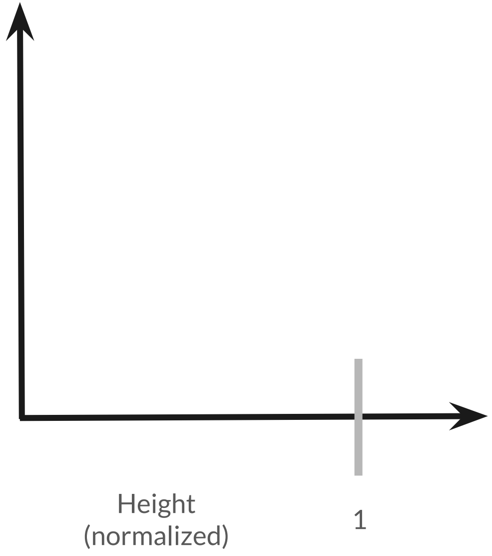
CIS 635 Knowledge Discovery & Data Mining

- Curse of Dimensionality
- Principal Component Analysis (PCA)

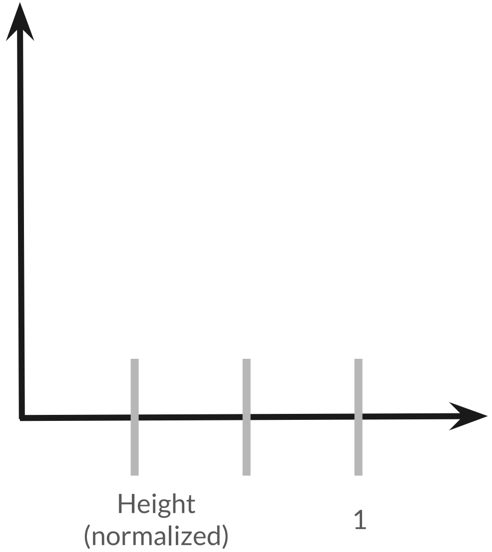
Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]



Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]
- **3 equal bins (aka numeric to categorical)**



Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]
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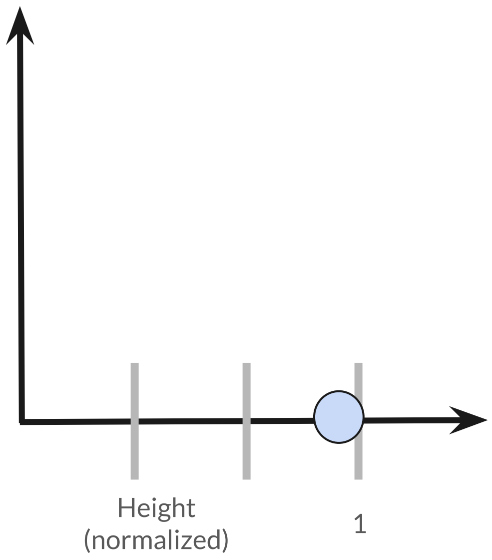
- **The tallest person in the class**



Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]
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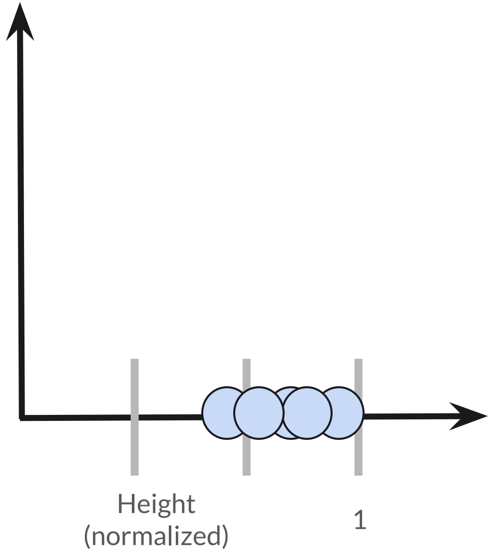
- **All of us**



Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]
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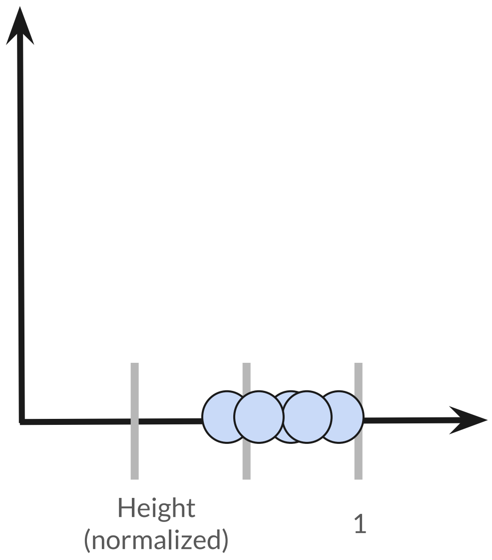
- **I don't think we have someone with 0.5 times height than the tallest**



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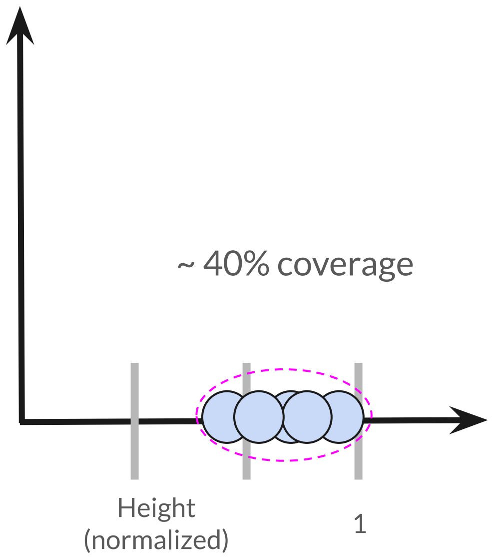
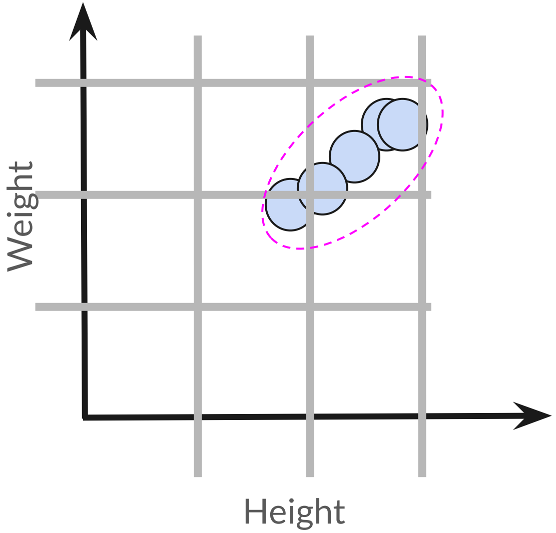
- I don't think we have someone with 0.5 times height than the tallest
- **Is ~40% domain coverage a reasonable assumption?**



Curse of Dimensionality

- We have added Weight as our second feature dimension
- Do you find the samples represent our class?
- What's the domain coverage now?



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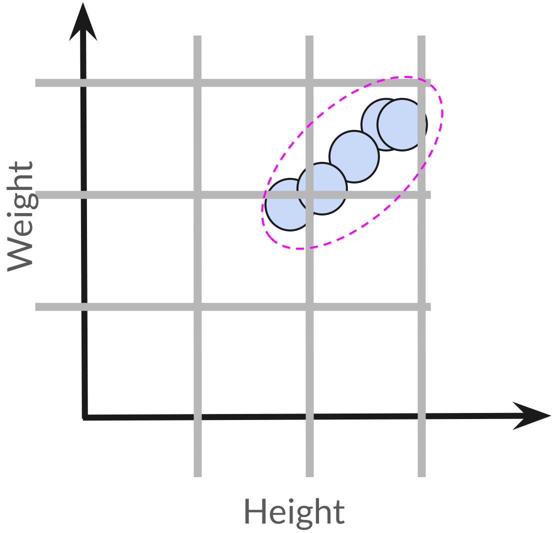
- **Is ~10% a reasonable assumption?**



