Random Projections

2IMM20 - Foundations of data mining
TU Eindhoven, Quartile 3, 2017-2018

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Why reduce the dimension?

Representation of input data often is often high dimensional (images, documents, etc.)

There are two main reasons to reduce the dimension:

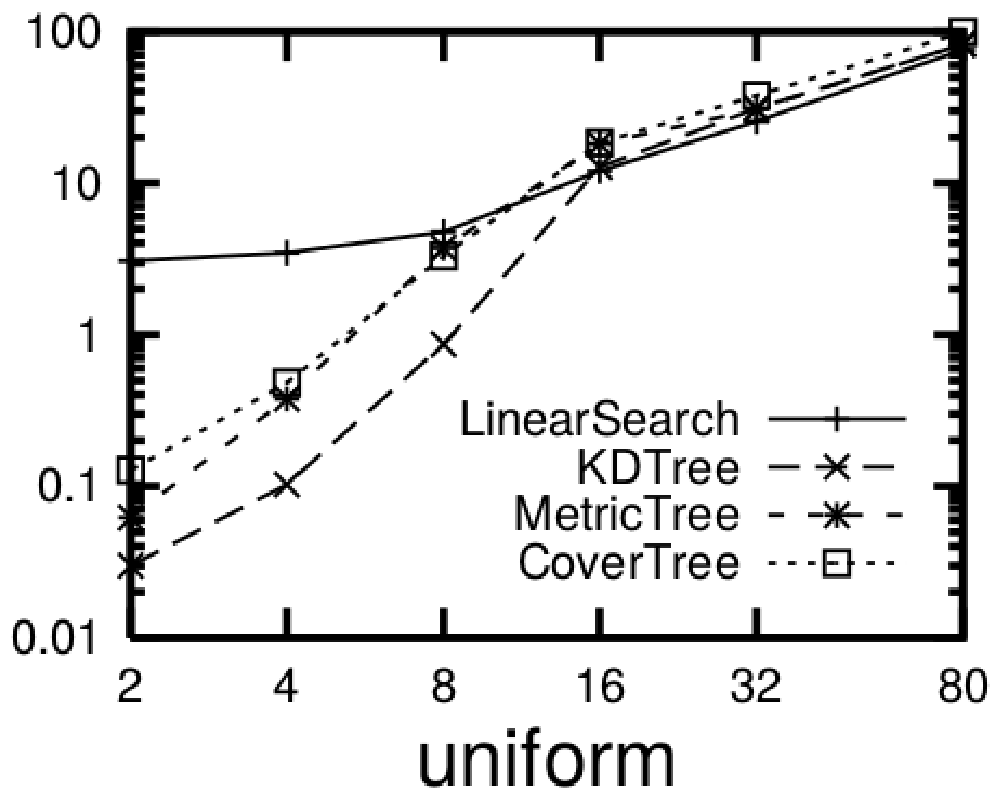
- some algorithms have **running time** exponential in the dimension
- we want to **visualize** inherent structure in the data

Overview of this lecture

- Nearest-neighbor searching
- Embedding and Distortion
- Achlioptas' Random Projection
- Projection onto a subspace
- Random Rotation (Expectation)
- Analysis of a fixed distance (Expectation)
- Law of large numbers
- Concentration of measure
- Analysis of a fixed distance
- Analysis of the Distortion
- Alternative Projection Matrix

Nearest neighbor searching

CPU-time to query the k-nearest neighbors vs. dimension of the data



Source: Ashraf M. Kibriya and Eibe Frank "An Empirical Comparison of Exact Nearest Neighbour Algorithms" PKDD 2007

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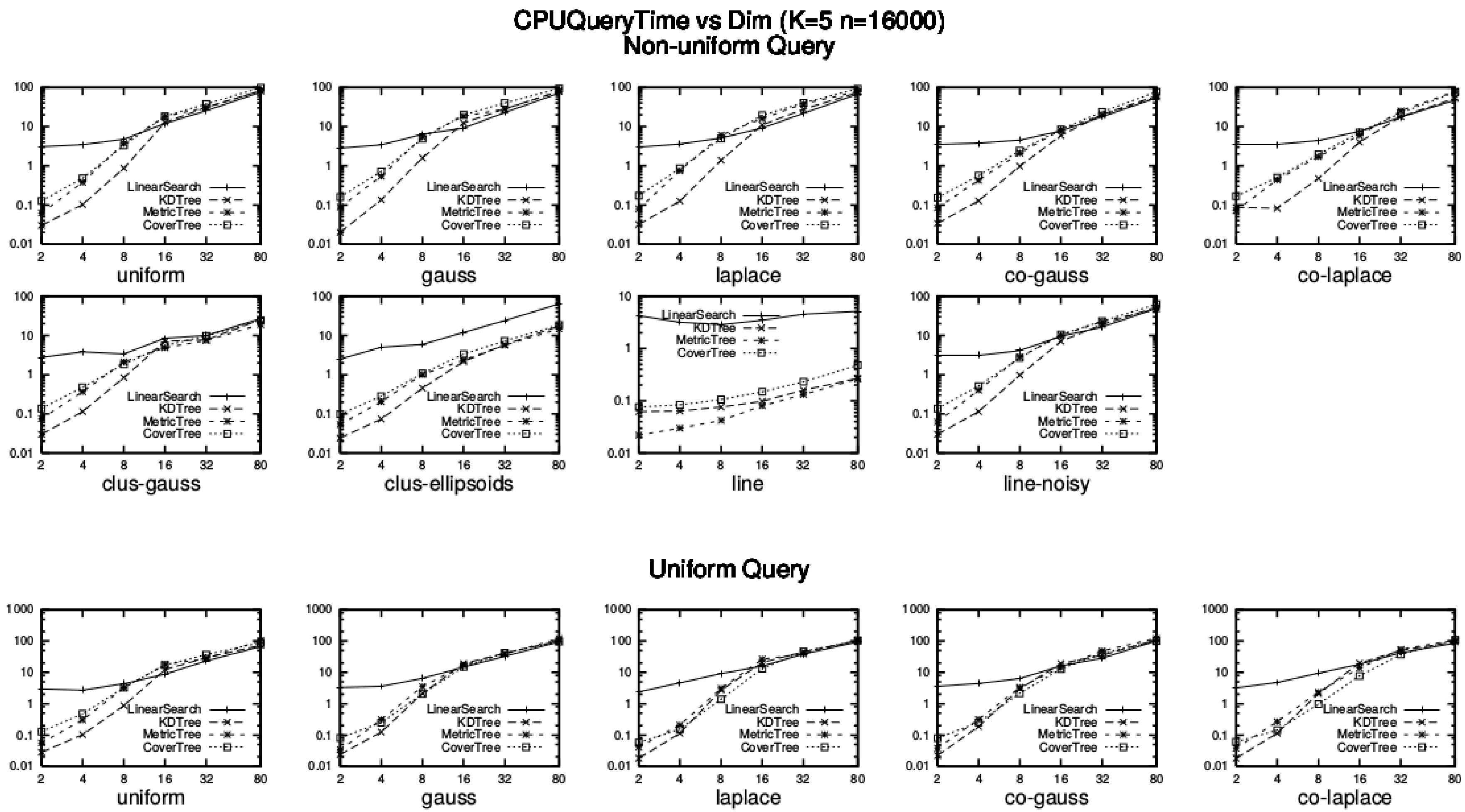

