Modern Algorithms for Machine Learning

Lecture 1 (Part II): Nearest Neighbour and Dimensionality Reduction

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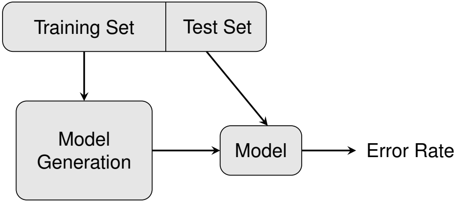
Outline

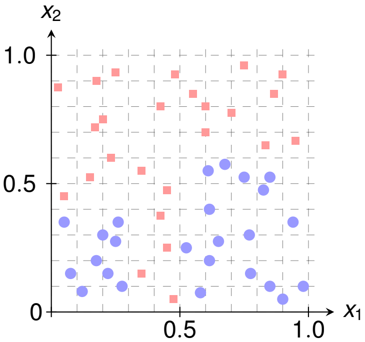
Machine learning model (Supervised Learning)



- Training data: used to build a model or classifier for the data.
- Test data: helps validate it.
- Overfitting:
  - ML algorithms tune their model to the training set (and not the general data that the training set represents);
  - test data helps restricting overfitting.
- Feature selection: which to use to input into ML algorithm?
- Training set creation: where do labels for data come from?

The Model (A bit more formal...)

- Let $\mathcal{X} = \mathbb{R}^d$ (domain set)
- Let $\mathcal{Y} = \{-1, +1\}$ (label set)
- Let $S = ((\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_m, y_m))$ (training set)



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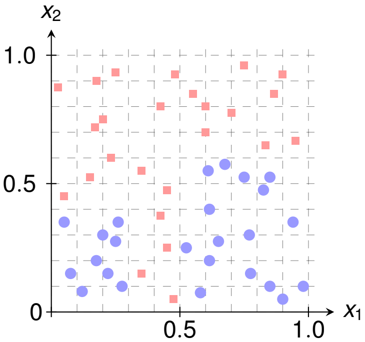

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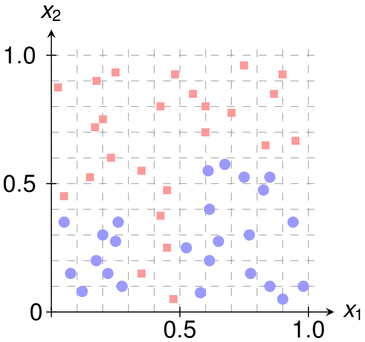

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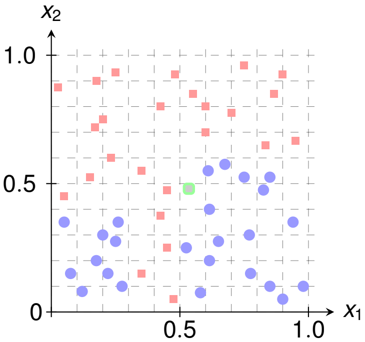

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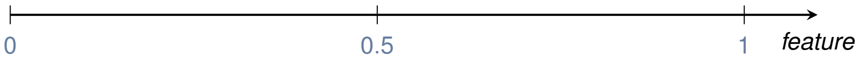

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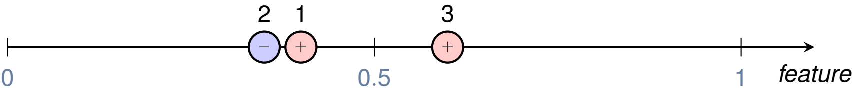

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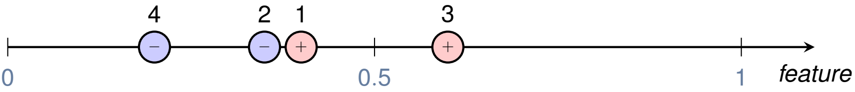

