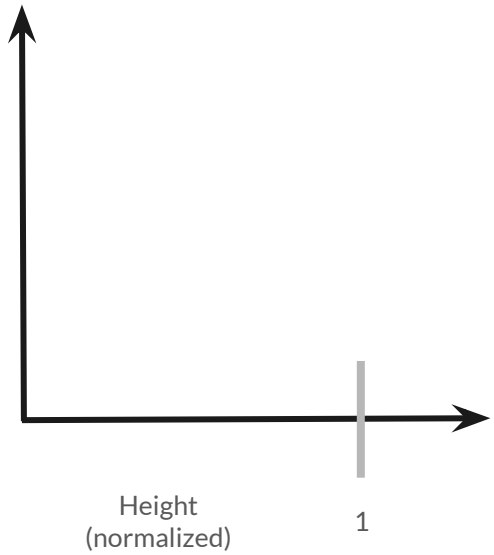
CIS 678 Machine Learning

- Curse of Dimensionality
- Linear Dimensionality Reduction (PCA)

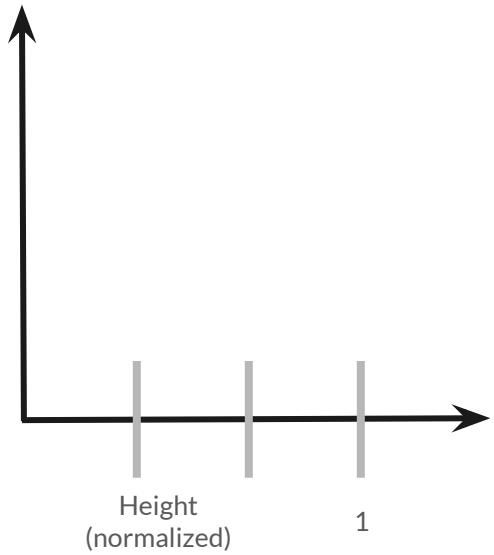
Curse of Dimensionality

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



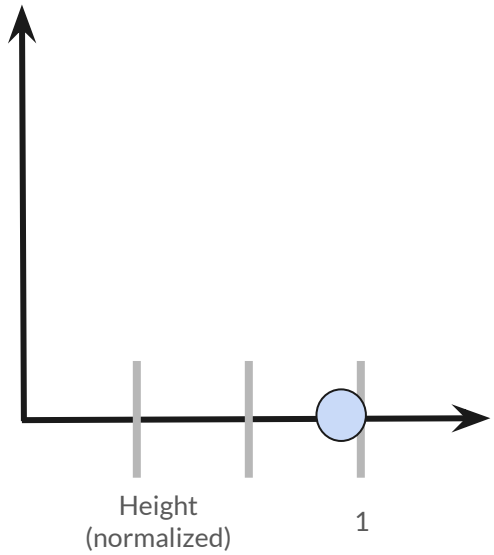
Curse of Dimensionality

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



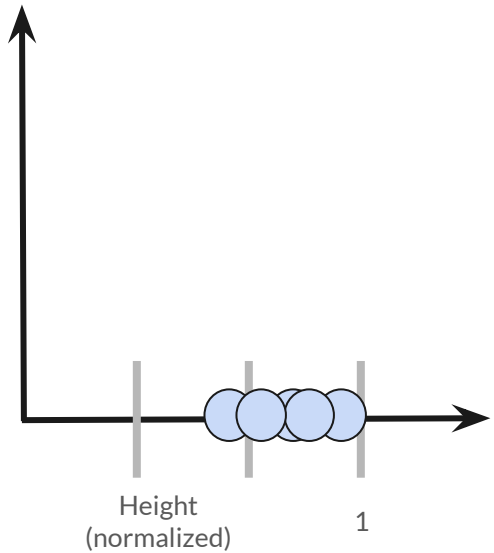
Curse of Dimensionality

- x axis : Heights (min-max normalized: [0-1]
- 3 equal bins (aka numeric to categorical)
- **The tallest person in the class**