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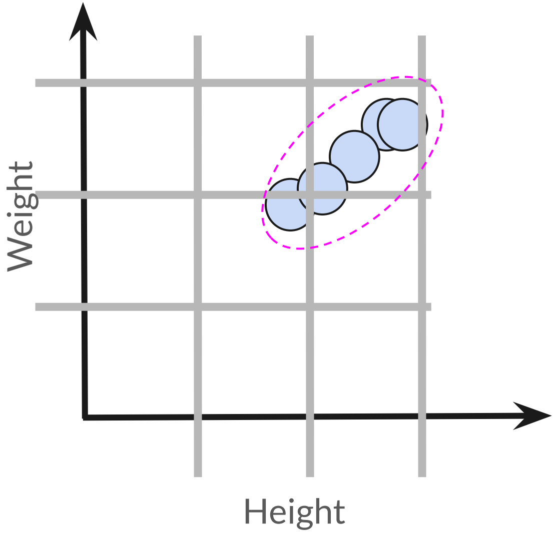

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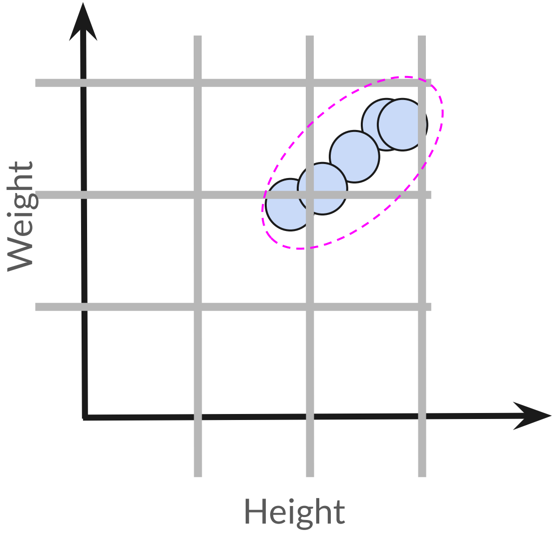

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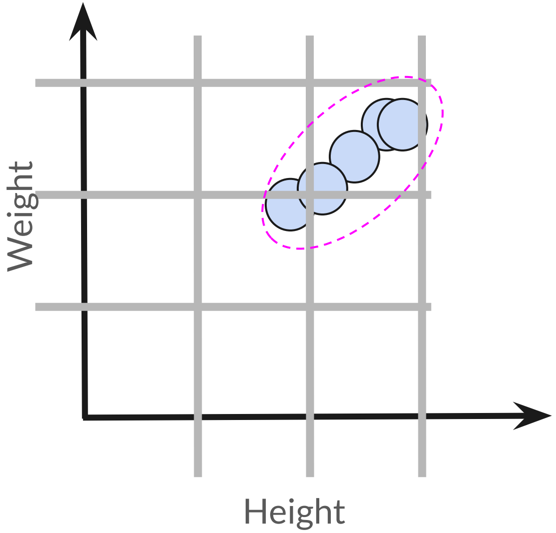

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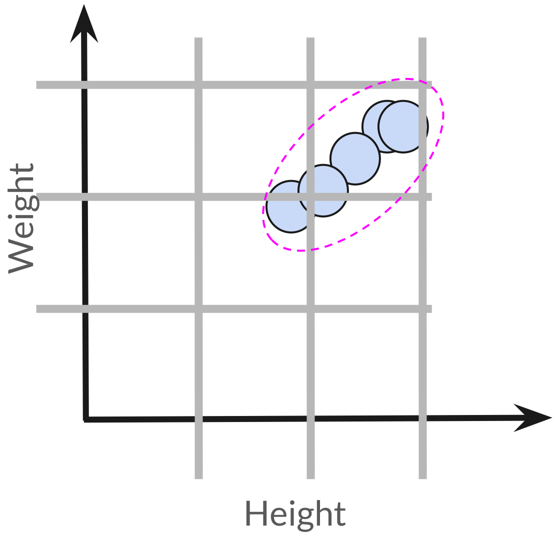

