2,1) = 2*(1,0) + 1*(0,1)

Summarizing Redundant Information



(2,1) = 1*(2,1) + 0*(2,-1)
(4,2) = 2*(2,1) + 0*(2,-1)

Summarizing Redundant Information



(2,1) = 1*(2,1) + 0*(2,-1)
(4,2) = 2*(2,1) + 0*(2,-1)

(Is it the most general? These vectors aren't orthogonal)

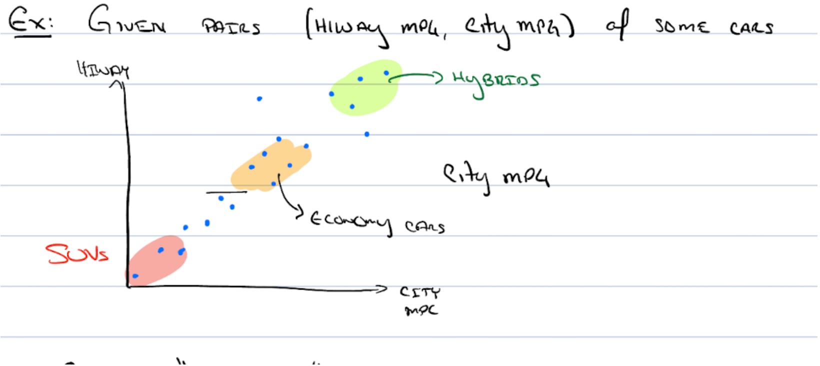
Our Tour Through Unsupervised Land

Structure	Probabilistic	Not Probabilistic
"Cluster"	GMM	k-Means
"Subspace"	Factor Analysis	PCA

We can impose other structures. These are popular.

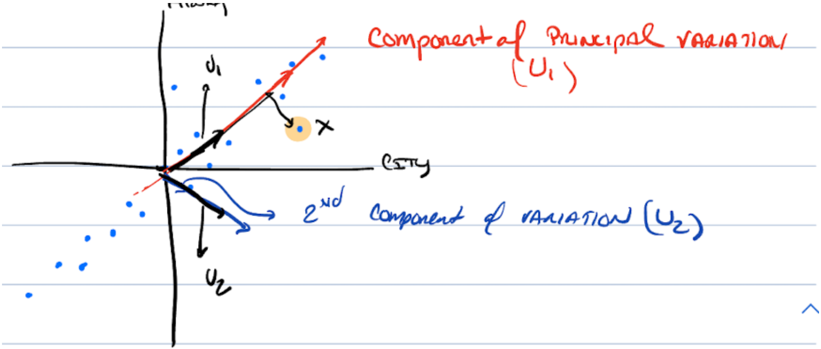
PCA Example: MPG

Given pairs (Highway MPG, City MPG) of some cars.



Question: What is "good" MPG?

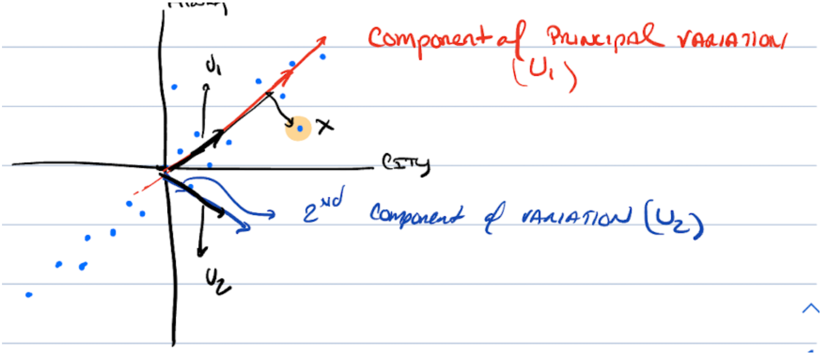
Center the data



We *center* the data, i.e., as preprocessing.

$$x^{(i)} \mapsto x^{(i)} - \mu \text{ where } \mu = \frac{1}{n}\sum_{i=1}^{n} x^{(i)}.$$

Finding Components



By convention, $\|u_1\| = \|u_2\| = 1$ by convention.

- u_1 is the first **principal component** "how good is the MPG"
- u_2 is the second, and roughly the difference.

