# Machine Learning 1.10: The Curse of Dimensionality

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# Curse of dimensionality

- Named by Richard Bellman
  ("Adaptive Control Processes: A Guided Tour", 1961)
  (Inventor of dynamic programming – later lecture)

- Short version: More dimensions $\implies$ need more data
  (dimension = feature)

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- Short version: More dimensions $\implies$ need more data
  (dimension = feature)
- Why?
- How much more?

# Combinatorics

- Imagine a problem:
  - Feature vector of length $n$
  - Binary – answers to *yes*/*no* questions
  - Any output

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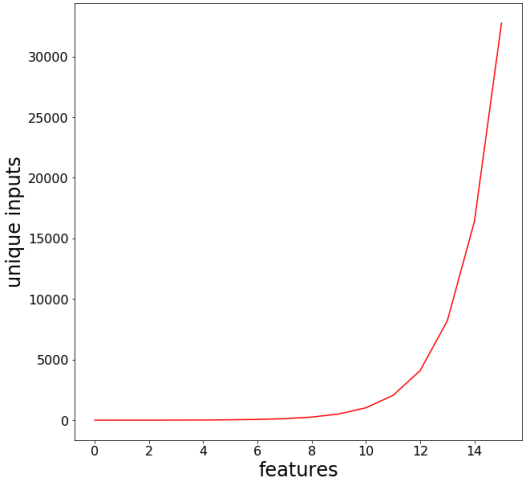
- There are $2^n$ possible inputs
- If you have 1000 unique exemplars:

| n | coverage |
|---|---|
| 10 | 100.0% |
| 50 | 40.0% |
| 100 | 10.0% |
| 500 | 0.4% |
| 1000 | 0.1% |



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# Coverage

- Machine learning assumption:
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- But:
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  Similar feature vector $\implies$ similar answer
- But:
  Low coverage $\implies$ nothing is similar
- There is still something "most similar" and "least similar" however...

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# Distance in $100D$ space

- 1000 points in $nD$ space, uniform distribution, $x \in [0,1]^n$
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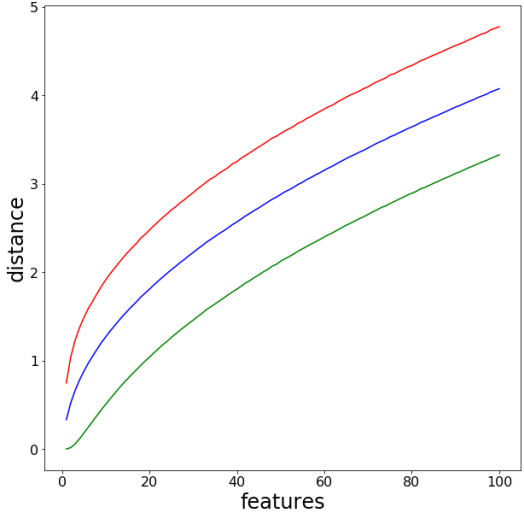

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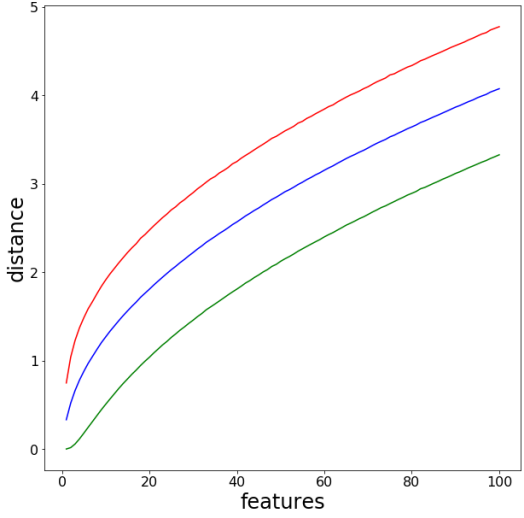
- Distance increases, range does not.
- $\frac{\texttt{maximum}}{\texttt{minimum}}$ decreases.

- Everything starts to look the same!