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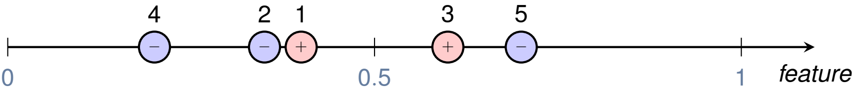

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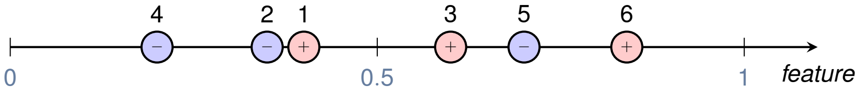

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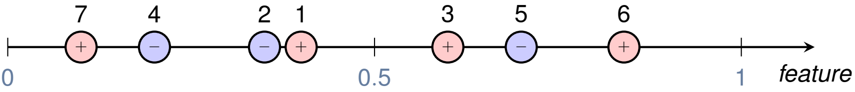

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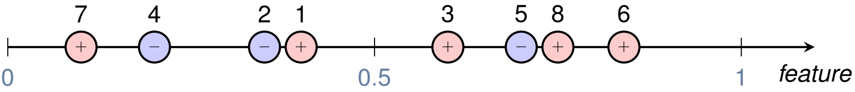

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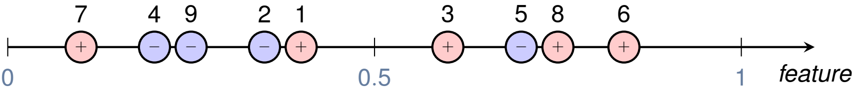

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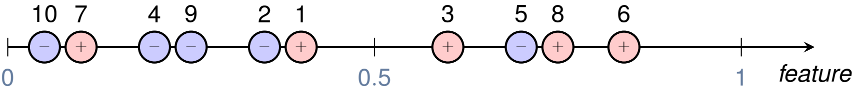

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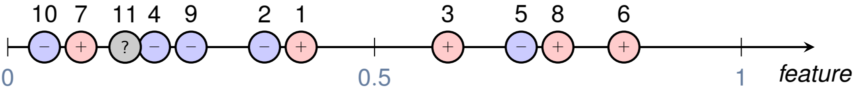

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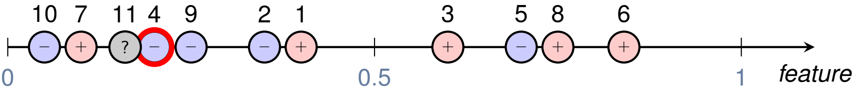

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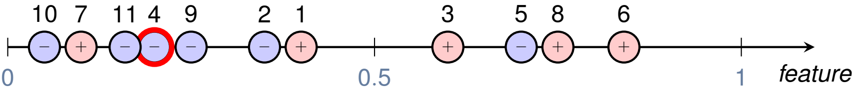

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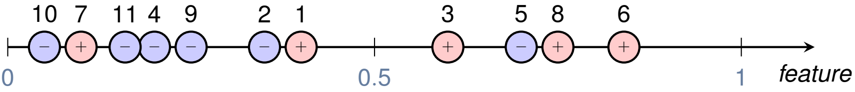

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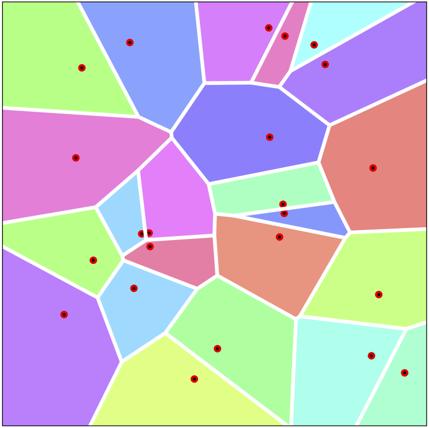
k-NN

input: a training sample $S = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)$
output: for every point $\mathbf{x} \in \mathcal{X}$,
return the majority label among $\{y_{\pi_i(\mathbf{x})} : i \le k\}$