Recall: any point can be written in an orthogonal basis:

$$x = \alpha_1 u_1 + \alpha_2 u_2$$

Goals

- How do we find these directions?
- Some caveats about how to use these?
- Reduce dimensions: Think about $D = 1000$ reduced to $d = 10$.

Preprocessing

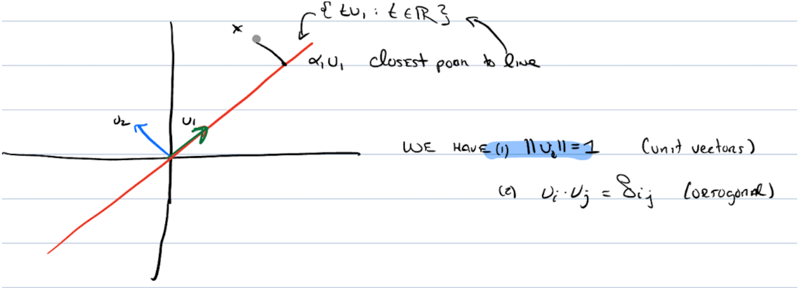
Given $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ we preprocess:

- **Center the data** $x^{(i)} \mapsto x^{(i)} - \mu$
- **Recale the data** May need to rescale components, e.g., "Feet per gallon" v. "Miles per Gallon"

$$x^{(i)} \mapsto \frac{x^{(i)} - \mu}{\sigma}.$$

We will assume from now on that the data is preprocessed.

PCA As Optimization



How do you find the closest point to the line?

$$\alpha_1 = \operatorname*{argmin}_{\alpha} \|x - \alpha u_1\|^2$$
$$= \operatorname*{argmin}_{\alpha} \|x\|^2 + \alpha^2 \|u_1\|^2 - 2\alpha u_1^T x$$

Then, differentiate wrt α, set to 0, and use $\|u_1\|^2$, which leads to:

$$2\alpha - 2u_1^T x = 0 \implies \alpha = u_i^T x.$$

Generalize to higher dimensions

Suppose we have a $u_1, \ldots, u_k \in \mathbb{R}^d$ with $u_i \cdot u_j = \delta_{i,j}$. Then,

$$= \underset{\alpha_1,\ldots,\alpha_k \in R}{\operatorname{argmin}} \|x - \sum_{i=1}^{k} \alpha_i u_i\|^2$$

$$= \underset{\alpha_1,\ldots,\alpha_k \in R}{\operatorname{argmin}} \|x\|^2 + \sum_{i=1}^{k} \alpha_i^2 - 2\alpha_i(u_i \cdot x)$$

These are k independent minimizations, so $\alpha_i = u_i \cdot x$.

- This process is also known as **projecting** on to the set spanned by the vectors $\{u_1, \ldots, u_k\}$.
- We call $\|x - \sum_{i=1}^{k} \alpha_i u_i\|^2$ the **residual**.

Finding PCA

There are two ways you can find PCA:

- Maximize the projected subspace of the data. (we see more)

$$\max_{u \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (u \cdot x^{(i)})^2.$$

- Minimize the residual

$$\min_{u \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - u \cdot x^{(i)})^2.$$

We need to recall some more linear algebra to solve this.

Recall: Eigenvalue decomposition

Let $A \in \mathbb{R}^{d\times d}$ be symmetric (and square) then there exists $U, \Lambda \in \mathbb{R}^{d\times d}$ such that

$$A = U\Lambda U^T \text{ in which } UU^T = I \text{ and } \Lambda \text{ is diagonal.}$$

- If $U = [u_1, \dots, u_d]$, $UU^T = I$ can also be written $u_i \cdot u_j = \delta_{i,j}$.
- In this decomposition,

  $$\Lambda_{i,i} = \lambda_i \text{ is called an } \textbf{eigenvalue}.$$

  and by convention, we order them $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$.
- For $i = 1, \dots, d$, u_i is the eigenvector associated with λ_i:

  $$Au_i = \lambda u_i \text{ since } Au_i = U\Lambda U^T u_i = \lambda_i Ue_i = \lambda u_i$$

  here e_i is the ith standard basis vector.