Curse of Dimensionality

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



Curse of Dimensionality

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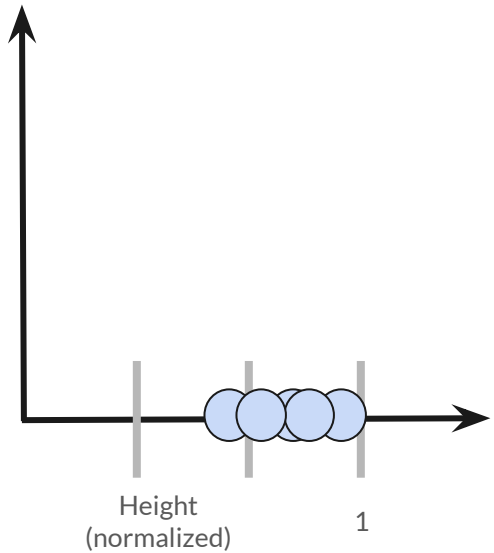
- All of **us**
- **I don't think we have someone with 0.5 times height than the tallest**



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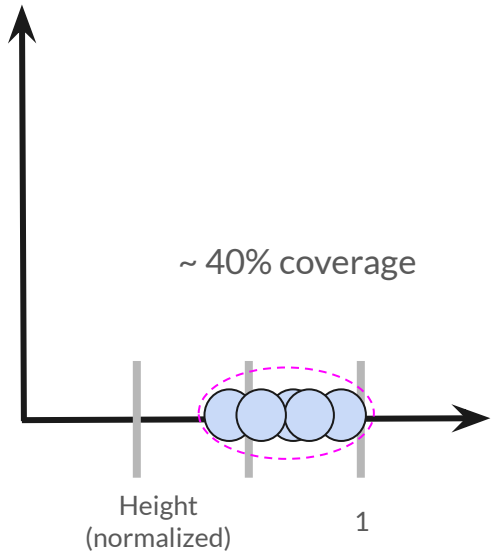
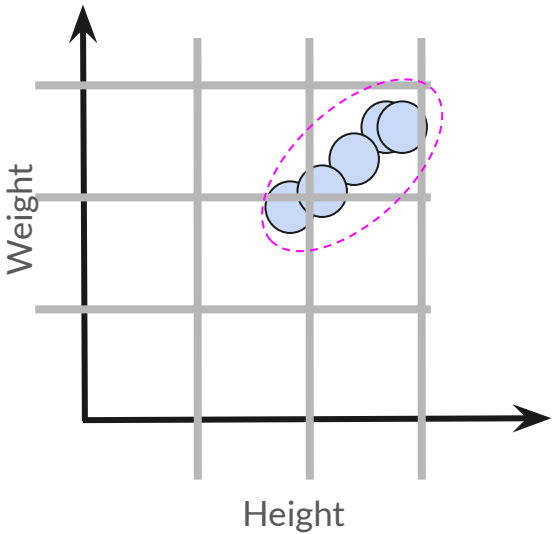
- I don't think we have someone with 0.5 times height than the tallest
- **Is ~40% domain coverage a reasonable assumption?**



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?
- Is ~10% a reasonable assumption?
- See how numbers dropped from ~40% to ~10%
- **The other way, the empty space grew up from ~60% to ~90%**



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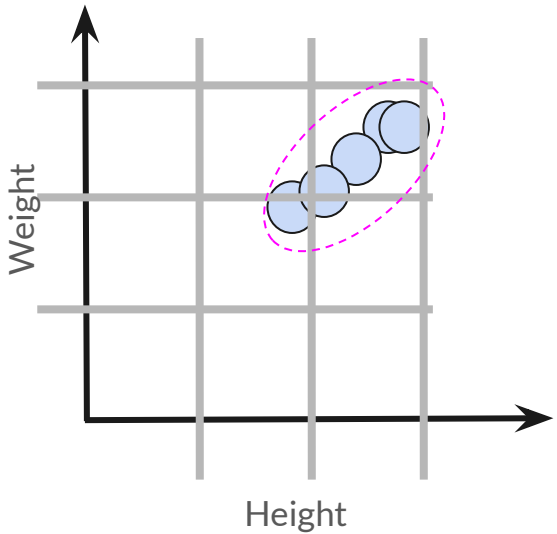
- **What's the number would look like if we add 2 more dimensions?**



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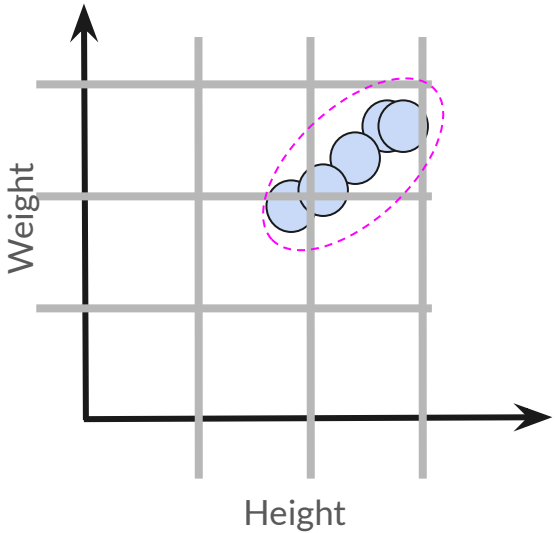
- **Empty space grows exponentially with the increase in adding new features.**



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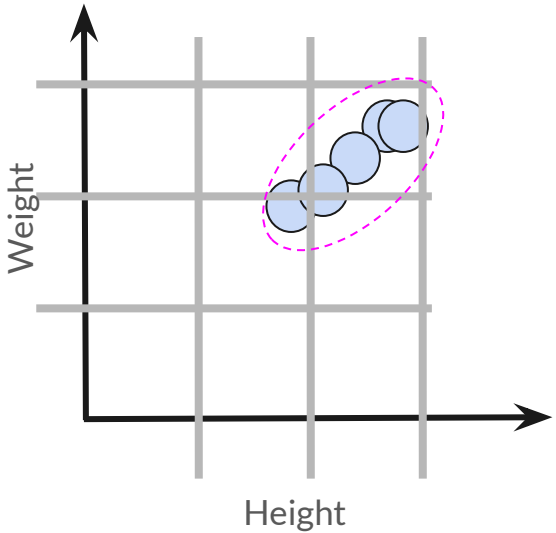
- **What's the number would look like if we add 2 more dimensions?**

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



Dimensionality Reduction (Linear)

- Principal Component Analysis (PCA)

Covariance

-

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

Covariance

-

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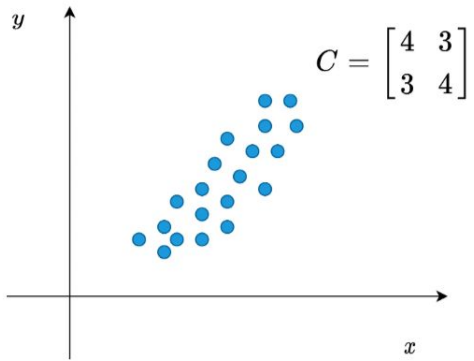
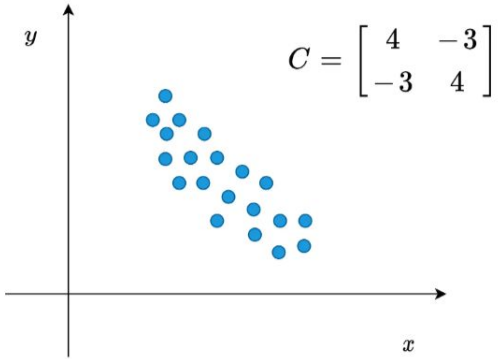
$$Cov(x,y) = \frac{\Sigma(x_i - \bar{x})(y_i - y)}{N-1}$$

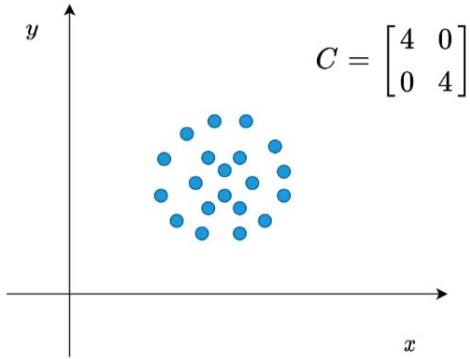
Positive Covariance



Negative Covariance



Zero Covariance

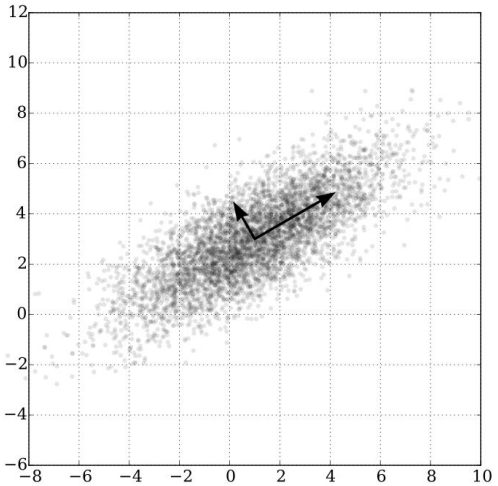


[5 Things you should know about Covariance]

PCA

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 ..

PCA steps

1. Apply standard scalar (normalization)
2. Estimate Covariance (matrix), **A**
3. Compute Eigenvalues and Eigenvectors of the Covariance Matrix
4. Solve the linear equation (right)

$$AX = \lambda X$$

$$AX - \lambda X = 0$$

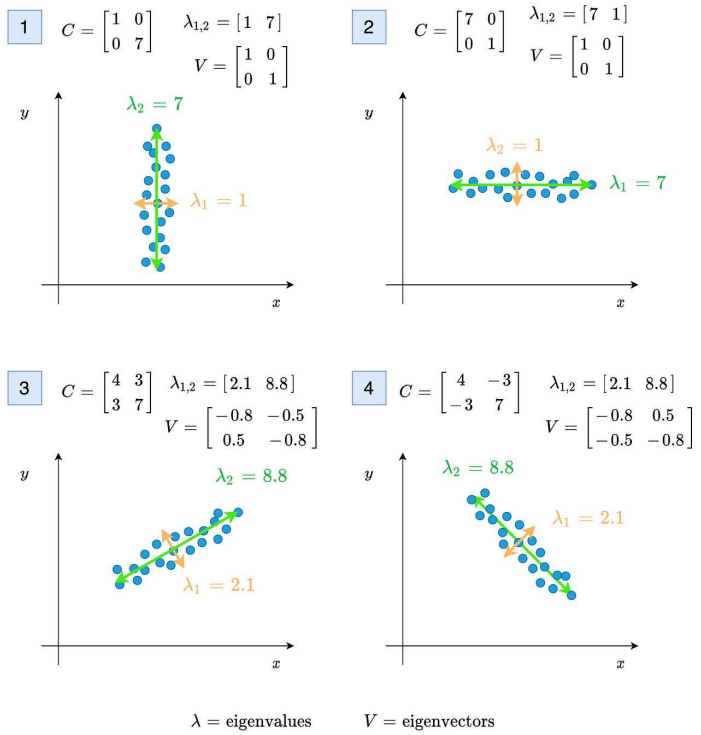
or

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

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

PCA

[Notebook presentation]



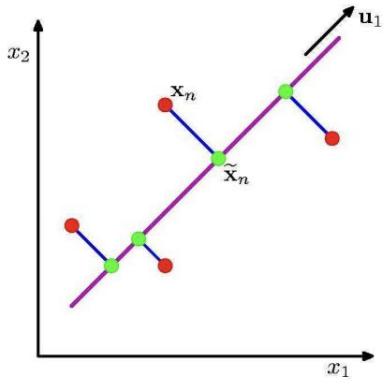
[ref]

Optimization

- 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

Two techniques (in general):

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



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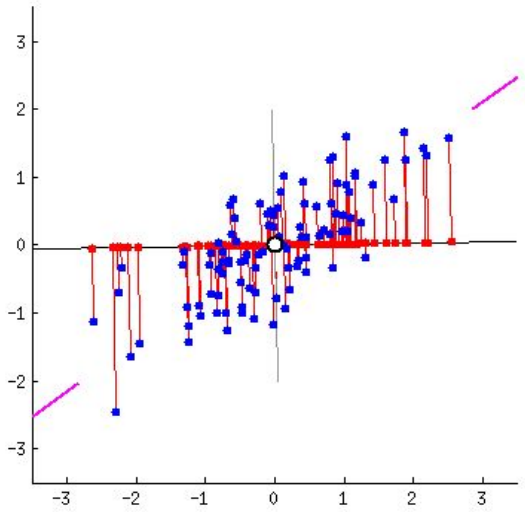


ref

Standard PCA: Variance maximization

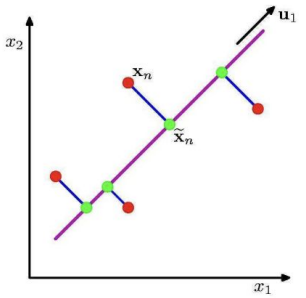
- One dimensional example
- Objective: maximize projected variance w.r.t. $\mathbf{U}_1$

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

  - 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