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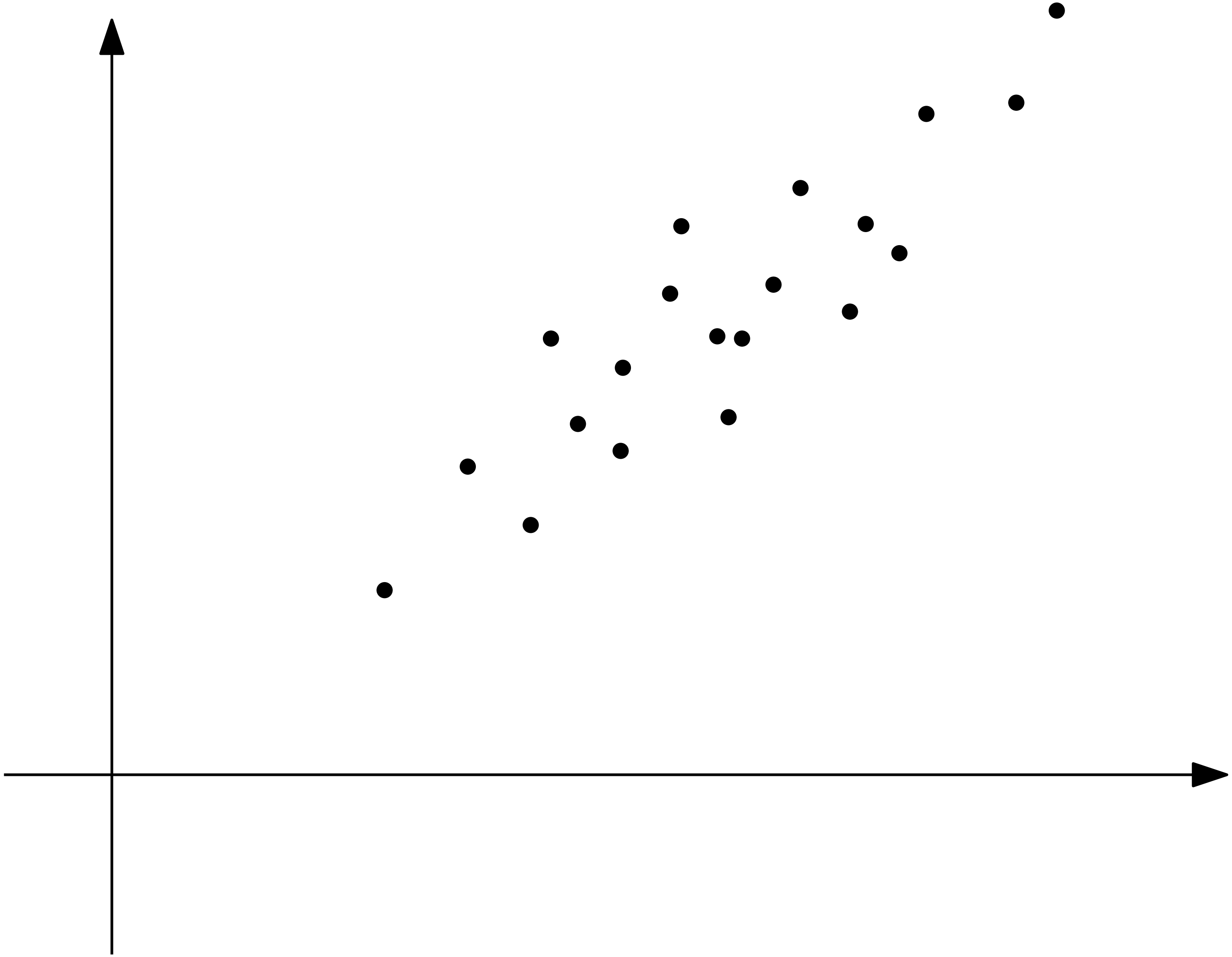
Principal Component Analysis (PCA)

Example: $d = 2, k = 1$



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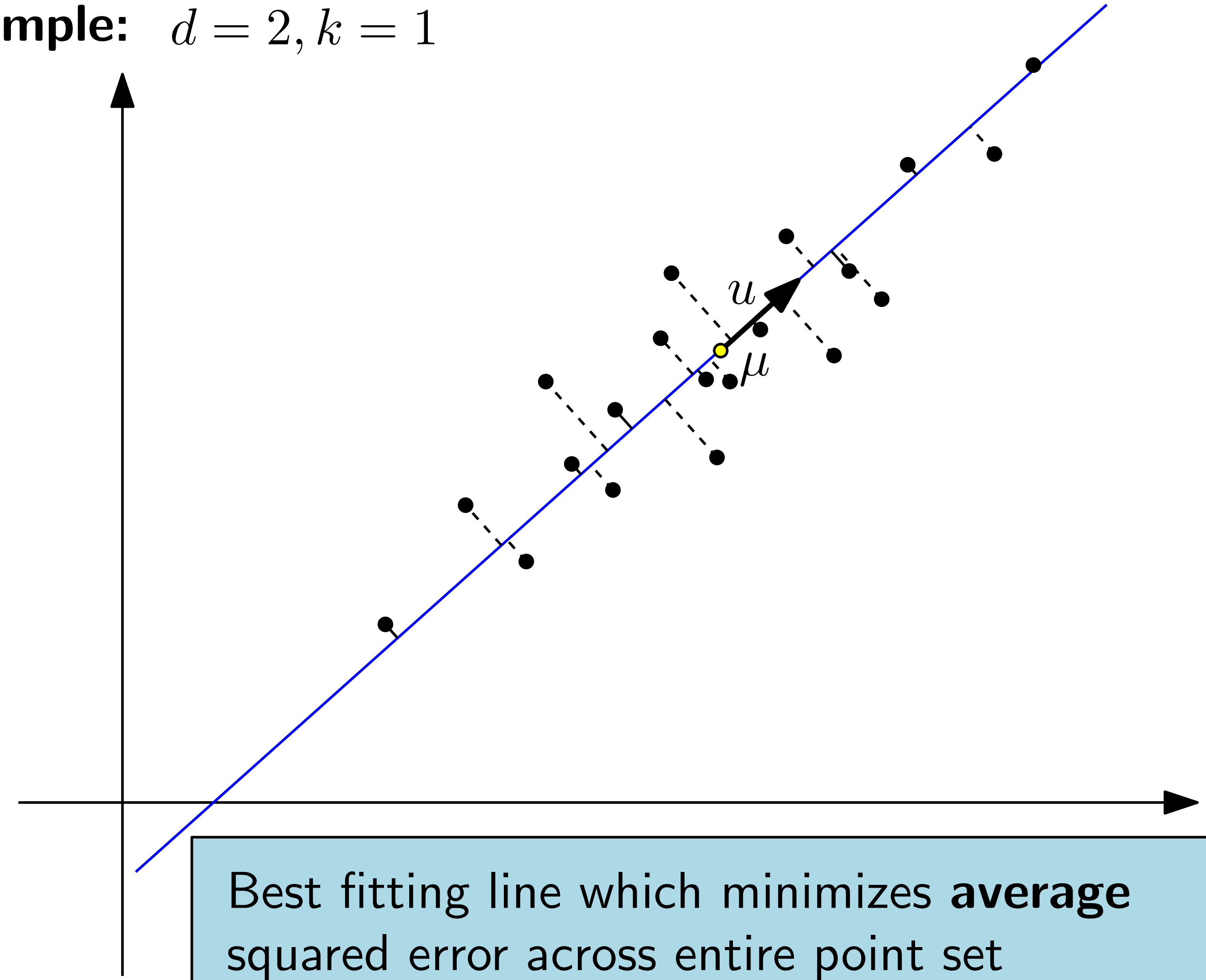

Best fitting line which minimizes **average** squared error across entire point set

Random Projection

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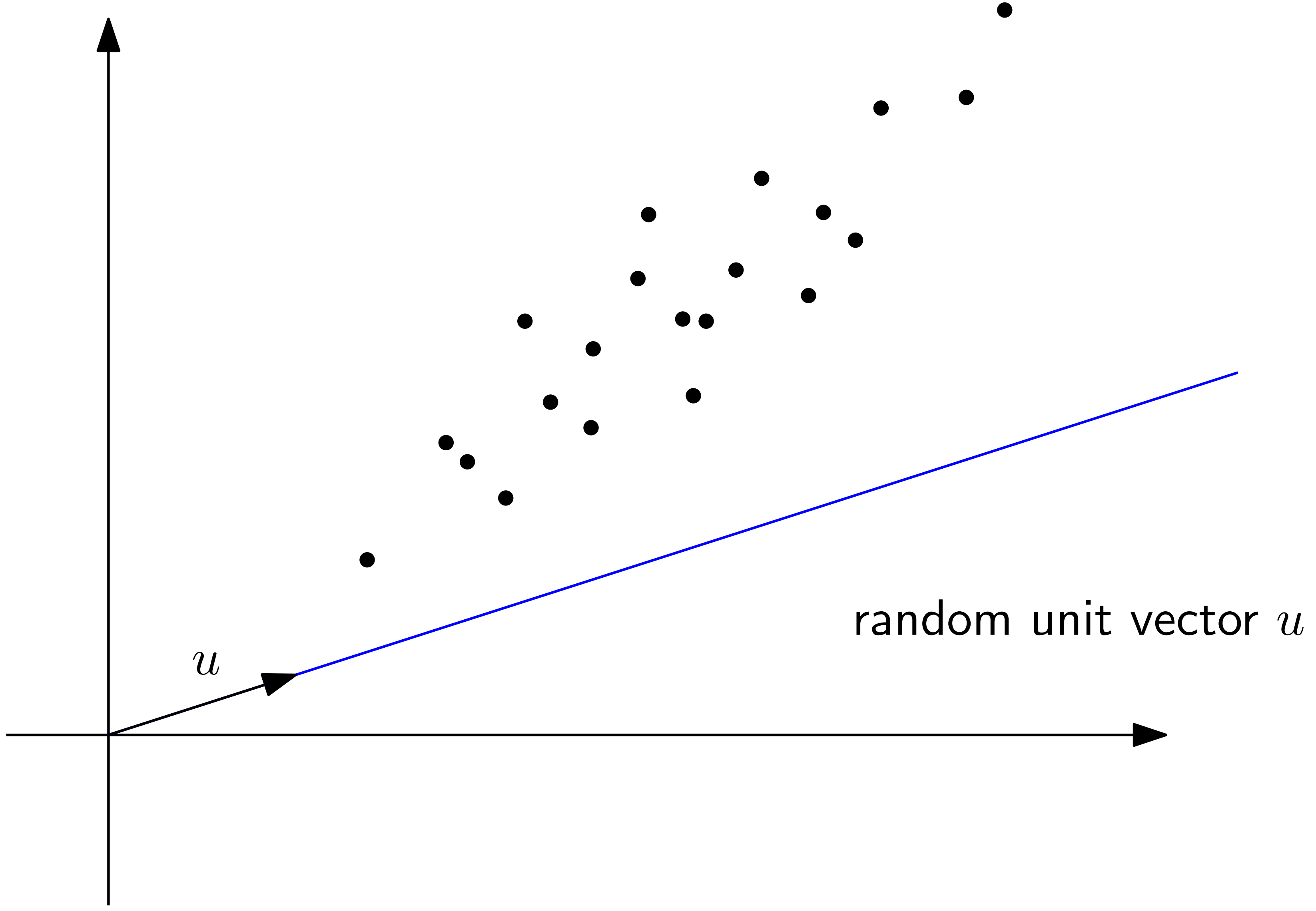

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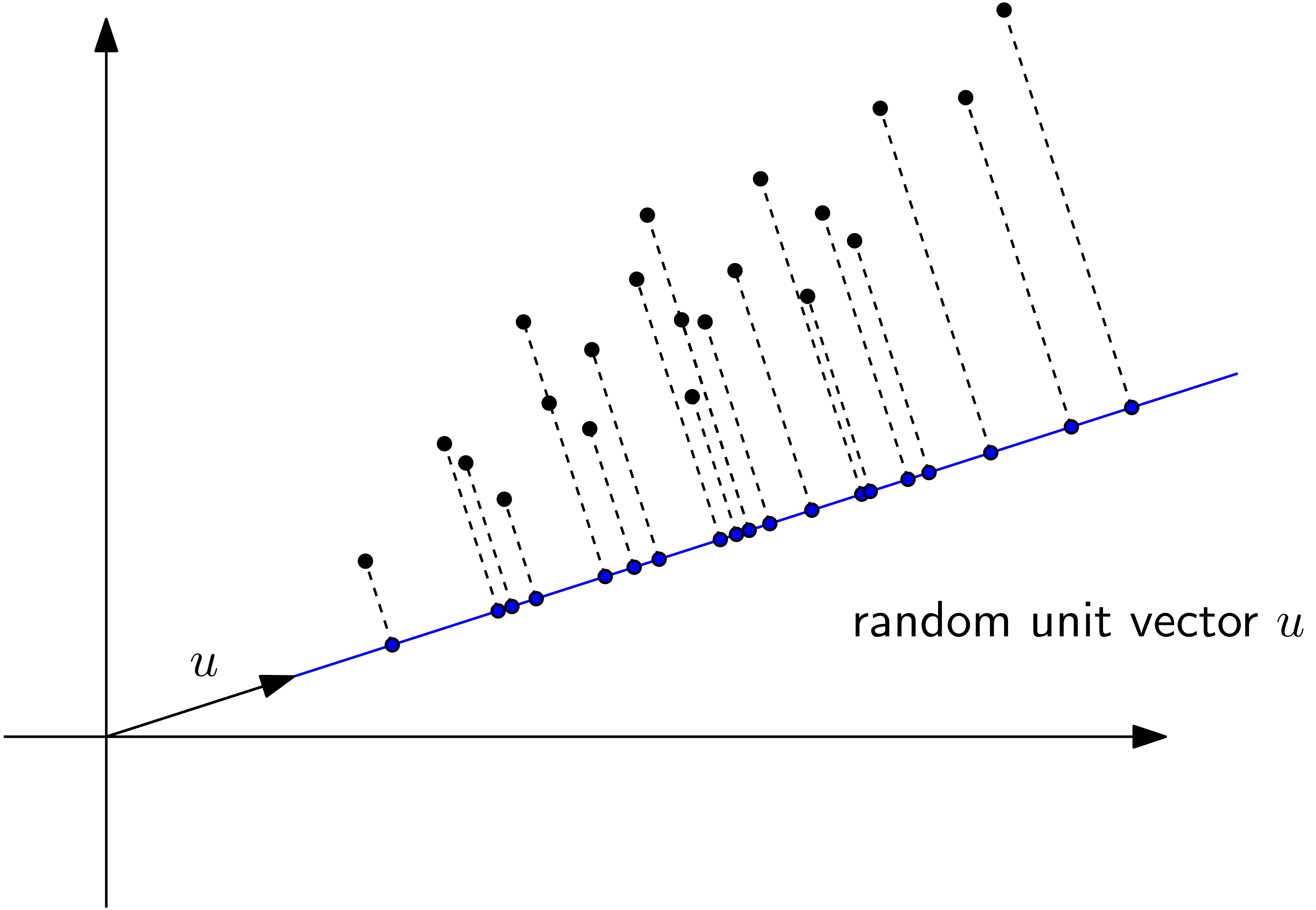