Recall: Eigenvalue decompositions

Given $x \in \mathbb{R}^d$ and $A = U\Lambda U^T$ we can express x in the basis:

$$x = \sum_{j=1}^{d} \alpha_j u_j$$

As before, using $u_i \cdot u_j = \delta_{i,j}$, we compute $x^T A x$

$$= x^T U\Lambda \sum_{j=1}^{d} \alpha_j e_j = x^T U \sum_{j=1}^{d} \lambda_j \alpha_j e_j = x^T \left(\sum_{j=1}^{d} \lambda_j \alpha_j u_j \right) = \sum_{j=1}^{d} \lambda_j \alpha_j^2$$

Since $\|x\|^2 = x^T x = \sum_{j=1}^{d} \alpha_j^2 = \|\alpha\|^2$, we can write:

$$\max_{x:\|x\|^2=1} x^T A x \text{ is equivalent to } \max_{\alpha:\|\alpha\|^2=1} \sum_{j=1}^{d} \alpha_j^2 \lambda_j.$$

Eigenvectors

So which x attains a maximum?

$$\max_{x:\|x\|^2=1} x^T A x \text{ is equivalent to } \max_{\alpha:\|\alpha\|^2=1} \sum_{j=1}^{d} \alpha_j^2 \lambda_j.$$

- Taking $x = u_1$ works, why?
- What if $\lambda_1 = \lambda_2$, is it unique?
  - Potential instability, when λ_1 is close to λ_2 issues can happen!

Back to PCA!

$$\max_{u \in \mathbb{R}^d : \|u\|^2 = 1} \frac{1}{n} \sum_{i=1}^{n} (u \cdot x^{(i)})^2$$

We can write:

$$\frac{1}{n} \sum_{i=1}^{n} (u \cdot x^{(i)})^2 = \frac{1}{n} \sum_{i=1}^{n} u^T x^{(i)} (x^{(i)})^T u = u^T \left(\underbrace{\frac{1}{n} \sum_{i=1}^{n} x^{(i)} (x^{(i)})^T}_{C} \right) u.$$

C is the covariance of the data, since we subtracted the mean.

> The first eigenvector of the data's covariance matrix is the principal component

More PCA

- **Multiple Dimensions** What if we want multiple dimensions? We keep the top-k.

$$\max_{U \in \mathbb{R}^{k \times d} : UU^T = I_k} \frac{1}{n} \sum_{u=1}^{n} \| Ux^{(i)} \|^2.$$

More PCA

- **Multiple Dimensions** What if we want multiple dimensions? We keep the top-k.

$$\max_{U \in \mathbb{R}^{k \times d} : UU^T = I_k} \frac{1}{n} \sum_{u=1}^{n} \| Ux^{(i)} \|^2.$$

- **Reduce dimensionality**. How do we represent data with just those $k < d$ scalars α_j for $j = 1, \dots, k$

$$x = \alpha_1 u_1 + \alpha_2 u_2 + \cdots + \alpha_d u_d \text{ keep only } (\alpha_1, \dots, \alpha_k)$$

  - Lurking instability: what if $\lambda_j = \lambda_{j+1}$?

More PCA

- **Multiple Dimensions** What if we want multiple dimensions? We keep the top-k.

$$\max_{U \in \mathbb{R}^{k \times d} : UU^T = I_k} \frac{1}{n} \sum_{u=1}^{n} \| Ux^{(i)} \|^2.$$

- **Reduce dimensionality**. How do we represent data with just those $k < d$ scalars α_j for $j = 1, \ldots, k$

$$x = \alpha_1 u_1 + \alpha_2 u_2 + \cdots + \alpha_d u_d \text{ keep only } (\alpha_1, \ldots, \alpha_k)$$

  - Lurking instability: what if $\lambda_j = \lambda_{j+1}$?

- **Choose k?** One approach is "amount of explained variance"

$$\frac{\sum_{j=1}^{k} \lambda_j}{\sum_{i=1}^{n} \lambda_i} \geq 0.9 \text{ note } \mathrm{tr}(C) = \sum_{i=1}^{n} C_{i,i} = \sum_{i=1}^{n} \lambda_i$$

Recall $\lambda_j \geq 0$ since C is a covariance matrix.

Recap of PCA

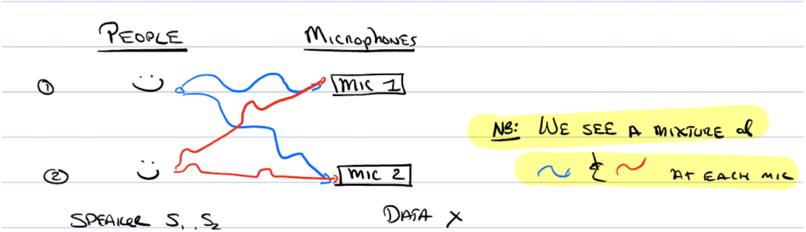
- Project the data onto a subspace: Find the subspace that captures as much of the data as possible (or doesn't explain the least amount).
- Dimensionality reduction and visualization
- Note: The preprocessing (especially centering) featured in our interpretation.

Independent Component Analysis

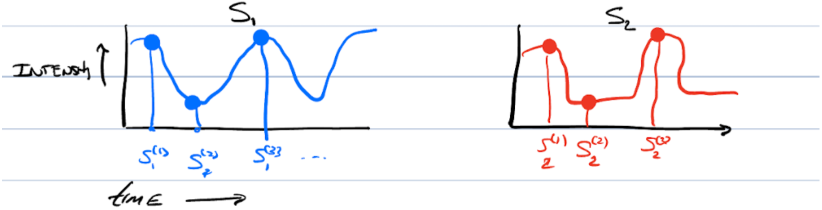
ICA: Independent Component Analysis

- The high-level story (the cocktail party problem)
- The key technical issues (on distributions) and likelihoods
- Model

Cocktail Party Problem



The Data



$S_j^{(t)}$ is the intensity at time t from speaker j.

We do **not** observe $S^{(t)}$ directly, only $x^{(t)}$ the microphones.

Our model is.

$$x_j^{(t)} = a_{j,1} S_1^{(t)} + a_{j,2} S_2^{(t)}.$$

"Microphone j at time t $\left(x_j^{(t)}\right)$ receives a mixture of speaker 1 at time t $\left(S_1^{(t)}\right)$ and speaker 2 at time t $\left(S_2^{(t)}\right)$."

Our Model

We can write out model succinctly as:

$$x^{(t)} = As^{(t)} \text{ for } t = 1, \ldots, n$$

- The blue values are observed: $x^{(t)}$.
- The red values are latent: A and $s^{(t)}$.
- Given x, our goal is to estimate s and A.

For simplicity, we assume number of speakers equals the number of microphones.

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

We call A the **mixing matrix** and $W = A^{-1}$ is the unmixing matrix.

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

We call A the **mixing matrix** and $W = A^{-1}$ is the unmixing matrix. We write

$$W = \begin{pmatrix} w_1^T \\ w_2^T \\ \vdots \\ w_d^T \end{pmatrix} \text{ so that } S_j^{(t)} = w_j \cdot x^{(t)}.$$

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

Some caveats:

- We assume A does **not** vary with time and is full rank.

More formal model

- **Given:** $x^{(1)}, \dots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \dots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

Some caveats:

- We assume A does **not** vary with time and is full rank.
- There are *inherent ambiguities*:
  - We can't determine speaker id (could swap 1 and 2!)

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

Some caveats:

- We assume A does **not** vary with time and is full rank.
- There are *inherent ambiguities*:
  - We can't determine speaker id (could swap 1 and 2!)
  - We can't determine absolute intensity:

$$(cA)(c^{-1}s^{(t)}) = As^{(t)} \text{ for any } c \neq 0.$$

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

Some caveats:

- We assume A does **not** vary with time and is full rank.
- There are *inherent ambiguities*:
  - We can't determine speaker id (could swap 1 and 2!)
  - We can't determine absolute intensity:

$$(cA)(c^{-1}s^{(t)}) = As^{(t)} \text{ for any } c \neq 0.$$

- Speakers cannot be Gaussian! Maybe surprising:

$$x^{(t)} \sim \mathcal{N}(\mu, AA^T) \text{ then if } U^T U = I \text{ then } AU \text{ generates same data.}$$

Nevertheless, we can recover something meaningful–and the whole algorithm is just MLE with gradient descent.