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# Never enough

- Poor coverage = failing similarity
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- Consider nearest neighbours (set point to same class as nearest)
- First dimension, x[0]:
  $x[0] < \frac{1}{3} \implies$ class 0,
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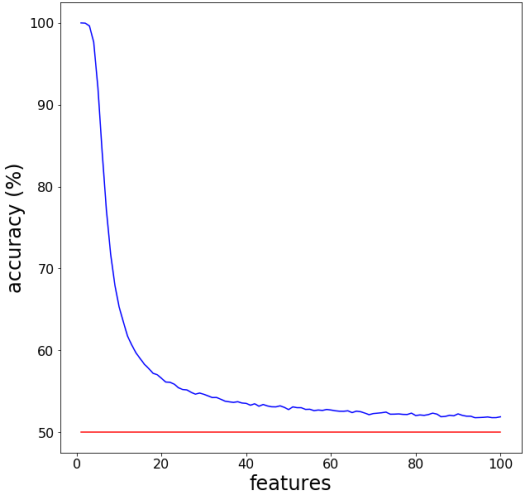
- This should be easy, but...



## Not the distributions as well...

- Affects probability distributions
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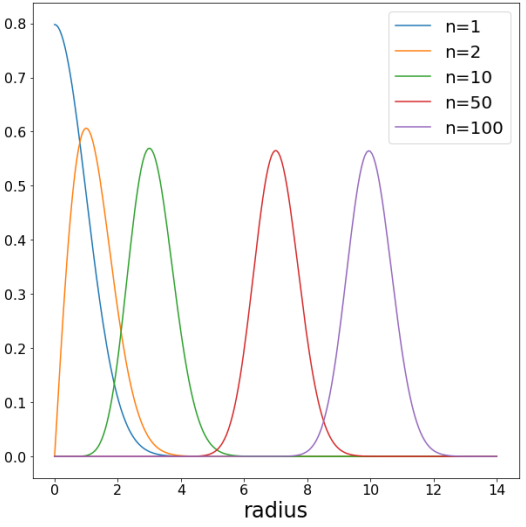
- Distribution of distances from mean?
  (called a $\chi$ (chi) distribution)



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# Not the distributions as well. . .

- Affects probability distributions
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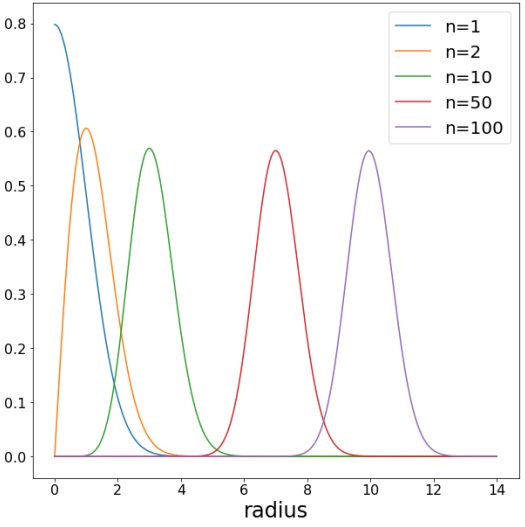
- Draw samples from distribution
- Distribution of distances from mean?
  (called a $\chi$ (chi) distribution)
- High dimensions: Samples are in a thin shell, avoiding the mean!



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# Avoiding the curse

- Affects all models
- Solutions:
  - Feature selection
  - Feature engineering
  - Problem doesn't exist for real data!
    (manifolds; which is not to say it's just going to solve itself)
- Related to regularisation

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# Feature selection

- Select a small number of features to use, ignore rest
- Three approaches:
  - **Model selection**: Train model with many subsets of the features and select best
  - **Filtering**: Use an estimate of feature usefulness and filter accordingly
  - **Embedded**: An algorithm with feature selection built in
- Using problem structure is better – later lectures

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  1. Start with empty set
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- **Stepwise regression**: Above with a regression model, e.g. Logistic regression
- Gets stuck in local minima

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- Questionable value, but fast:
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$$\left| \frac{\mathbb{E}\left[(x_i - \mu_{x_i})(y - \mu_y)\right]}{\sqrt{\mathbb{E}\left[(x_i - \mu_{x_i})^2\right]\mathbb{E}\left[(y - \mu_y)^2\right]}} \right| > t$$

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- "Usefulness" depends on other variables:
  - Two variables might contain same information $\implies$ including both is pointless
  - A variable might be useless on it's own, useful with others

- Too crude (linear) for interesting problems
- Other correlation metrics...