Source: SS&BD

Special Case: 1-NN



- For $k = 1$, the produced decision boundaries are Voronoi-cells
- Any new point will be classified according to the centre of each cell

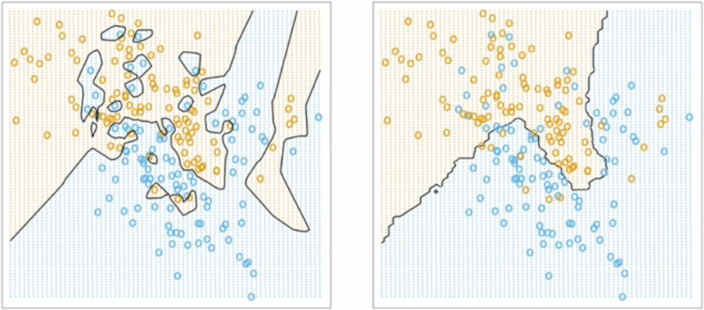
How many Neighbours should we choose?

Source: Lecture by Ulrike von Luxburg

$k = 1$ $k = 15$

How many Neighbours should we choose?

For small k, k-NN overfits the data!



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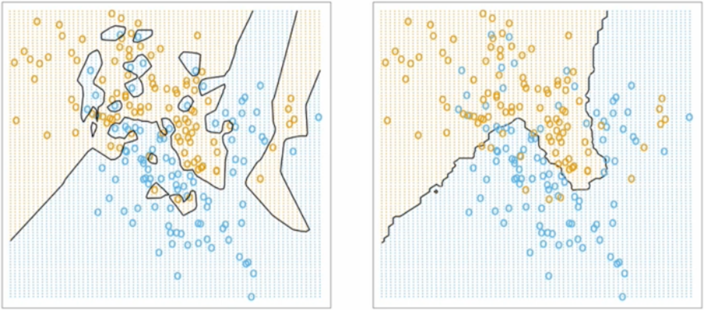

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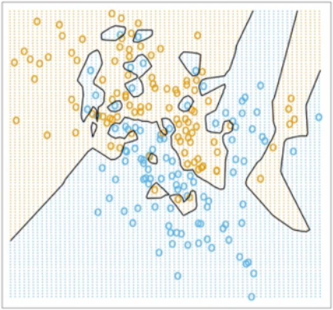
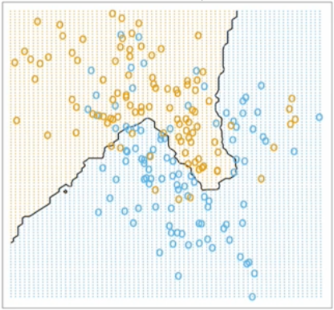
Question: What happens if $k = n$, where n is the total number of points in our training set?

How many Neighbours should we choose?

For small k, k-NN overfits the data!

Rule-of-thumb: $k \approx \log n$ is good





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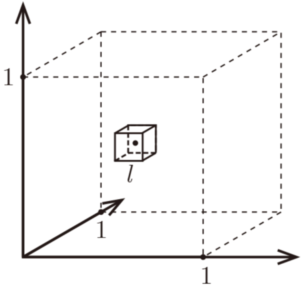
Curse of Dimensionality



Source: Kilian Weinberger

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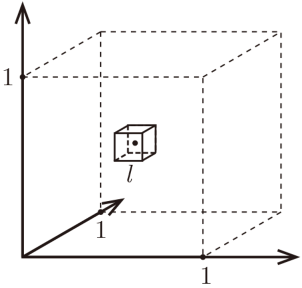

Source: Kilian Weinberger

- Suppose $n = 1000$ points are "randomly" spread across $[0, 1]^d$

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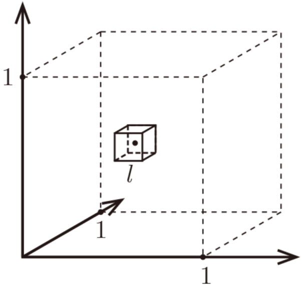