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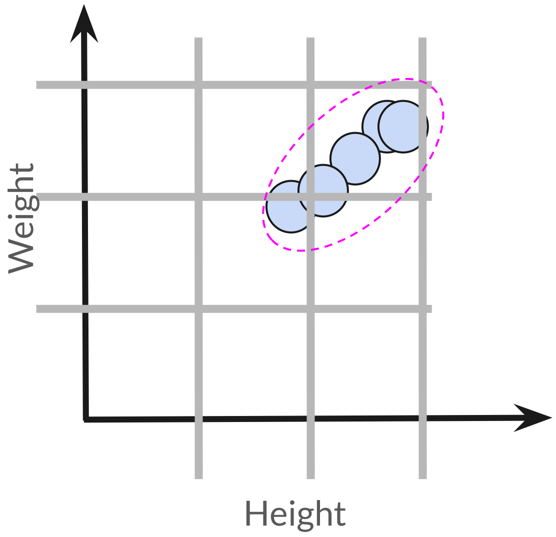
- Empty space grows exponentially with the increase in adding new features.
- **Data distribution becomes sparse, and difficult to learn a good model.**



Dimensionality Reduction

General idea

- You have some data of feature dimension size, **|*D*|**

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<u>General idea</u>

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- You want to compress them to of size, **|*d*|**
- **|*d*| < |*D*|**

Dimensionality Reduction

- Linear
  - Principal Component Analysis (PCA)
  - SVD
- Neural Networks
  - Auto Encoders
  - RBMs

Covariance

- Variance relationship between a pair of variables

$$cov_{x,y} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{N - 1}$$

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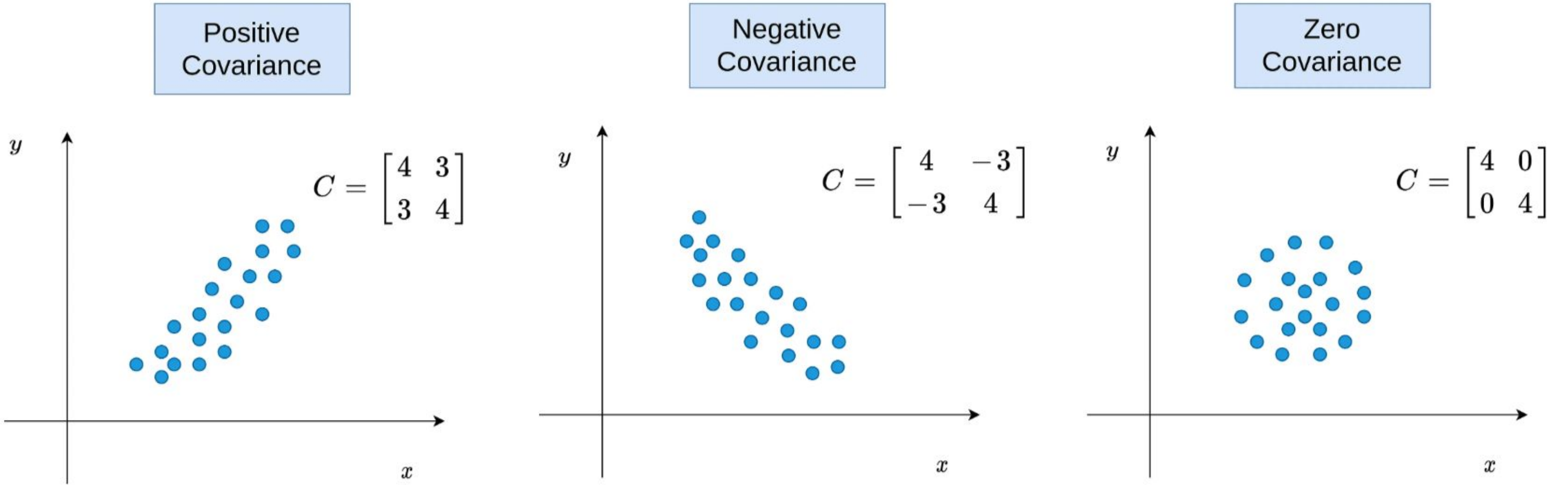
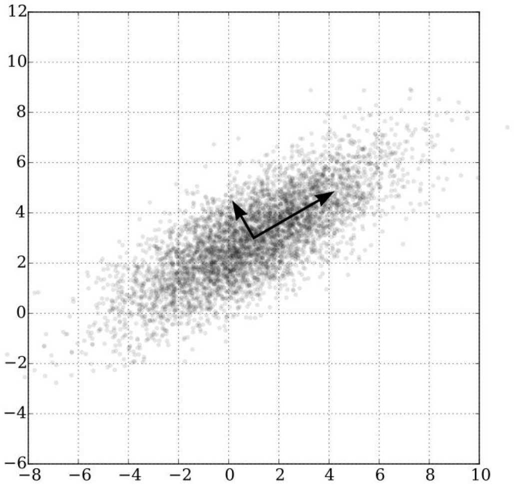