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# Feature selection: Embedded

- Algorithm does it as part of learning
- Good trade off between performance/speed

- Best example: Random forests
  - Feature/split selection is feature filtering
  - Significant part of why they perform so well

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# Feature engineering

- Use domain knowledge to design new features
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# Feature engineering

- Use domain knowledge to design new features
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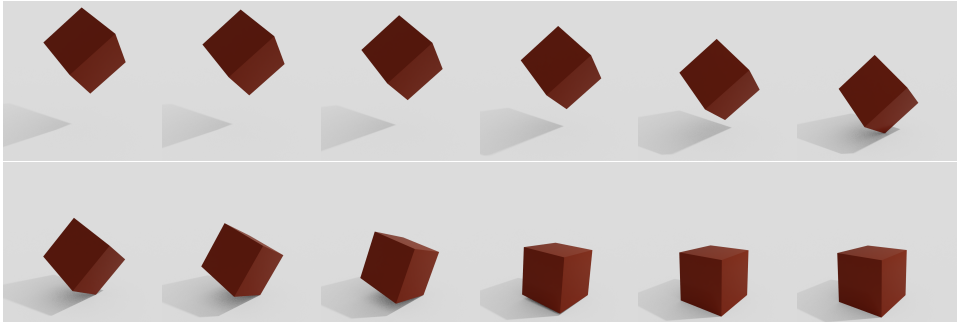
- Example: Radius trick to fit a circle with Logistic regression
- Often about **invariance**
- Can massively improve performance...
  ...but requires domain knowledge

# Real data

Consider a video of a cube falling:



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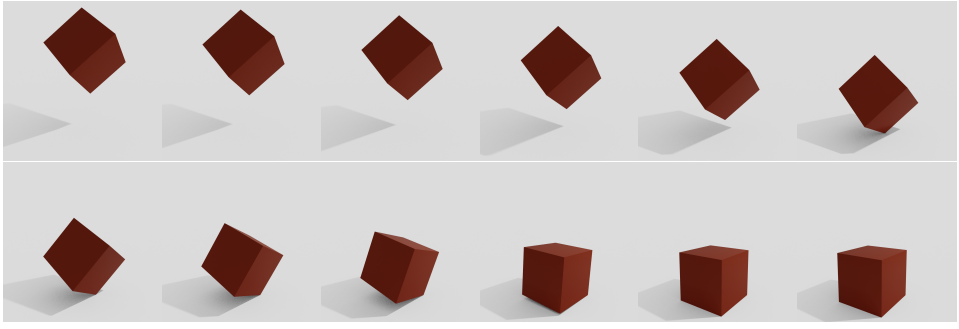

- How many dimensions does each frame have?
- Formally: 3145728: $1024 \times 1024$ images, 3 channels per pixel
- Actually: 6: 3 for position of cube, 3 for orientation of cube (everything else is a (complex) function of these 6 parameters)
- **Real data is mostly low dimensional**!

# Manifolds

- Manifold: Low dimensional surface embedded in higher dimensional space
- Real data typically lies on a manifold
  (in MI we generalise maths definition slightly: Manifold dimensionality can vary)