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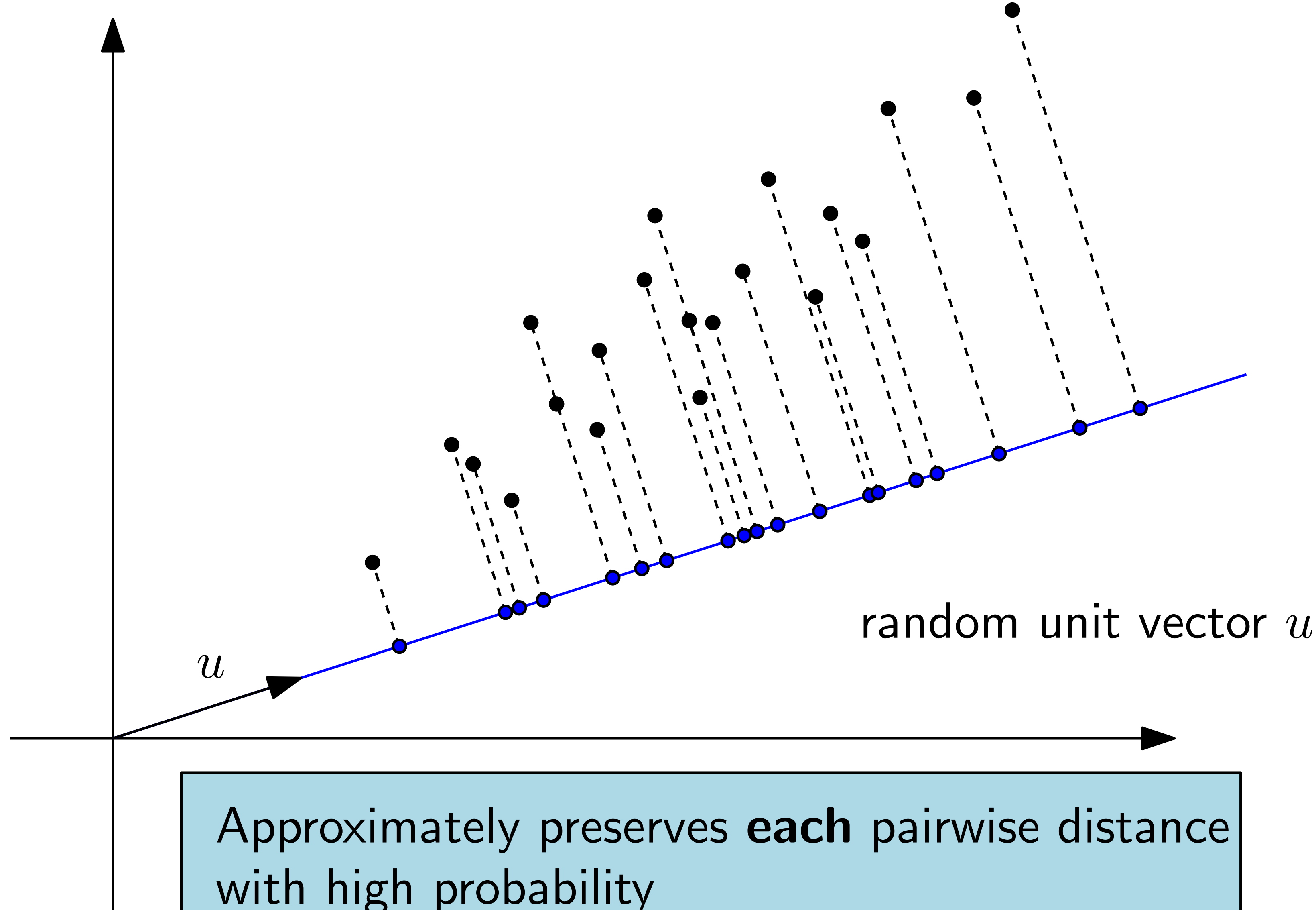

Approximately preserves **each** pairwise distance with high probability

Embedding and Distortion

Given a point set $X \in \mathbb{R}^d$, we call a function $f : X \to \mathbb{R}^k$ an **embedding** of X. We define

$$\text{expansion}(f) = \max_{x,y \in X} \frac{\|f(x) - f(y)\|}{\|x - y\|}$$

$$\text{contraction}(f) = \max_{x,y \in X} \frac{\|x - y\|}{\|f(x) - f(y)\|}$$

The **distortion** of f is defined as the product of the expansion and the contraction of f.

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Note that for all $x, y \in X$ we have

$$\frac{1}{\beta}\|x - y\| \leq \|f(x) - f(y)\| \leq \alpha\|x - y\|$$

where α denotes the expansion and β denotes the contraction

Achlioptas' Random Projection (Algorithm)

Input: set of points $P = \{p_1, \ldots, p_n\} \subseteq \mathbb{R}^d$, value of k
Output: set of points $Q = \{q_1, \ldots, q_n\} \subseteq \mathbb{R}^k$

Algorithm:

- Generate a random $k \times d$ matrix $\mathbf{R}$ by choosing

$$r_{i,j} = \begin{cases} +1 & \text{with probability } \frac{1}{2} \\ -1 & \text{with probability } \frac{1}{2} \end{cases}$$

- For each $i = 1, \ldots, n$, compute $q_i = \frac{1}{\sqrt{k}} \mathbf{R} p_i$

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Theorem:

Let $k_0 = \frac{4+2\beta}{\varepsilon^2/2 - \varepsilon^3/3} \log n$, for given $\varepsilon, \beta > 0$. If $k \geq k_0$ then with probability at least $1 - \frac{1}{n^\beta}$, we have for all $p_i, p_j \in P$ that

$$(1-\varepsilon)\|p_i - p_j\|^2 \leq \|q_i - q_j\|^2 \leq (1+\varepsilon)\|p_i - p_j\|^2$$

History: Embedding Lemma

Random projections were invented by Johnson and Lindenstrauss.

Lemma (Johnson and Lindenstrauss, 1984):
Given $\varepsilon > 0$ and an integer n, let k be a positive integer $k \geq k_0 = O\left(\frac{\log n}{\varepsilon^2}\right)$. For every set of points $P = \{p_1, \ldots, p_n\} \subseteq \mathbb{R}^d$ there exists $f : \mathbb{R}^d \to \mathbb{R}^k$ such that for all $p_i, p_j \in P$

$$(1 - \varepsilon)\|p_i - p_j\|^2 \leq \|f(p_i) - f(p_j)\|^2 \leq (1 + \varepsilon)\|p_i - p_j\|^2.$$

Note: The proof uses a random projection to show that f exists. For historical reasons, the JL-lemma only talks about the existence of f.

Linear Algebra: Rotation

In general:
A matrix is a rotation iff it is orthogonal

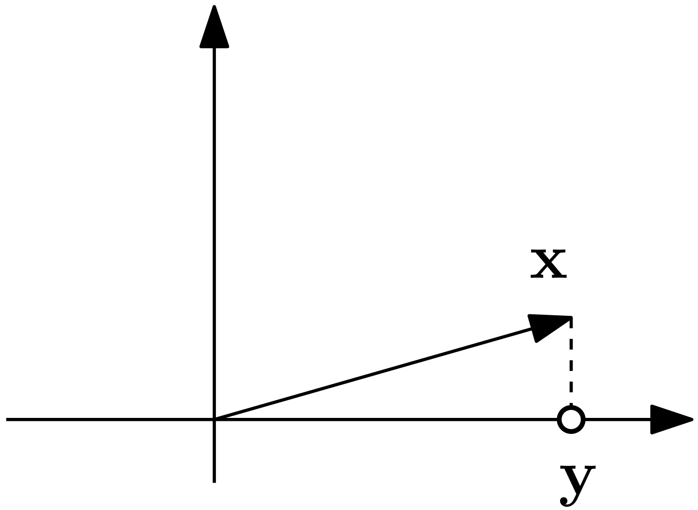
$$\mathbf{R} = \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} \\ r_{2,1} & r_{2,2} & r_{2,3} \\ r_{3,1} & r_{3,2} & r_{3,3} \end{pmatrix} = \begin{pmatrix} \mathbf{r_1} \\ \mathbf{r_2} \\ \mathbf{r_3} \end{pmatrix}$$