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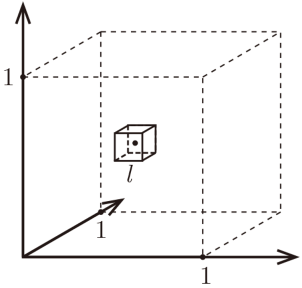

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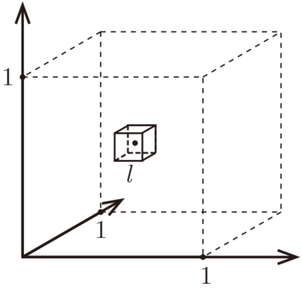
d	ℓ
2	0.1
10	0.63
100	0.955
1000	0.9954

Curse of Dimensionality



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- Suppose $n = 1000$ points are "randomly" spread across $[0, 1]^d$
- If we want to find the 10 nearest neighbour, how large must be the subcube be?

d	ℓ
2	0.1
10	0.63
100	0.955
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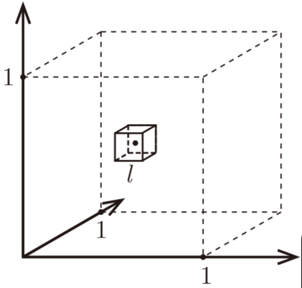
To find the closest neighbour, we need to search the entire space!

Curse of Dimensionality



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In high dimensions, almost all points have the same (far) distance!

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+ does not use any training/learning phase
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– results may crucially depend on the choice of distance function and k
– finding nearest neighbour is costly ($\rightsquigarrow$ KD-trees, locality-sensitive hashing)
– very slow with large k or high-dimensional data (course of dimensionality)

We will now learn a powerful pre-processing method called **Dimensionality Reduction**!

Outline

Mathematical Tools

- **Matrices and Geometry**
  - Data points (predictions, observations, classifications) encoded in matrices/vectors
  - This allows geometric representation that is the basis of many ML methods
  - Networks and graphs $\Leftrightarrow$ adjacency matrices

  Inner product, Hyperplanes, Eigenvectors

- **Probability Theory**
  - Sampling-based algorithms
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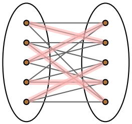
  - Incomplete data, noisy/corrupted data can be modelled by a random processes

  Random Variables, Chernoff Bounds, hashing



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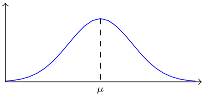

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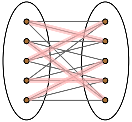

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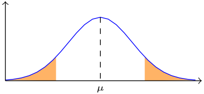

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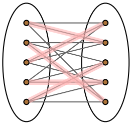

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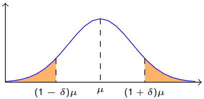
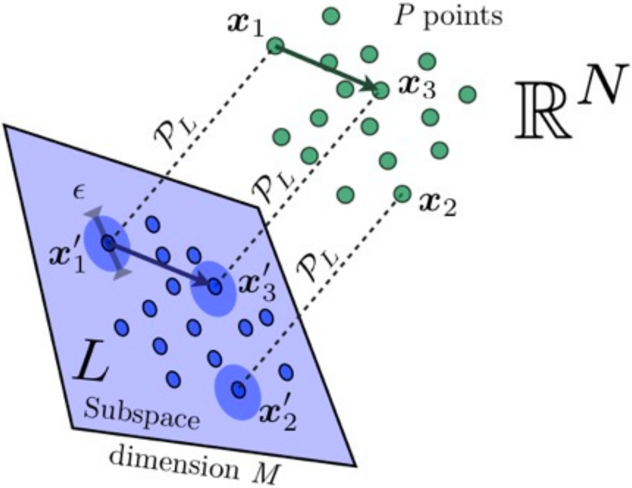
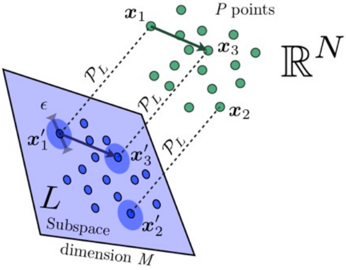