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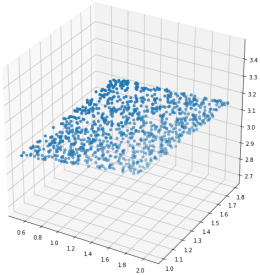
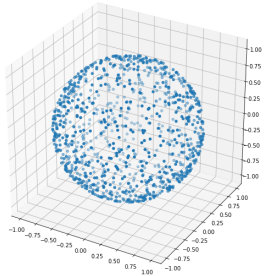
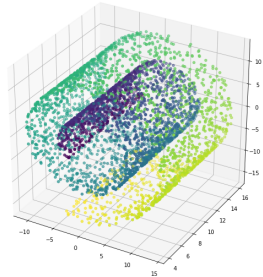
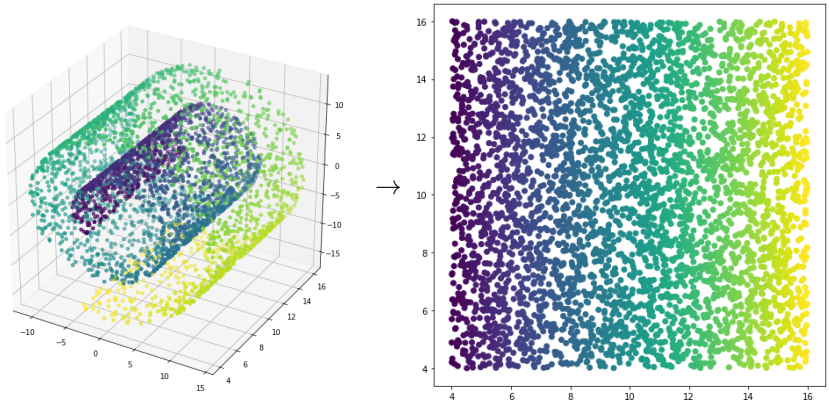
- e.g. $2D$ manifolds embedded in $3D$ space:

# Dimensionality reduction I

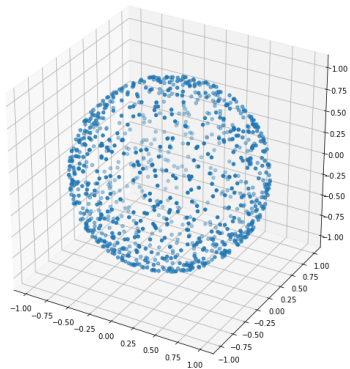
- Assign a coordinate system to the manifold, use that instead:




- Also used for visualisation (e.g. you used PCA previously)

# Dimensionality reduction II

- Doesn't work if you have loops however!



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# Principal component analysis

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  "On Lines and Planes of Closest Fit to Systems of Points in Space"
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- Simple, fast
- Great for visualisation and dimensionality reduction
- Linear manifolds only (e.g. $4D$ hyper-cube embedded in $12D$ space)
- Still valuable for non-linear manifolds
- Note: Related to factor analysis

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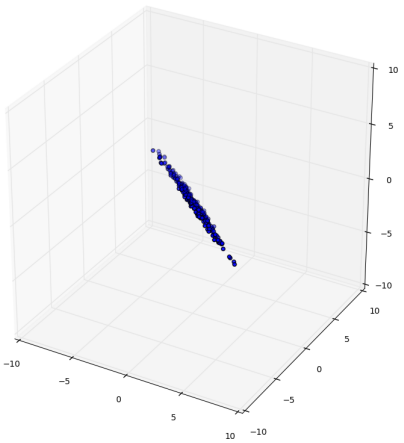
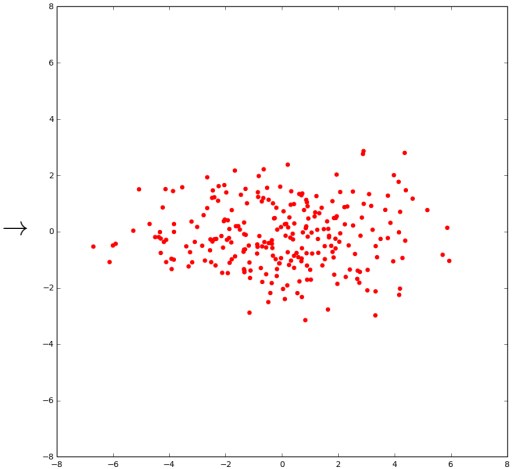
# Example



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- What is the optimal $\hat{d}$?