This means its row vectors are..
(1) pairwise orthogonal: $\mathbf{r_i} \cdot \mathbf{r_j} = 0$
(2) unit vectors: $\|\mathbf{r_i}\| = 1$

Furthermore, it holds that $\mathbf{R}^{-1} = \mathbf{R}^{\mathbf{T}}$ and that the length of any vector is preserved under $\mathbf{R}$

Linear Algebra: Axis-orthogonal Projection

Project a vector $\mathbf{x}$ into first dimension:



$$\mathbf{P} \cdot \mathbf{x} = \mathbf{y}$$

Transformation matrix:

$$\mathbf{P} = \begin{pmatrix} 1 & 0 \end{pmatrix}$$

In general:

An axis-orthogonal projection is an identity matrix with some 'collapsed' dimensions

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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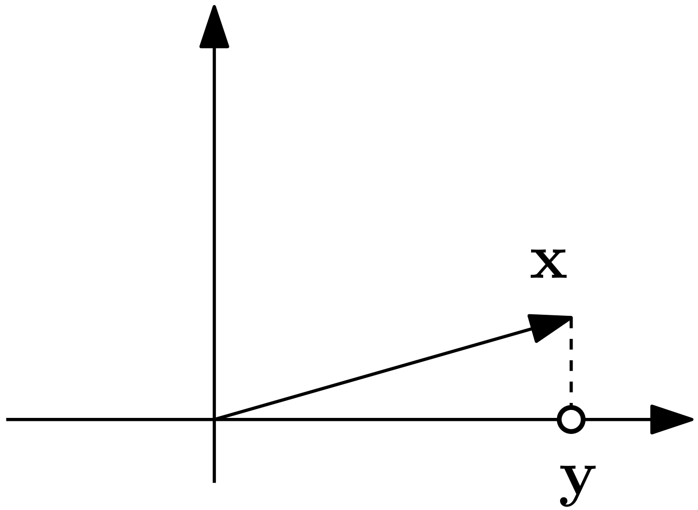

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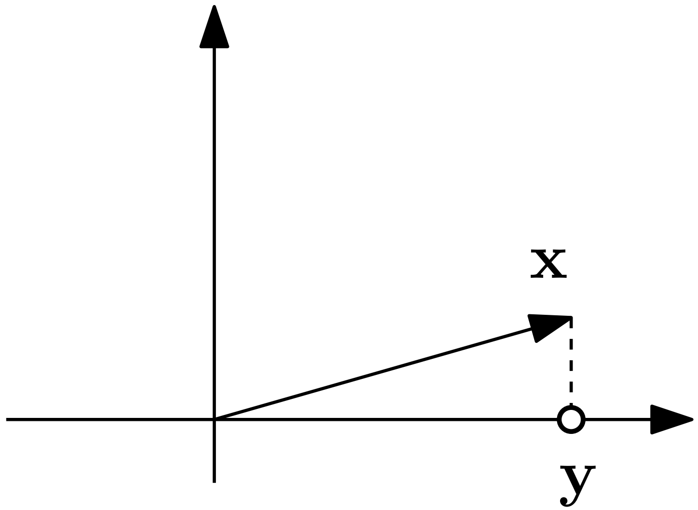

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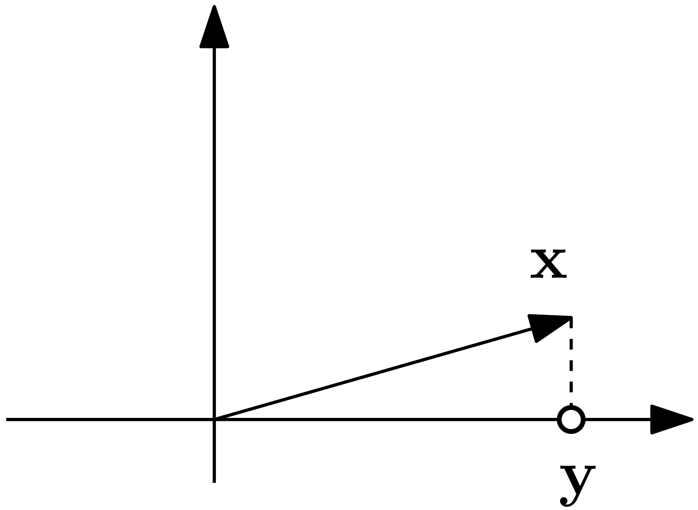

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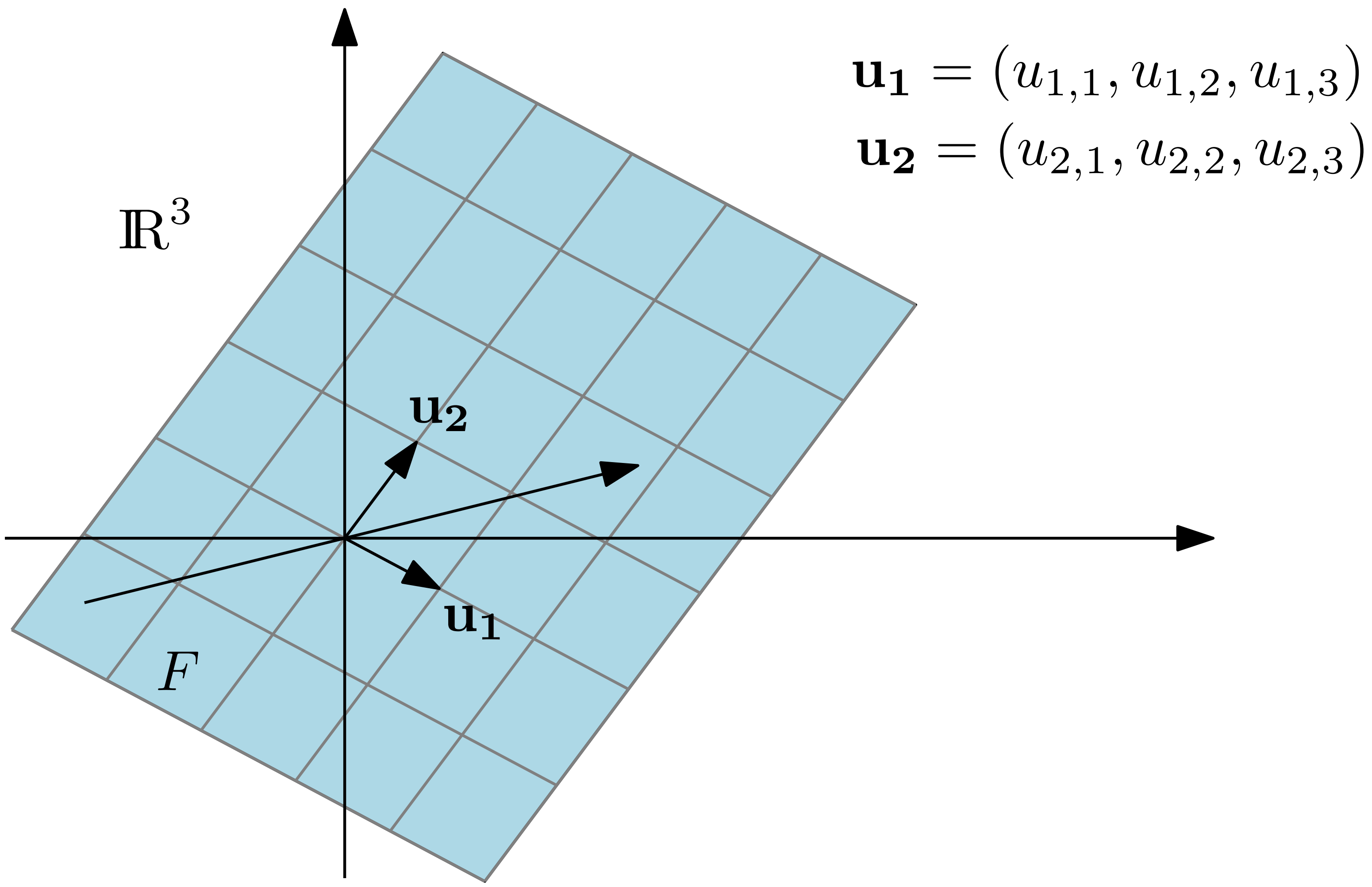
$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

Linear Algebra: Projection onto subspace

Let F be a k-dimensional linear subspace of $\mathbb{R}^d$ spanned by orthonormal vectors $\mathbf{u_1}, \ldots, \mathbf{u_k}$ and let $\mathbf{R}$ be the projection onto F



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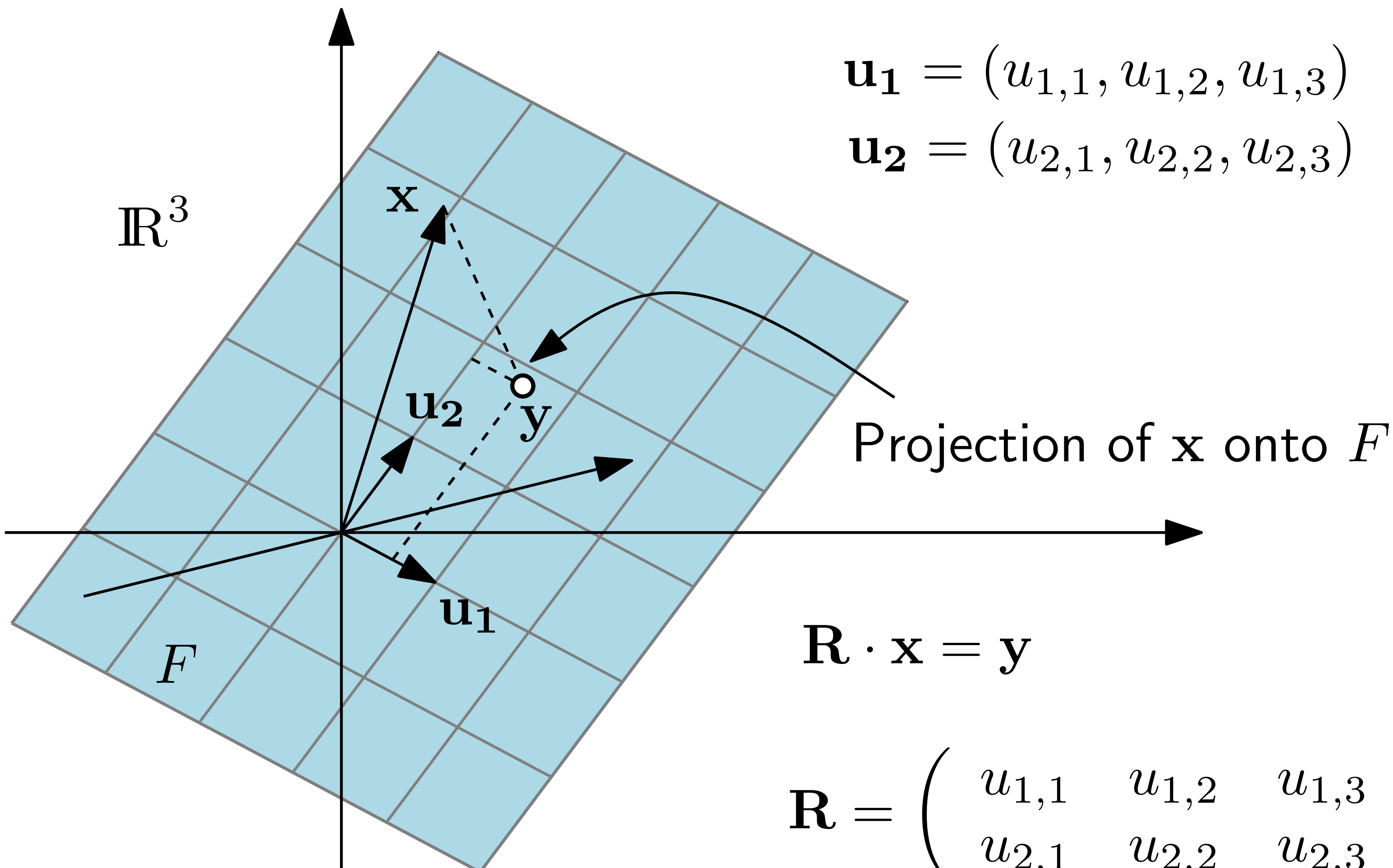
$$\mathbf{u_1} = (u_{1,1}, u_{1,2}, u_{1,3})$$
$$\mathbf{u_2} = (u_{2,1}, u_{2,2}, u_{2,3})$$



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Linear Algebra: Projection onto subspace

A projection onto a subspace can be viewed as rotation followed by an axis-orthogonal projection

To see this, let's rewrite $\mathbf{R} = \mathbf{P} \cdot \mathbf{M}$ with

- $\mathbf{M}$: rotation to align each $\mathbf{u_i}$ with standard basis vector $\mathbf{v_i}$
- $\mathbf{P}$: orthogonal projection onto first k coordinates

To find the rotation matrix $\mathbf{M}$, note that for $i = 1, \ldots, k$

$$\mathbf{M} \cdot \mathbf{u_i} = \mathbf{v_i} \quad \Leftrightarrow \quad \mathbf{M^{-1}} \cdot \mathbf{v_i} = \mathbf{u_i} \quad \Leftrightarrow \quad \mathbf{M^T} \cdot \mathbf{v_i} = \mathbf{u_i}$$

- since $\mathbf{v_i}$ is the i'th standard basis vector, $\mathbf{M^T v_i}$ is the ith column vector of $\mathbf{M^T}$
- thus, $\mathbf{u_i}$ is the ith row vector of $\mathbf{M}$ for $i = 1, \ldots, k$

Analysis of Achlioptas' Random Rotation

We can think of Achlioptas transformation as a rotation $\mathbf{M}$ followed by a projection $\mathbf{P}$ onto the first k dimensions.

$$f(p) = \frac{1}{\sqrt{k}}\mathbf{R}p = \frac{\sqrt{d}}{\sqrt{k}}\frac{1}{\sqrt{d}}\mathbf{R}p = \frac{\sqrt{d}}{\sqrt{k}}\mathbf{P}\mathbf{M}p$$

Example: $k = 2, d = 4$

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\mathbf{M} = \frac{1}{\sqrt{d}}\begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & r_{1,4} \\ r_{2,1} & r_{2,2} & r_{2,3} & r_{2,4} \\ r_{3,1} & r_{3,2} & r_{3,3} & r_{3,4} \\ r_{4,1} & r_{4,2} & r_{4,3} & r_{4,4} \end{pmatrix}$$

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But is $\mathbf{M}$ a rotation?