More formal model

- **Given:** $x^{(1)}, \ldots, x^{(n)} \in \mathbb{R}^d$ where d is the number of speakers and microphones.
- **Do:** Find $s^{(1)}, \ldots, s^{(n)} \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$

$$x^{(t)} = As^{(t)}.$$

Some caveats:

- We assume A does **not** vary with time and is full rank.
- There are *inherent ambiguities*:
  - We can't determine speaker id (could swap 1 and 2!)
  - We can't determine absolute intensity:

$$(cA)(c^{-1}s^{(t)}) = As^{(t)} \text{ for any } c \neq 0.$$

- Speakers cannot be Gaussian! Maybe surprising:

$$x^{(t)} \sim \mathcal{N}(\mu, AA^T) \text{ then if } U^T U = I \text{ then } AU \text{ generates same data.}$$

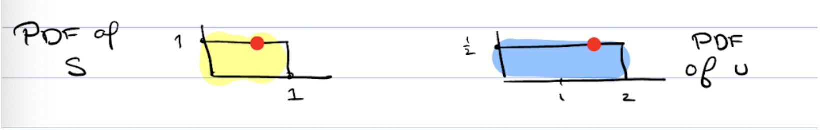
Nevertheless, we can recover something meaningful–and the whole algorithm is just MLE with gradient descent.We need one fact first.

Detour: Density under linear transformations

Consider

$$s \sim \text{Uniform}[0,1] \text{ and } u = 2s.$$

What is the PDF of u? Tempted to write $P_u(x/2) = P_s(x)$ – but this is incorrect:



$$P_s(x) = \begin{cases} 1 & \text{if } x \in [0,1] \\ 0 & \text{otherwise} \end{cases} \text{ and } P_u(x) = \frac{1}{2} p_s\left(\frac{x}{2}\right).$$

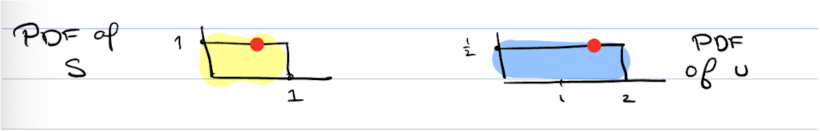
The key issue is the *normalization constant* here $\frac{1}{2}$.

Detour: Density under linear transformations

Consider

$$s \sim \text{Uniform}[0,1] \text{ and } u = 2s.$$

What is the PDF of u? Tempted to write $P_u(x/2) = P_s(x)$ – but this is incorrect:



$$P_s(x) = \begin{cases} 1 & \text{if } x \in [0,1] \\ 0 & \text{otherwise} \end{cases} \text{ and } P_u(x) = \frac{1}{2} p_s\left(\frac{x}{2}\right).$$

The key issue is the *normalization constant* here $\frac{1}{2}$. For matrix A:

$$P_u(x) = p_s(A^{-1}x)\left|\det(A^{-1})\right| = P_s(Wx)\left|\det(W)\right|.$$

Here, $\det(A^{-1}) = \frac{1}{\det(A)}$

Now the ICA Model is MLE

Goal: write signals in terms of observed quantities:

$$p(s) = \prod_{j=1}^{d} p_s(s_j) \qquad \text{sources are iid.}$$

Now the ICA Model is MLE

Goal: write signals in terms of observed quantities:

$$p(s) = \prod_{j=1}^{d} p_s(s_j) \qquad \text{sources are iid.}$$

$$p(x) = \prod_{j=1}^{d} p_s(w_j \cdot x)\,|\det(W)| \qquad \text{Use the previous slide}$$

Technical: Use non-rotationally invariant distribution. We set

$$p_s(x) \propto g'(x) \text{ for } g(x) = \frac{1}{1+e^{-x}}.$$

With this, we can solve the following with gradient descent:

$$\ell(W) = \sum_{t=1}^{n} \sum_{j=1}^{d} \log g'\left(w_j \cdot x^{(t)}\right) + \log|\det(W)|\,.$$

Summary of Lecture

- We saw PCA: workhorse of dimensionality reduction. The structure was "subspaces"
- We saw ICA: Key idea for homework, and introduced this concept of up to symmetry.