Intuition behind Dimensionality Reduction



Source: Laurent Jacques

Dimensionality Reduction: Basic Setup



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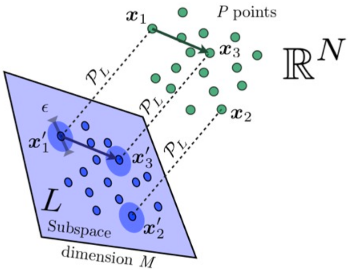

- Given P points $x_1, x_2, \ldots, x_P \in \mathbb{R}^N$
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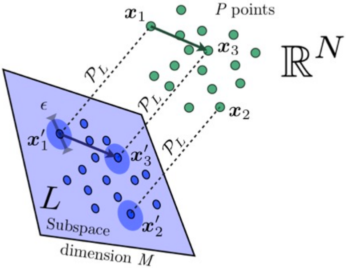

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Goal: Distances are approximately preserved, i.e.,

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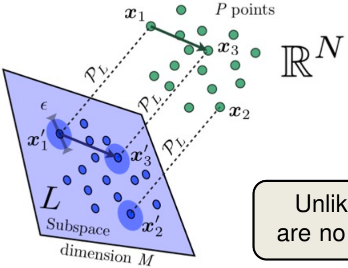

Unlike other methods like PCA, there are no assumptions on the original data.

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Theorem

Let $x_1, x_2, \ldots, x_p \in \mathbb{R}^N$ be arbitrary. Pick any $\epsilon = (0, 1)$. Then for some $M = O(\log(P)/\epsilon^2)$, there is a polynomial-time algorithm that, with probability at least $1 - \frac{2}{P}$, computes $x_1', x_2', \ldots, x_P' \in \mathbb{R}^M$ such that

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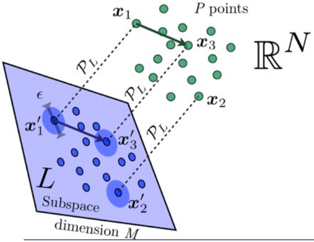
How to construct $x'_1, x'_2, \ldots, x'_P$?

Key Tool: Random Projection Method



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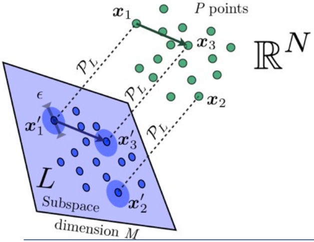
Definition of $f : \mathbb{R}^N \to \mathbb{R}^M \qquad (M \ll N)$



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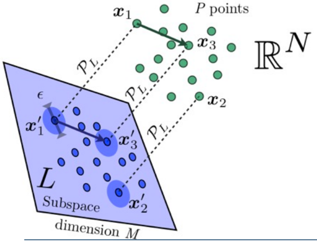

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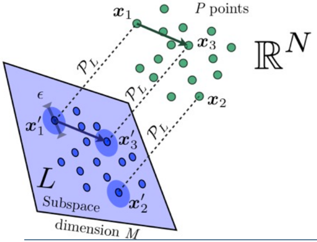

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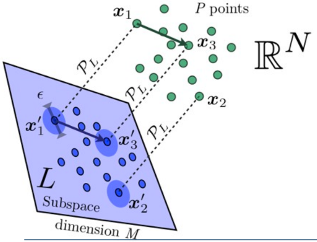

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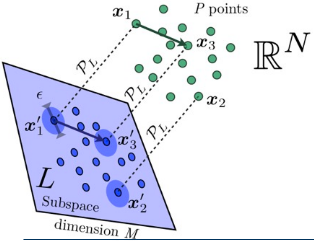

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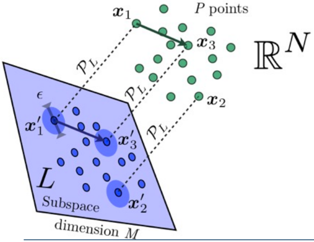

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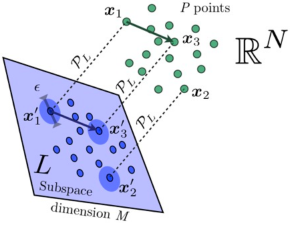

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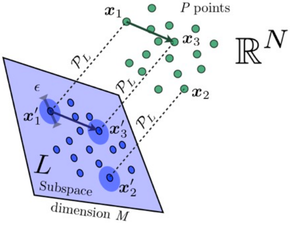

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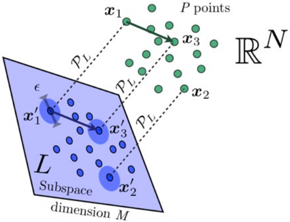

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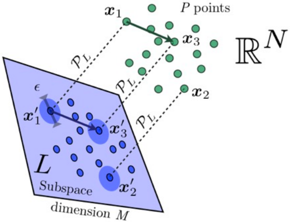

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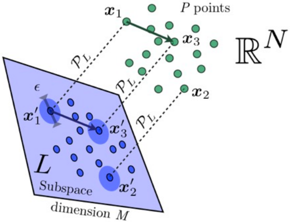

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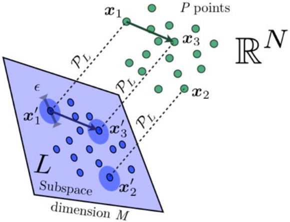

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$$(1-\epsilon)\cdot\|x_i\| \le \|L(x_i)\| \le (1+\epsilon)\cdot\|x_i\| \quad \text{for all } i. \qquad \square$$

Outline

Proof of JL-Lemma (1/4)

Johnson-Lindenstrauss Lemma

Let $w \in \mathbb{R}^N$ with $\|w\| = 1$. Then for some $M = O(\log(P)/\epsilon^2)$, we have

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- Hence

$$\|f(w)\|^2 = \sum_{i=1}^{M} X_i^2,$$

where the X_i's are independent $\mathcal{N}(0,1)$ random variables.

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- Since $X_1^2, \dots, X_M^2$ are independent,

$$\mathbf{E}\left[e^{tX}\right] = \mathbf{E}\left[e^{t\sum_{i=1}^{M} X_i^2}\right] = \mathbf{E}\left[\prod_{i=1}^{M} e^{tX_i^2}\right] \stackrel{!}{=} \prod_{i=1}^{M} \mathbf{E}\left[e^{(tX_i^2)}\right]$$

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- With $M = 6 \ln P/\epsilon^2$, the last term becomes $\frac{2}{P^3}$.
- Lower bound is derived similarly $\Rightarrow$ proof complete $\square$

Example: Target Dimension M of JL-Lemma

Recall: $M \leq \frac{6 \ln P}{\epsilon^2}$

ϵ	Number of Points P	Target Dimension M
1/2	1,000	166
1/2	10,000	221
1/2	100,000	276
1/2	1,000,000	331
1/2	10,000,000	387
1/10	1,000	4145
1/10	10,000	5526
1/10	100,000	6907
1/10	1,000,000	8298
1/10	10,000,000	9670

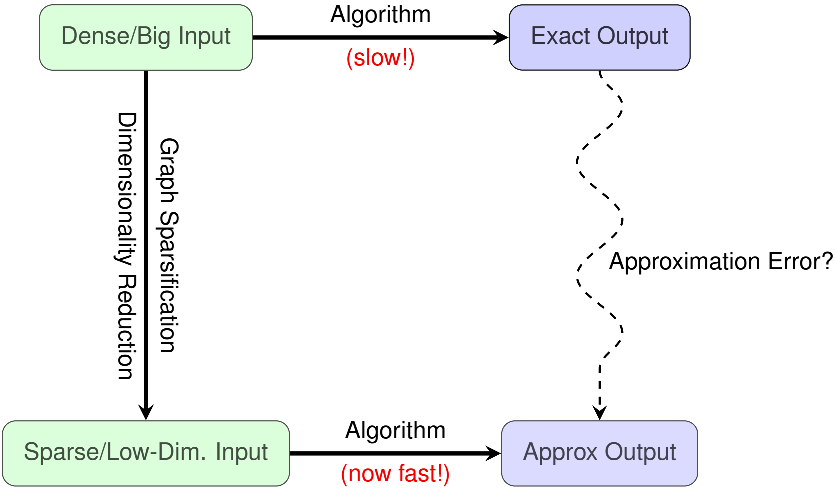
General Comments on the JL-Lemma

- Use Random Projection to a Subspace
  - similar to projection on the bottom k eigenvalues, but with different aim here
  - exploits redundancy in “Wide-Data” (high-dimensional data)
  - also powerful method in approximation algorithms (example: MAX-CUT)

- Why do we use a Random Projection?
  - If projection f is chosen deterministically, easy to find vectors u, v with $\|u - v\|$ large but $f(u) = f(v)$.

  $\Rightarrow$ Randomisation prevents the input to foil a specific deterministic algorithm

Generic Application of Preprocessing



Applications of the JL-Lemma

- Streaming Algorithms
- Preprocessing of many Machine Learning Methods

. . .

Random Projection, Margins, Kernels, and Feature-Selection

Avrim Blum

Department of Computer Science,
Carnegie Mellon University, Pittsburgh, PA 15213-3891

Abstract. Random projection is a simple technique that has had a number of applications in algorithm design. In the context of machine learning, it can provide insight into questions such as "why is a learning problem easier if data is separable by a large margin?" and "in what sense is choosing a kernel much like choosing a set of features?" This talk is intended to provide an introduction to random projection and to survey some simple learning algorithms and other applications to learning based on it. I will also discuss how, given a kernel as a black-box function, we can use various forms of random projection to extract an explicit small feature space that captures much of what the kernel is doing. This talk is based in large part on work in [BB05, BBV04] joint with Nina Balcan and Santosh Vempala.

Outline

Nearest Neighbour Algorithm

Dimensionality Reduction

Proof of JL-Lemma (advanced)

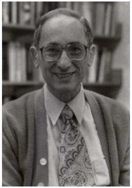
Chernoff Bounds and Concentration of Measure (Bonus Material)

Appendix

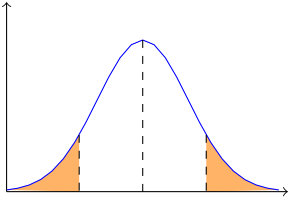
Chernoff Bounds

- Chernoffs bounds are "strong" bounds on the tail probabilities of sums of independent random variables (random variables can be discrete or continuous)
- usually these bounds decrease exponentially as opposed to a polynomial decrease in Markov's or Chebysheff's inequality (see example later)
- have found various applications in:
  - Random Projections
  - Approximation and Sampling Algorithms
  - Learning Theory (e.g., PAC-learning)
  - Statistics

  ⋮



Hermann Chernoff (1923-)



A Simple Chernoff Bound for Uniform Coin Flips

Uniform Chernoff Bound

Let $X_1, \ldots, X_n$ be independent random variables with $\mathbf{Pr}[X_i = 1] = \mathbf{Pr}[X_i = -1] = 1/2$. Let $X := \sum_{i=1}^{n} X_i$. Then for any $\lambda > 0$,

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- This is a simple yet important setting, since r.v.'s are identical and symmetric
- Bound on $\mathbf{Pr}[X \leq -\lambda]$ follows by symmetry
- Bounds for the case $\mathbf{Pr}[X_i = 1] = \mathbf{Pr}[X_i = 0] = 1/2$ through substitution, see below

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Corollary

Let $X_1, \ldots, X_n$ be independent random variables with $\mathbf{Pr}[X_i = 0] = \mathbf{Pr}[X_i = 1] = 1/2$. Let $X := \sum_{i=1}^n X_i$ and $\mu := \mathbf{E}[X] = n/2$. Then for any $\lambda > 0$,

$$\mathbf{Pr}[X \geq \mu + \lambda] \leq e^{-2\lambda^2/n}.$$

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- The uniform Chernoff bound (Corollary) with $\mu = 50, \lambda = 25$ gives:

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Chernoff bound yields a more accurate result but needs independence!

Recipe for Deriving Chernoff Bounds

Main Steps

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4. Optimise the value of t to obtain best tail bound

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   - Therefore,

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$$\mathbf{Pr}\left[\, X \geq \lambda \,\right] \leq e^{\lambda^2/(2n) - \lambda^2/n} = e^{-\lambda^2/(2n)}. \qquad \square$$

Extension to Non-Uniform Random Variables

Hoeffding's inequality

Let $X_1, \ldots, X_n$ be n independent random variables with $X_i \in [a_i, b_i]$ for each $1 \leq i \leq n$. Let $X := \sum_{i=1}^n X_i$ and $\mu = \mathbf{E}[X] = \sum_{i=1}^n \mathbf{E}[X_i]$. Then, for any $\delta \geq 0$,

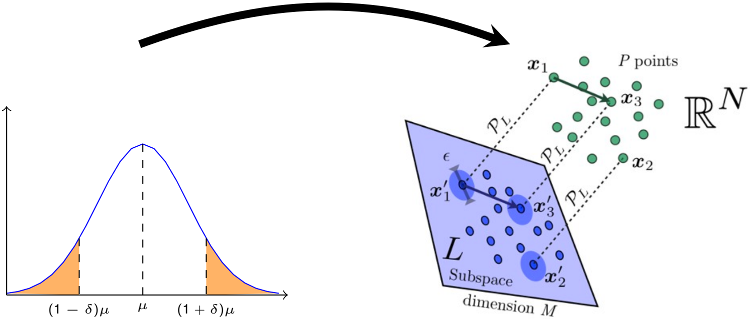
$$\mathbf{Pr}[|X - \mu| \geq \delta] \leq 2 \cdot \exp\left(-\frac{2\delta^2}{\sum_{i=1}^n (b_i - a_i)^2}\right).$$

Further Extensions:

- Chernoff Bounds for sum of random variables with unbounded range (e.g., geometric random variables)
- Martingales (Azuma-Hoeffding's Inequality, Method of Bounded Independent Differences)
- Talagrand's Inequality (Measure Concentration and Expansion)
- ...

The last two extensions apply even to settings where the random variables are not independent.

Summary: Measure Concentration and Randomised Algorithms



- sums of independent random variables
- Chernoff Bounds: concrete tail inequalities that are exponential in the deviation
- Proof Method: Moment Generating Function & Markov's Inequality

- Random Projection Method
  - multiply by a random matrix
  - preserves distances up to $1 \pm \epsilon$
  - new dimension $\mathcal{O}(\log P/\epsilon^2)$

Outline

Appendix A: Moment Generating Functions

Moment-Generating Function

The moment-generating function of a random variable X is

$$M_X(t) = \mathbf{E}\left[e^{tX}\right], \qquad \text{where } t \in \mathbb{R}.$$

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Lemma

1. If X and Y are two r.v.'s with $M_X(t) = M_Y(t)$ for all $t \in (-\delta, +\delta)$ for some $\delta > 0$, then the distributions X and Y are identical.
2. If X and Y are independent random variables, then

$$M_{X+Y}(t) = M_X(t) \cdot M_Y(t).$$

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Proof of 2:

$$M_{X+Y}(t) = \mathbf{E}\left[e^{t(X+Y)}\right] = \mathbf{E}\left[e^{tX} \cdot e^{tY}\right] \overset{(!)}{=} \mathbf{E}\left[e^{tX}\right] \cdot \mathbf{E}\left[e^{tY}\right] = M_X(t)M_Y(t) \qquad \square$$

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