Analysis of Achlioptas' Random Rotation

$\mathbf{M}$ is a rotation if and only if the product of $\mathbf{M}$ and its transpose is the identity (i.e., $\mathbf{M}$ is orthogonal)

$$\mathbf{M}\mathbf{M}^{\mathbf{T}} = \mathbf{I}$$

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(1) each pair of row vectors is orthogonal

(2) each row vector has unit length

Let $\mathbf{r_i} = \frac{1}{\sqrt{d}}(r_{i,1}, \ldots, r_{i,d})$ be the ith row vector of $\mathbf{M}$

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Analysis of Achlioptas' Random Rotation

(continued)

Recall that each $r_{i,j}$ is a discrete random variable:

$$r_{i,j} = \begin{cases} +1 & \text{with probability } \frac{1}{2} \\ -1 & \text{with probability } \frac{1}{2} \end{cases}$$

Let's analyze expected values of the matrix entries of $\mathbf{MM^T}$

We will need the expected value of $r_{i,j}$:

$$\forall i, j : \mathrm{E}\left[r_{i,j}\right] = -1 \cdot \tfrac{1}{2} + 1 \cdot \tfrac{1}{2} = 0$$

Analysis of Achlioptas' Random Rotation

(continued)

(1) the expected angle between each pair of row vectors is orthogonal: $\forall i \neq j : \mathrm{E}\left[\langle \mathbf{r_i}, \mathbf{r_j} \rangle\right] = 0$

Analysis of Achlioptas' Random Rotation

(continued)

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Proof:

By linearity of expectation

$$\mathrm{E}\left[\langle \mathbf{r_i}, \mathbf{r_j} \rangle\right] = \mathrm{E}\left[\sum_{t=1}^{d} \frac{r_{i,t}}{\sqrt{d}} \cdot \frac{r_{j,t}}{\sqrt{d}}\right] = \frac{1}{d} \sum_{t=1}^{d} \mathrm{E}\left[r_{i,t} \cdot r_{j,t}\right]$$

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for $i \neq j$ it holds that $r_{i,t}$ and $r_{j,t}$ are independent random variables, therefore

$$\mathrm{E}\left[\langle \mathbf{r_i}, \mathbf{r_j} \rangle\right] = \frac{1}{d} \sum_{t=1}^{d} \mathrm{E}\left[r_{i,t}\right] \cdot \mathrm{E}\left[r_{j,t}\right] = 0$$

□

Analysis of Achlioptas' Random Rotation

(continued)

(2) the expected squared length of each row vector is 1:

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Analysis of Achlioptas' Random Rotation

(continued)

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Note that $r_{i,t}^2$ is also a random variable and its expected value is:

$$\mathrm{E}\left[r_{i,t}^2\right] = (-1)^2 \cdot \tfrac{1}{2} + (1)^2 \cdot \tfrac{1}{2} = 1$$

Analysis of Achlioptas' Random Rotation

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Therefore, $\mathrm{E}\left[\langle \mathbf{r_i}, \mathbf{r_i} \rangle\right] = 1$ $\square$

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- Next we want to analyze the effect of the random projection on a distance between two points
- Therefore we analyze for fixed $p_i, p_j \in P$ the expectation of its squared length in the projection

$$\mathrm{E}\left[\|f(p_i) - f(p_j)\|^2\right]$$

Analysis of a fixed distance d_{ij} (Expectation)

Claim: For fixed $p_i, p_j \in P : \mathrm{E}\left[\|f(p_i) - f(p_j)\|^2\right] = \|p_i - p_j\|^2$

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Since f is a linear transformation, we have that

$$\mathrm{E}\left[\|f(p_i) - f(p_j)\|^2\right] = \mathrm{E}\left[\|f(p_i - p_j)\|^2\right] = \mathrm{E}\left[\|f(\alpha)\|^2\right]$$

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By the definition of f

$$\|f(\alpha)\|^2 = \left\|\frac{\sqrt{d}}{\sqrt{k}}\mathbf{PM}\alpha\right\|^2 = \frac{d}{k}\|\mathbf{PM}\alpha\|^2 = \frac{d}{k}\sum_{i=1}^{k}(\mathbf{r_i}\alpha)^2$$

where $\mathbf{r_i} = \frac{1}{\sqrt{d}}(r_{i,1}, \ldots, r_{i,d})$ is the ith row vector of $\mathbf{M}$, as defined earlier.

Analysis of a fixed distance d_{ij} (Expectation)

(continued)

by linearity of expectation

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$$\mathrm{E}\left[(\mathbf{r_i}\alpha)^2\right] = \mathrm{E}\left[\left(\sum_{j=1}^{d}\frac{1}{\sqrt{d}}r_{i,j}a_j\right)^2\right] = \mathrm{E}\left[\frac{1}{d}\left(\sum_{j=1}^{d}r_{i,j}a_j\right)^2\right]$$

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We recursively expand the inner quadratic expression

$$\begin{aligned}\left(\sum_{j=1}^{d}r_{i,j}a_j\right)^2 &= (r_{i,1}a_1)^2 + 2r_{i,1}a_1\left(\sum_{j=2}^{d}r_{i,j}a_j\right) + \left(\sum_{j=2}^{d}r_{i,j}a_j\right)^2\\ &= \dots\\ &= \sum_{j=1}^{d}(r_{i,j}a_j)^2 + \sum_{j=1}^{d-1}\sum_{l=j+1}^{d}2r_{i,j}a_jr_{i,l}a_l\end{aligned}$$

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Plugging back into the equation..

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$$= \frac{1}{d}\sum_{j=1}^{d} a_j^2 = \frac{1}{d}\|\alpha\|^2$$

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Now, plugging back the definition of α

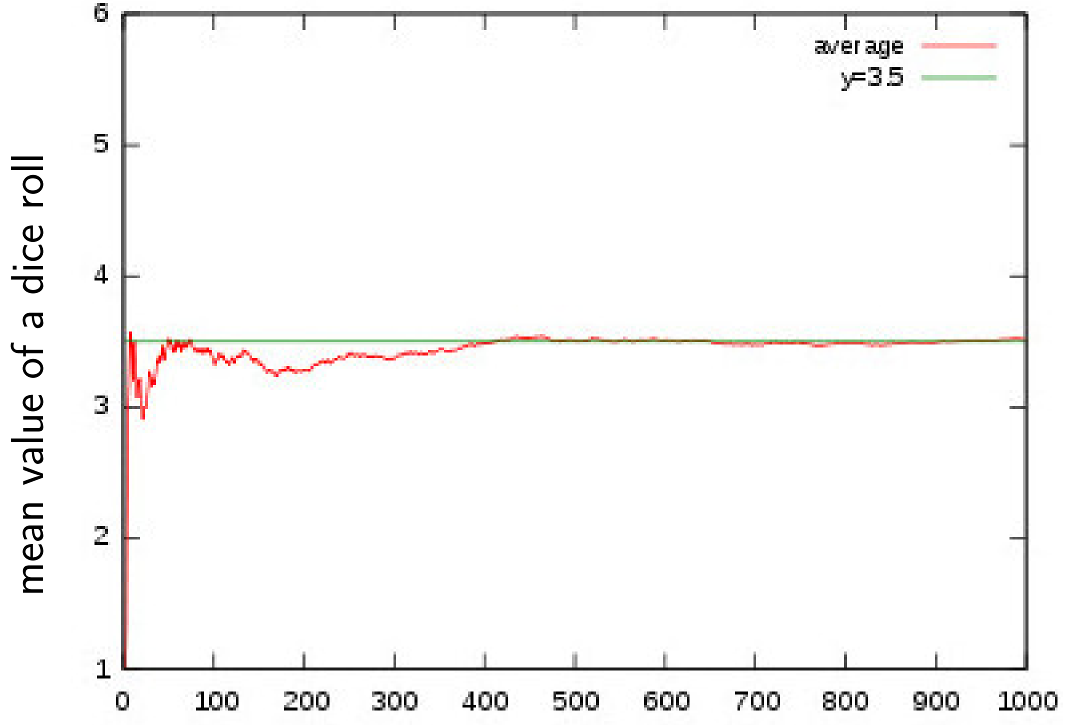
$$\mathrm{E}\left[\|f(p_i) - f(p_j)\|^2\right] = \|p_i - p_j\|^2$$

$\square$

Law of Large Numbers

Let $X_1, \ldots, X_n$ be n samples of a random variable X.
The law of large numbers states that

$$\Pr\left[\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \mathrm{E}\left[X\right]\right| \geq \varepsilon\right] \leq \frac{\mathrm{Var}\left(X\right)}{n \cdot \varepsilon^2}$$