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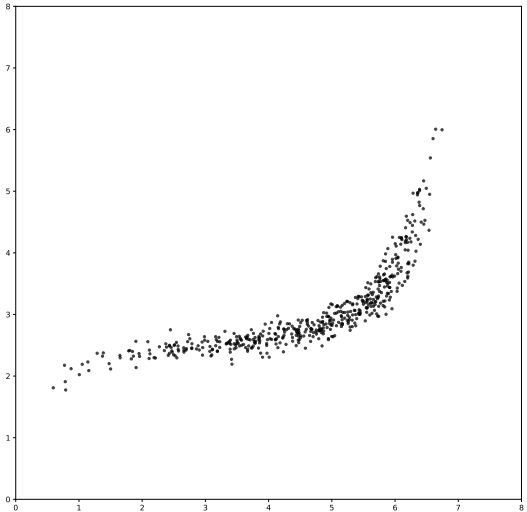
# Visualise I

- Simplest case: 2D to 1D



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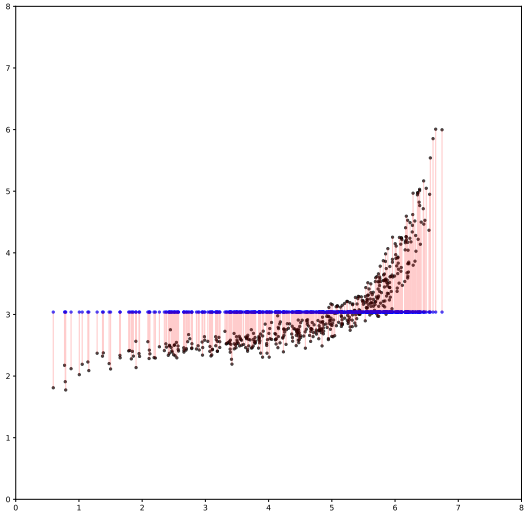

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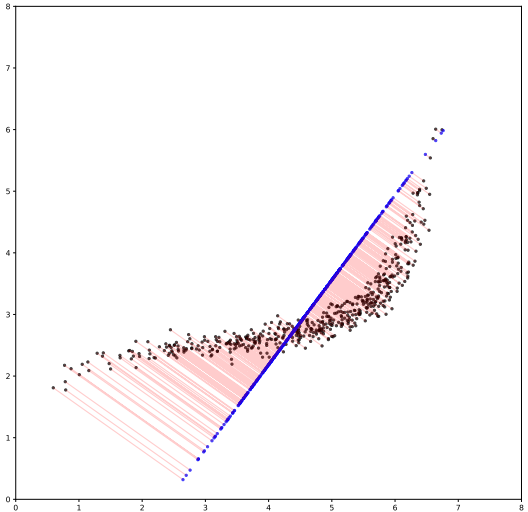

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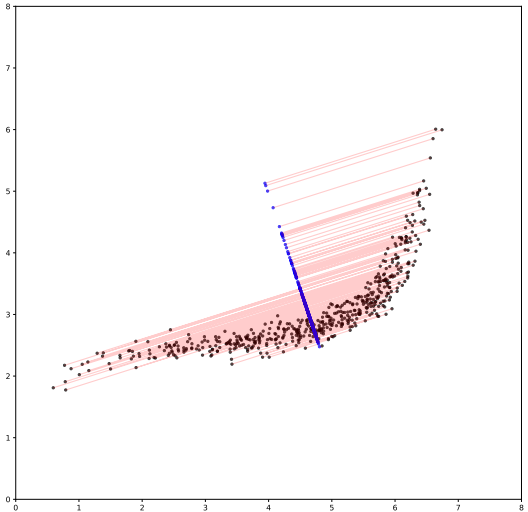

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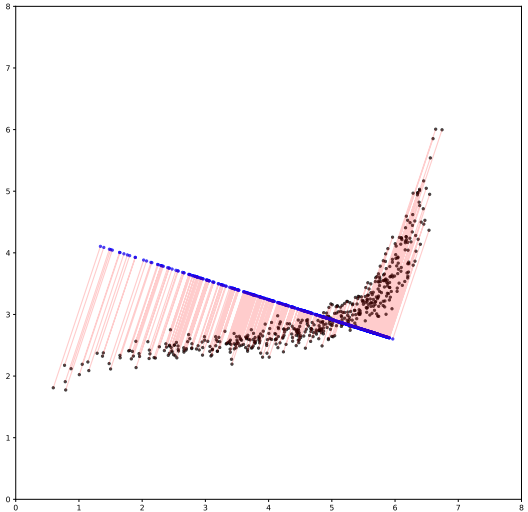
- Best orientation?