[5 Things you should know about Covariance]()

Principal Component Analysis (PCA)

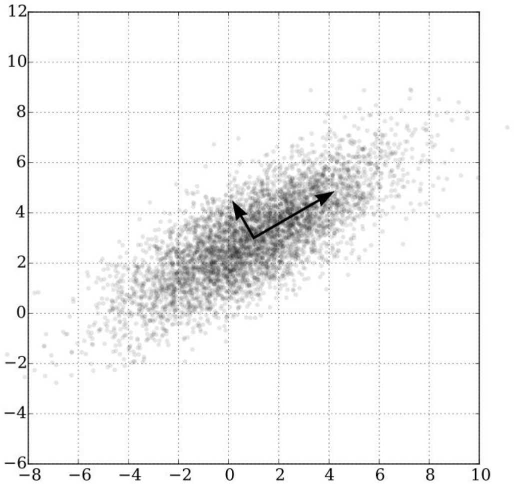
General idea: 2D Gaussian example

- Features ***x*** and ***y*** shows some relationships



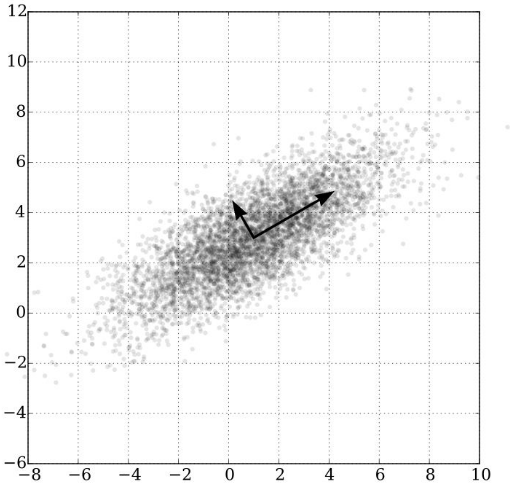
General idea: 2D Gaussian example

- Features ***x*** and ***y*** shows some relationships
- This 2D Gaussian has its own coordinates (off the reference cartesian coordinates ***x'*** and ***y'***; right?)



General idea: 2D Gaussian example

- Features **x** and **y** shows some relationships
- This 2D Gaussian has its own coordinates (off the reference cartesian coordinates **x'** and **y'**; right?)
- **The principal components**



How to ..

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PCA steps

1. Let assume D_{mxn} is a given data matrix
2. Apply standard scalar (normalization)
3. Estimate Covariance (matrix), A_{nxn}
4. Compute Eigenvalues and Eigenvectors of the Covariance Matrix by solving the linear dynamical system at the right

If ***A*** is a *nxn* matrix, solving this linear dynamical system will give *n* **eigenvalues**, and n associated *n* **eigenvectors**

$$AX = \lambda X$$

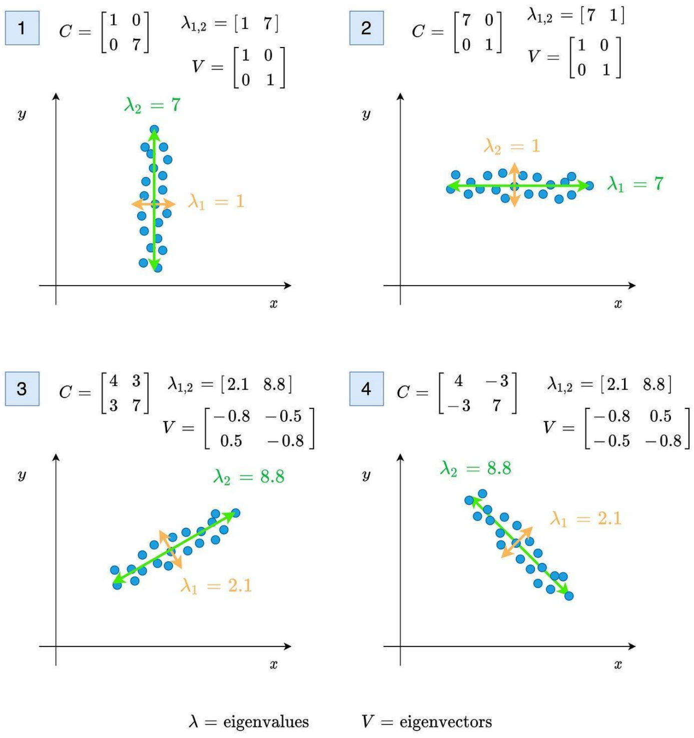
$$AX - \lambda X = 0$$

or

$$(A - \lambda I)\,X = 0$$

PCA

[Notebook presentation]()



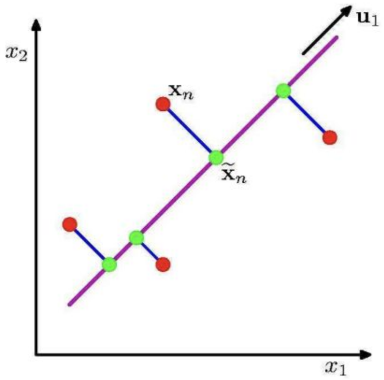
[ref]()

What are we optimizing?

- 2D example (red points)
- Green points are 1D projections/transformations
- We are reducing data definitions from 2D to 1D; this can be generalized from D to M dimensions

<u>Two techniques (in general):</u>

- Maximize variance
- Minimize errors (distance between each green-red paris)



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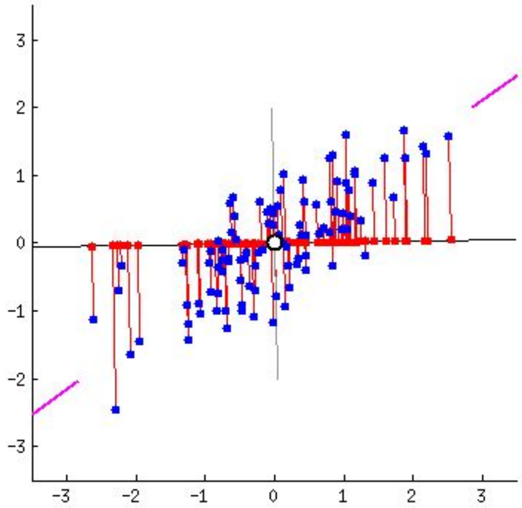

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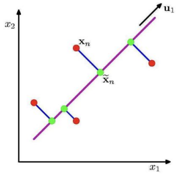
Standard PCA: Variance maximization



- One dimensional example
- Objective: maximize projected variance w.r.t. $\mathbf{U}_1$

$$\frac{1}{N}\sum_{n=1}^{N}\{\mathbf{u}_1^T\mathbf{x}_n - \mathbf{u}_1^T\bar{\mathbf{x}}\}^2 = \mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$$

  - where sample mean and data covariance are:

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n$$

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^T$$

- Must constrain $\|\mathbf{u}_1\|$: via Lagrange multiplier, maximize w.r.t $\mathbf{u}_1$

$$\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1 + \lambda(1 - \mathbf{u}_1^T\mathbf{u}_1)$$

- Optimal $\mathbf{u}_1$ is principal component (eigenvector with maximal eigenvalue)

ref