$n =$ number of trials

Concentration of mass in high dimensions

The unit hypercube: $[0,1]^d = \{(x_1, \dots, x_d) \mid x_i \in [0,1]\}$

Random vector $\mathbf{x} = (x_1, \dots, x_d) \in [0,1]^d$
(choose x_i independently and uniformly random in $[0,1]$)

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$$L := \frac{\|\mathbf{x}\|^2}{d} = \frac{1}{d} \sum_{i=1}^{d} x_i^2 \sim \frac{1}{3}$$

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This is the average of a random variable, since x_i are independent and identically distributed

(with $\mathrm{E}\left[x_i^2\right] = \int_0^1 x_i^2 = \left[\frac{1}{3}x^3\right]_0^1 = \frac{1}{3}$)

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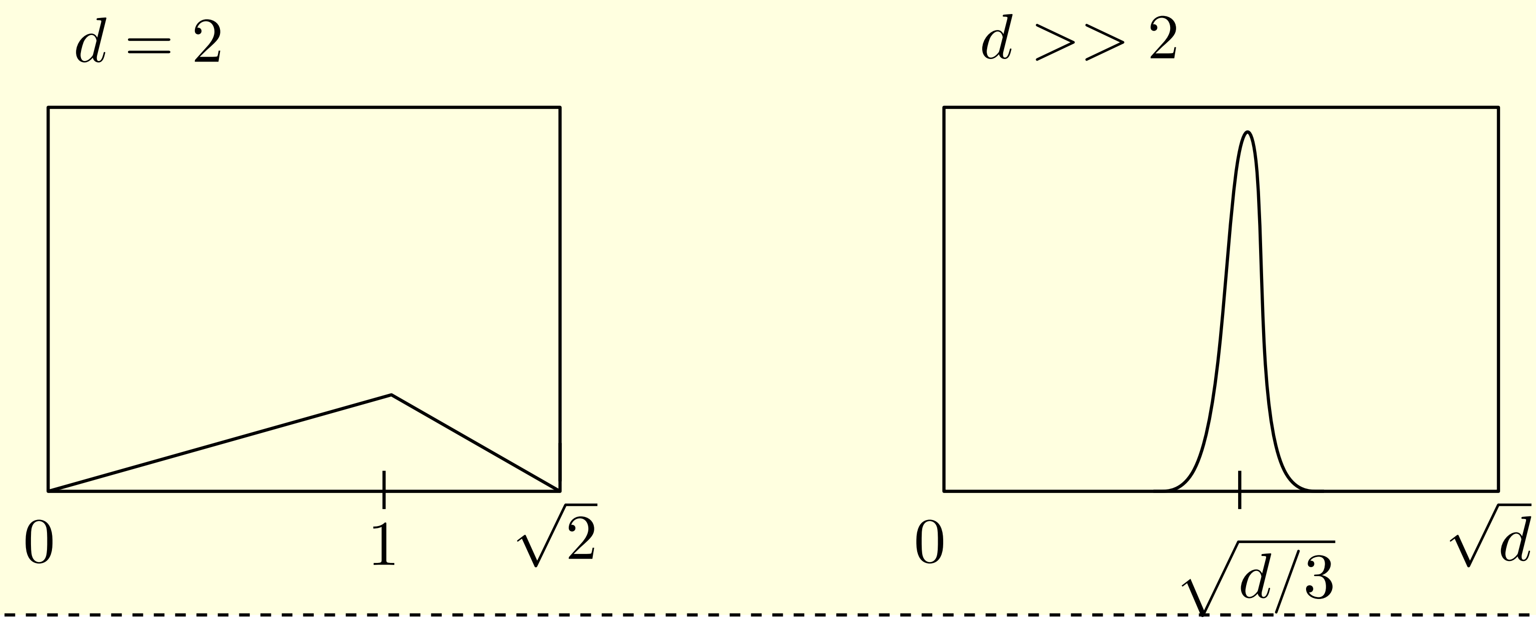
Distribution of the length of $\mathbf{x}$ in low vs. high dimensions



Analysis of a fixed distance d_{ij}

Failure probability for two fixed points p_i, p_j:

$$\Pr\left[\frac{\|f(p_i) - f(p_j)\|^2}{\|p_i - p_j\|^2} \notin [1-\varepsilon, 1+\varepsilon]\right]$$

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define $\alpha = \frac{p_i - p_j}{\|p_i - p_j\|}$ (note that α is a fixed unit vector)

$$\Pr\left[\|f(\alpha)\|^2 \notin [1-\varepsilon, 1+\varepsilon]\right]$$

Analysis of a fixed distance d_{ij}

(continued)

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One can use concentration of measure.

Analysis of a fixed distance d_{ij}

Using concentration of measure, Achlioptas shows the following lemma (we omit the full proof):

Lemma:

Let $r_{i,j}$ be chosen uniformly random from $\{-1, 1\}$, then for any $\varepsilon > 0$ and any unit vector $\alpha \in \mathbb{R}^d$,

$$\Pr\left[\|f(\alpha)\|^2 \notin [1-\varepsilon, 1+\varepsilon]\right] < 2 \cdot e^{(-\frac{k}{2}(\varepsilon^2/2-\varepsilon^3/3))}$$

Therefore, choosing

$$k \geq \frac{4+2\beta}{\varepsilon^2/2 - \varepsilon^3/3} \log n$$

is sufficient to ensure

$$\Pr\left[\frac{\|f(p_i) - f(p_j)\|^2}{\|p_i - p_j\|^2} \notin [1-\varepsilon, 1+\varepsilon]\right] = \Pr\left[\|f(\alpha)\|^2 \notin [1-\varepsilon, 1+\varepsilon]\right] \; < \; \frac{2}{n^{2+\beta}}$$

Analysis of the Distortion

Theorem:

Let $k_0 = \frac{4+2\beta}{\varepsilon^2/2-\varepsilon^3/3}\log n$, for given $\varepsilon, \beta > 0$. If $k \geq k_0$ then with probability at least $1 - \frac{1}{n^\beta}$, we have for all $p_i, p_j \in P$ that

$$(1-\varepsilon)\|p_i - p_j\|^2 \leq \|f(p_i) - f(p_j)\|^2 \leq (1+\varepsilon)\|p_i - p_j\|^2$$

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Proof :

- there are $\binom{n}{2}$ pairs of points in P
- bound the failure probability for two fixed points:

$$\Pr\left[\frac{\|f(p_i) - f(p_j)\|^2}{\|p_i - p_j\|^2} \notin [1-\varepsilon, 1+\varepsilon]\right] < \frac{2}{n^{2+\beta}}$$

- apply the union bound: $\binom{n}{2} \cdot \frac{2}{n^{2+\beta}} < \frac{n^2}{2} \cdot \frac{2}{n^{2+\beta}} = \frac{1}{n^\beta}$

Alternative Projection Matrix

Note:

For generating the matrix $\mathbf{R}$, other distributions are possible.
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Alternative Projection Matrix

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$$r_{i,j} = \sqrt{3} \begin{cases} +1 & \text{with probability } \frac{1}{6} \\ 0 & \text{with probability } \frac{2}{3} \\ -1 & \text{with probability } \frac{1}{6} \end{cases}$$

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What would be the advantage of this?

This generates a sparser matrix

Summary

- Nearest-neighbor searching
- Embedding and Distortion
- Achlioptas' Random Projection
- Projection onto a subspace
- Random Rotation (Expectation)
- Analysis of a fixed distance (Expectation)
- Law of large numbers
- Concentration of measure
- Analysis of a fixed distance
- Analysis of the Distortion
- Alternative Projection Matrix

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