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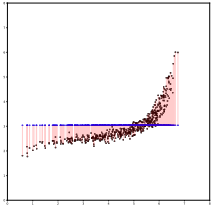
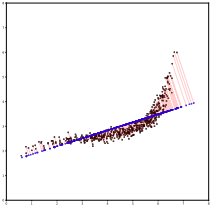
# Visualise II

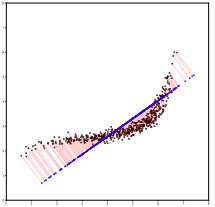
0°:



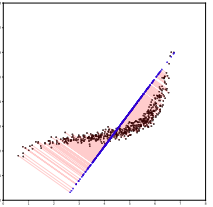
18°:



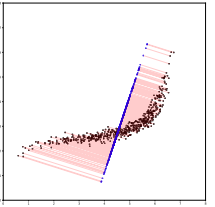
36°:



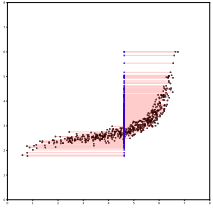
54°:



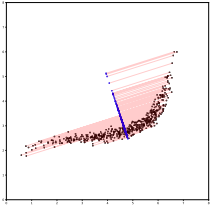
72°:



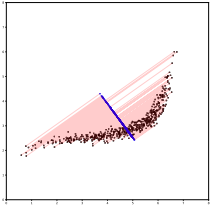
90°:



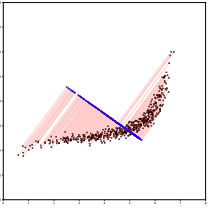
108°:



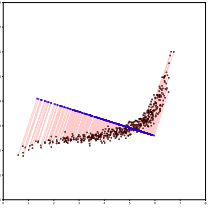
126°:



144°:



162°:



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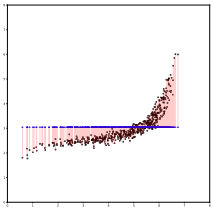
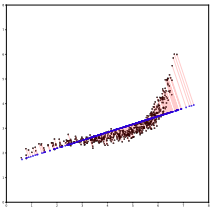


$\sigma^2 = 1.80$

18°:



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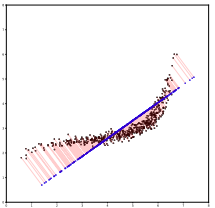
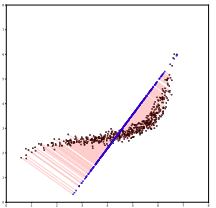
36°:



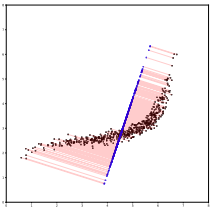
$\sigma^2 = 2.02$

54°:



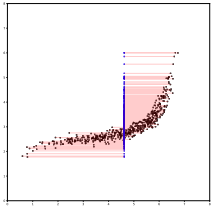
$\sigma^2 = 1.60$

72°:



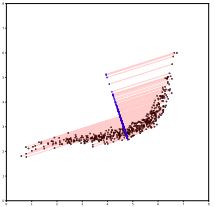
$\sigma^2 = 1.00$

90°:



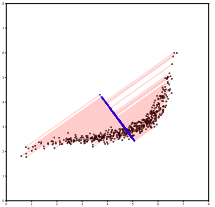
$\sigma^2 = 0.45$

108°:



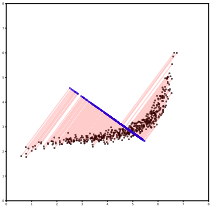
$\sigma^2 = 0.16$

126°:



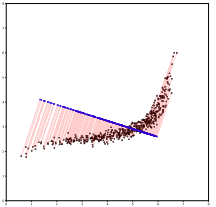
$\sigma^2 = 0.23$

144°:



$\sigma^2 = 0.65$

162°:



$\sigma^2 = 1.25$

# More principle components

- First principle component = direction with **maximum variance**

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- Second principle component:
  - Select another direction, maximising variance
  - **Orthogonal to first principle component**
  - Orthogonality = no shared (wasted) information

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# More principle components

- First principle component = direction with **maximum variance**
- Second principle component:
  - Select another direction, maximising variance
  - **Orthogonal to first principle component**
  - Orthogonality = no shared (wasted) information
- Repeat, orthogonal to all previous components each time

  (set of basis vectors – a rotation by convention)

(not actually coded like this)

# Energy

- Energy $= \sum_{i=1}^{n} \sigma_i^2$
  (sum of variance for all features)
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# Energy

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  (sum of variance for all features)
- Invariant to rotation!

- PCA is a rotation (followed by throwing away low variance dimensions)
- Maximises variance for each principle component

- PCA minimises lost energy
- Typically: Keep 99.9% of energy
- Select principle components until threshold passed

# Algorithm I

- Has analytic solution!

- The principle components = eigenvectors of covariance matrix
- Variance along eigenvector = eigenvalue

  $\therefore$
- PCA uses a eigendecomposition

# Algorithm II

- Subtract mean
- Eigendecomposition of covariance matrix
- Keep eigenvectors with largest eigenvalues
- Energy = sum of eigenvalues, either
  - Keep 99.9% (for dimensionality reduction)
  - Keep 2 or 3 (for visualisation)
- Multiply data with kept eigenvectors (rotation + deletion of low energy directions)

- Return to original space: (with information loss)
  Multiply with transpose of kept eigenvectors, add back mean

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# Algorithm III

```
data -= data.mean(axis=0, keepdims=True) # data[exemplar, feature]
covar = numpy.cov(data.T) # Symmetric

evals, evecs = numpy.linalg.eigh(covar)
# evals ordered lowest to highest, with evecs[:,i] matching evals[i]

energy = numpy.cumsum(evals)
start = 0
while energy[start+1] < 0.001 * energy[-1]: # Keep 99.9% of energy
    start += 1

project = evecs[:,start:][:,::-1].T # Create transform
projected = project.dot(data.T).T # Apply to data
```

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# PCA example

- Data set: Superconductors, 81 features
- Goal: Predict critical temperature

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# PCA example

- Data set: Superconductors, 81 features
- Goal: Predict critical temperature

- PCA: Reduced to 10 features (99.9% energy)

- Elastic net with 81 features: RMSE = 21.0 kelvin, training time 292 milliseconds
- Elastic net with 10 features: RMSE = 21.0 kelvin, training time 17.5 milliseconds

# Further manifold algorithms

All non-linear: (and all start with PCA, if only for initialisation!)

- t-SNE
- Isomap – Probably most common for visualisation
- Autoencoder – Probably most used for dimensionality reduction
- Probabilistic PCA
- Gaussian process latent variable model – Probably most theoretically sweet

# Other curse-avoiding approaches

- Learning features with convolutional NN
- Using structure (conditional independence)

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# Classic preprocessing

- Steps:
  1. Whitening

```
data -= data.mean(axis=0, keepdims=True)
data /= data.std(axis=0, keepdims=True)
```

     (subtract mean, divide by standard deviation)

  2. PCA

- Most algorithms: Improves performance (more accurate and faster!)

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# Summary

- The curse of dimensionality
  (beware your intuitions in high dimensions – they are wrong)
- Feature selection
- Feature engineering
- Manifolds & dimensionality reduction

# Further reading

- "A Few Useful Things to Know about Machine Learning", by P. Domingos, `https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf`