Today.

Modelling.

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An Analysis of the Power of PCA.

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An Analysis of the Power of PCA.

Musing about “heuristics” in the real world.

Two populations.

DNA data:

Two populations.

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human1: A $\cdots$ C $\cdots$ T $\cdots$ A

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DNA data:

human1: A $\cdots$ C $\cdots$ T $\cdots$ A
human2: C $\cdots$ C $\cdots$ A $\cdots$ T

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Single Nucleotide Polymorphism.

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Same population?

Two populations.

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Model: same popultion breeds.

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Model: same populution breeds.

Population 1: snp 843: Pr[A] = .4 , Pr[T] = .6
Population 2: snp 843: Pr[A] = .6 , Pr[T] = .4

Two populations.

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Individual: $x_1, x_2, x_3.., x_n$.

Two populations.

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Comment: snps could be movie preferences, populations could be types.

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E.g., republican/democrat, shopper/saver.

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Population 1: snp i: Pr[$x_i = 1$] = $p_i^{(1)}$
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Simpler Calculation:

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Population 1: Gaussion with mean $\mu_1 \in R^d$, variance σ in each dim.
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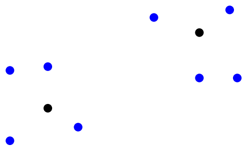

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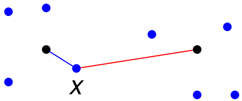

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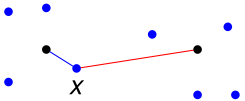

If $(\mu_1-\mu_2)^2 = d\varepsilon^2 >> \sigma^2$, then different.

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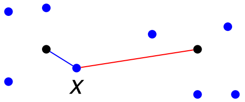

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$\rightarrow$ take $d >> \sigma^2/\varepsilon^2$

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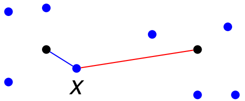

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Variance of estimator?

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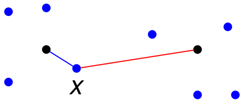

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Variance of estimator?
Roughly $d\sigma^4$.

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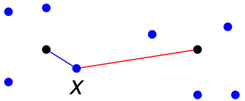

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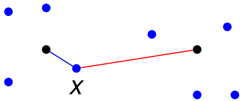

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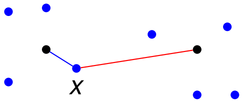

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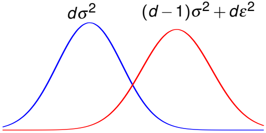

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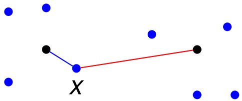

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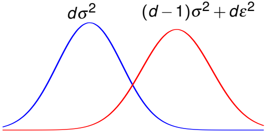

Signal $>>$ Noise. $\leftrightarrow d\varepsilon^2 >> \sqrt{d}\sigma^2$.

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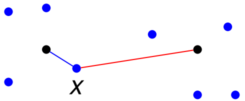

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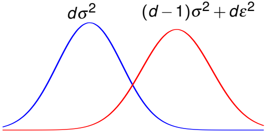

Signal $>>$ Noise. $\leftrightarrow$ $d\varepsilon^2 >> \sqrt{d}\sigma^2$. $d >> \sigma^4/\varepsilon^4$ suffices!

Projection

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Project x onto unit vector v in direction $\mu_2 - \mu_1$. x in population 1.

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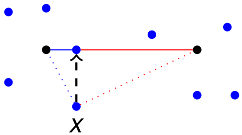

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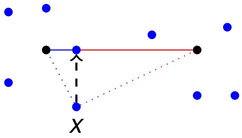

Std deviation is σ^2!

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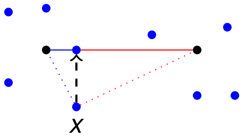

Std deviation is σ^2! versus $\sqrt{d}\sigma^2$!

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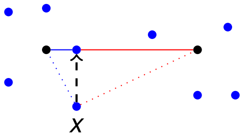
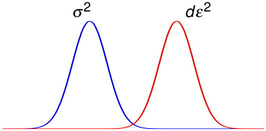


Std deviation is σ^2! versus $\sqrt{d}\sigma^2$!

No loss in signal!



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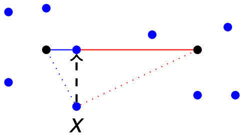
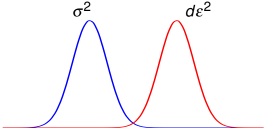


Std deviation is σ^2! versus $\sqrt{d}\sigma^2$!

No loss in signal!



$$d\varepsilon^2 >> \sigma^2.$$

Projection

Population 1: Gaussian with mean $\mu_1 \in R^d$, variance σ in each dim.
Population 2: Gaussian with mean $\mu_2 \in R^d$, variance σ in each dim.

Difference between humans σ per snp.
Difference between populations ε per snp.

Project x onto unit vector v in direction $\mu_2 - \mu_1$. x in population 1.

$$E[((x-\mu_1)\cdot v)^2] = \sigma^2$$
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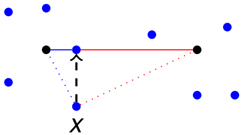

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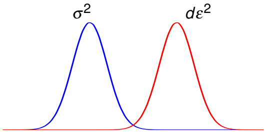

$d\varepsilon^2 >> \sigma^2$. $\quad \rightarrow d >> \sigma^2/\varepsilon^2$

Projection

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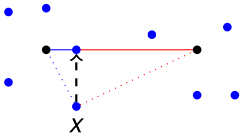

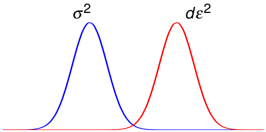

Std deviation is σ^2! versus $\sqrt{d}\sigma^2$!

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$d\varepsilon^2 >> \sigma^2$. $\rightarrow d >> \sigma^2/\varepsilon^2$

Versus $d >> \sigma^4/\varepsilon^4$.

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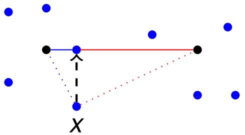

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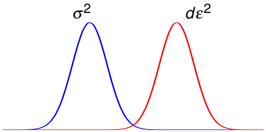

$d\varepsilon^2 >> \sigma^2$. $\quad \rightarrow d >> \sigma^2/\varepsilon^2$

Versus $d >> \sigma^4/\varepsilon^4$.

A quadratic difference in amount of data!

Don’t know much about...

Don’t know μ_1 or μ_2?

Don't know much about...

Don't know μ_1 or μ_2? Uh oh!

Without knowing the means?

Sample of n people.

Without knowing the means?

Sample of n people.

- Some (say half) from population 1,

Without knowing the means?

Sample of n people.

Some (say half) from population 1,

some from population 2.

Without knowing the means?

Sample of n people.

Some (say half) from population 1,

some from population 2.

Which are which?

Without knowing the means?

Sample of n people.

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Which are which?

Near Neighbors Approach

Without knowing the means?

Sample of n people.

Some (say half) from population 1,

some from population 2.

Which are which?

Near Neighbors Approach

Compute Euclidean distance squared.

Without knowing the means?

Sample of n people.
Some (say half) from population 1,
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Which are which?

Near Neighbors Approach

Compute Euclidean distance squared.   Cluster using threshold.

Without knowing the means?

Sample of n people.

Some (say half) from population 1,

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Which are which?

Near Neighbors Approach

Compute Euclidean distance squared.   Cluster using threshold.

Signal $E[d(x_1, x_2)] - E[d(x_1, y_1)]$

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Compute Euclidean distance squared. Cluster using threshold.

Signal $E[d(x_1, x_2)] - E[d(x_1, y_1)]$

should be larger than noise in $d(x, y)$

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Compute Euclidean distance squared. Cluster using threshold.

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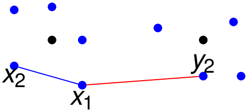
Where x's from one population, y's from other.



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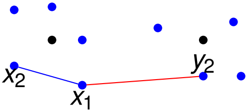

Signal $E[d(x_1, x_2)] - E[d(x_1, y_1)]$
should be larger than noise in $d(x, y)$
Where x's from one population, y's from other.

Signal is proportional $d\varepsilon^2$.

Without knowing the means?

Sample of n people.

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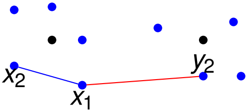
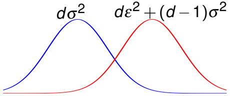


Signal is proportional $d\varepsilon^2$.

Noise is proportional to $\sqrt{d}\sigma^2$.



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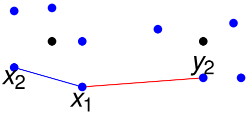

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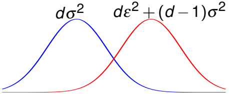

$d >> \sigma^4/\varepsilon^4$ $\rightarrow$ same type people closer to each other.

Without knowing the means?

Sample of n people.
Some (say half) from population 1,
some from population 2.

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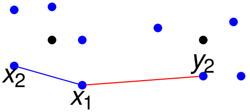

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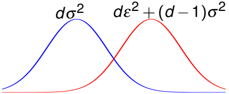

$d >> \sigma^4/\varepsilon^4$ $\rightarrow$ same type people closer to each other.

$d >> (\sigma^4/\varepsilon^4)\log n$ suffices for threshold clustering.

Without knowing the means?

Sample of n people.

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Which are which?

Near Neighbors Approach

Compute Euclidean distance squared. Cluster using threshold.

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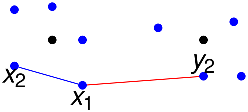

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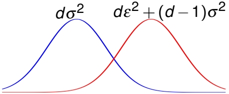

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$\log n$ factor for union bound over $\binom{n}{2}$ pairs.

Without knowing the means?

Sample of n people.

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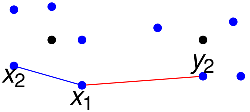

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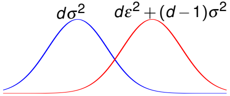

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Best one can do?

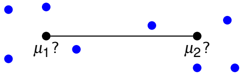
Principal components analysis.

Remember Projection!

Principal components analysis.

Remember Projection!

Still don't know μ_1 or μ_2?



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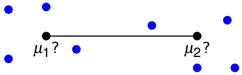

Principal component analysis(PCA):

Principal components analysis.

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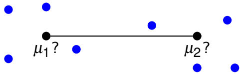

Principal component analysis(PCA):

Find direction, v, of maximum variance.

Principal components analysis.

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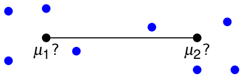

Principal component analysis(PCA):

Find direction, v, of maximum variance.

Maximize $\sum(x \cdot v)^2$ (zero center the points)

Principal components analysis.

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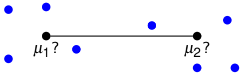

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Recall: $(x \cdot v)^2$ determines population well.

Principal components analysis.

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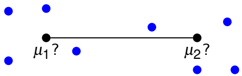

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Typical direction variance. $n\sigma^2$.

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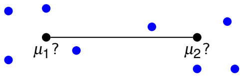

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Direction along $\mu_1 - \mu_2$,

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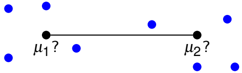

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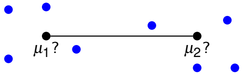

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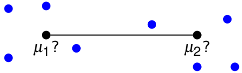

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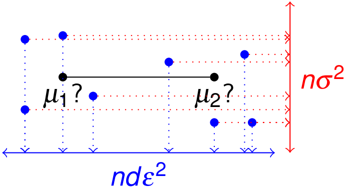
Need $nd\varepsilon^2 >> n\sigma^2$.



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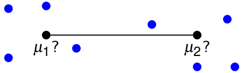

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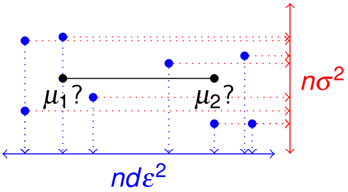

Need $nd\varepsilon^2 >> n\sigma^2$.

Need $d\varepsilon^2 >> \sigma^2 \equiv d >> \sigma^2/\varepsilon^2$ at least.

Principal components analysis.

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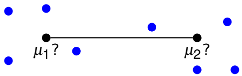

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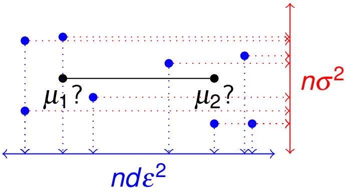

Need $d\varepsilon^2 >> \sigma^2 \equiv d >> \sigma^2/\varepsilon^2$ at least. Just signal difference here!

Principal components analysis.

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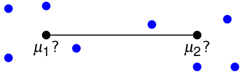

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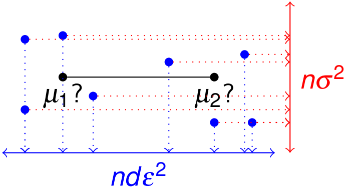

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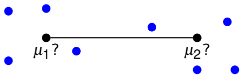

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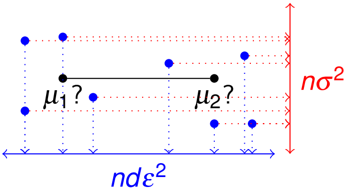

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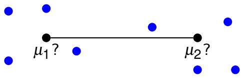
Principal components analysis.

Remember Projection!

Still don't know μ_1 or μ_2?



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Find direction, v, of maximum variance.

Maximize $\sum(x \cdot v)^2$ (zero center the points)

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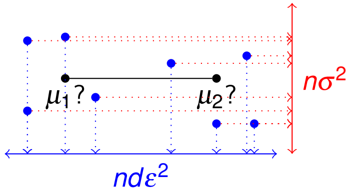

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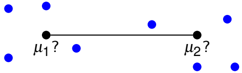

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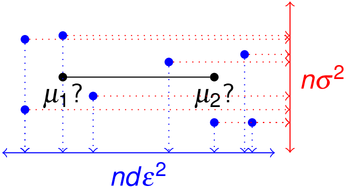

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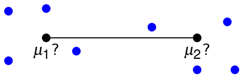

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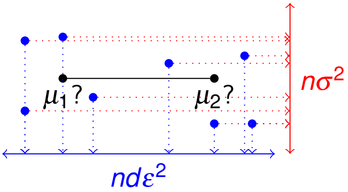

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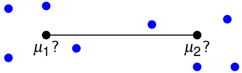

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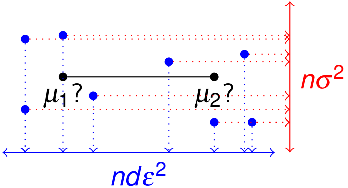

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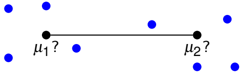

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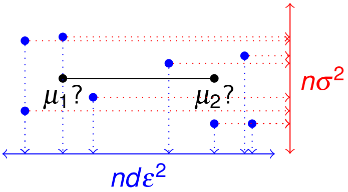

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Nets

“δ - Net”.

Nets

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Set $\mathscr{D}$ of directions

Nets

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where all others, v, are close to $x \in \mathscr{D}$.

Nets

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- Set $\mathscr{D}$ of directions
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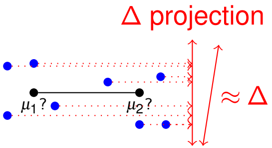

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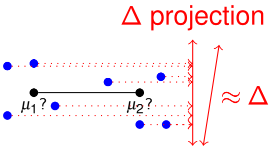

Signal $>>$ Noise times $\sqrt{\log N} = O(\sqrt{d \log \frac{d}{\delta}})$ to isolate direction.

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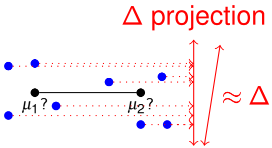

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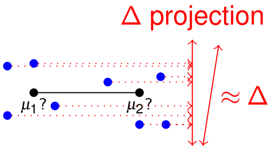

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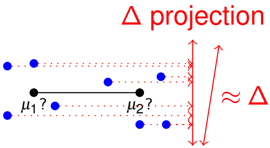

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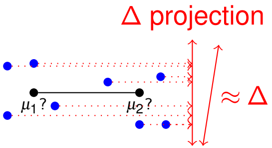

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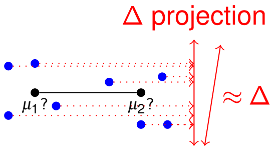

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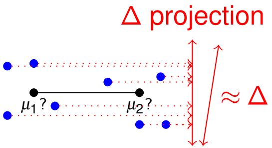

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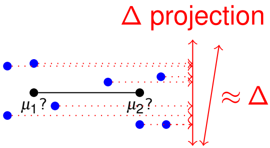

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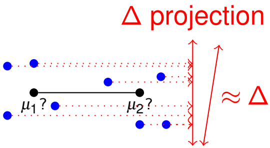

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PCA reduces d to "knowing centers" case, with extra sample points.

PCA calculation.

Matrix A where rows are points.

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First eigenvector of $B = A^T A$ is maximum variance direction.

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Power method:

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Choose random unit x.

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Choose random unit x.
Repeat: Let $x = Bx$. Scale x to unit vector.

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Expected projection of random x onto unit v?

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If no gap, then any vector in subspace of $[v_1, v_2]$ is fine.

Cluster Algorithm.

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Choose random partition.
Repeat: Compute means of partition. Project, cluster.

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Sizes of S_i? d is $\propto S_i$, advantage grows, $|S_1| = \Theta(n)$, others smaller.

Gaussian Shift advantage.

Let $\Delta = (p - q) \times$ imbalance.

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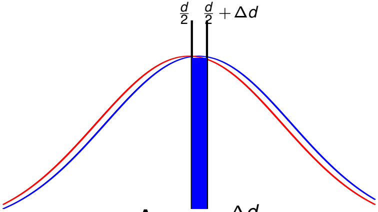
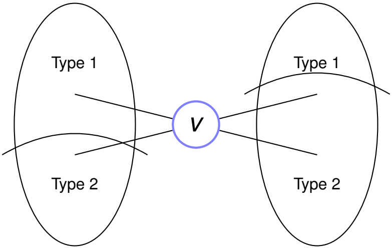


Area $\approx \frac{\Delta d}{\sqrt{d}}$

Assuming $\Delta d << \sqrt{d}$.



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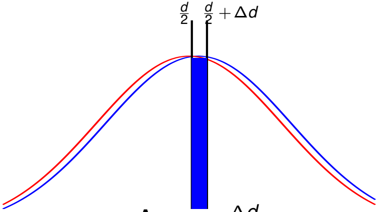

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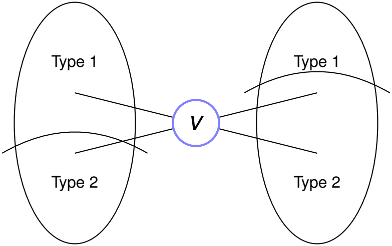

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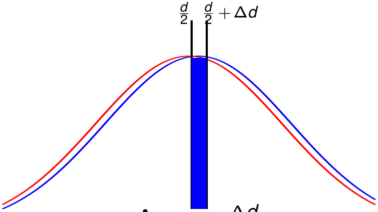

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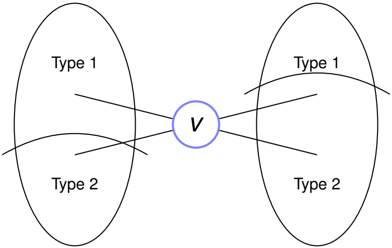

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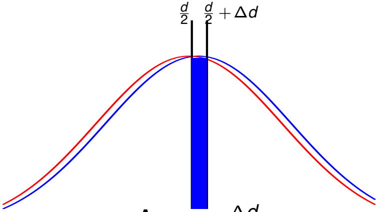

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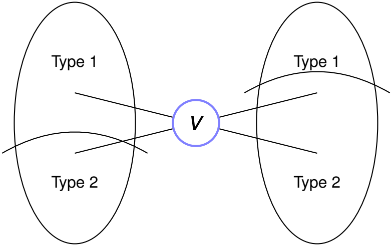

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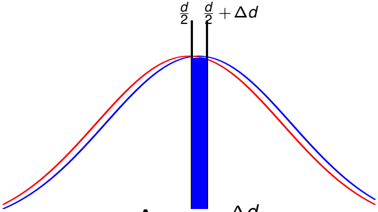

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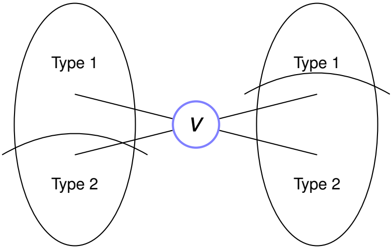


Original imbalance is $1/\sqrt{n}$ of the vertices.

If advantage $((p-q)/\sqrt{n})/\sqrt{d} >> 1/\sqrt{n}$, then imbalance increases.

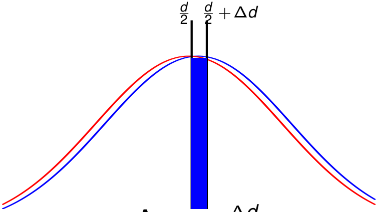
...and then gets better after that.

Roughly: $(p-q) \geq \sqrt{d}$.

Gaussian Shift advantage.

Let $\Delta = (p - q) \times$ imbalance.

Step 1: $\Delta = (p - q) \times \frac{1}{\sqrt{n}}$.



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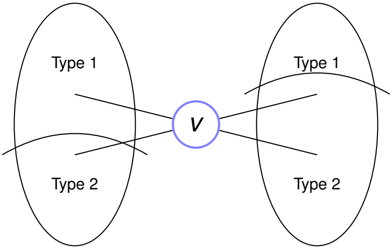

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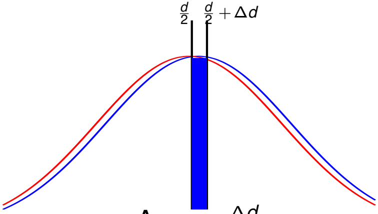

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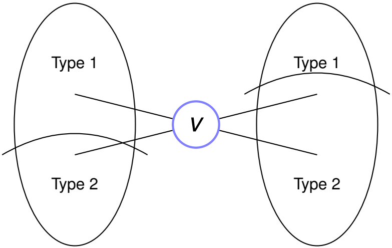

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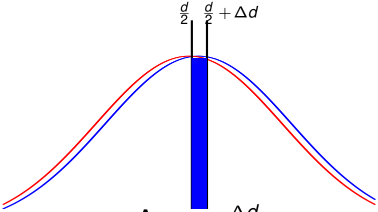

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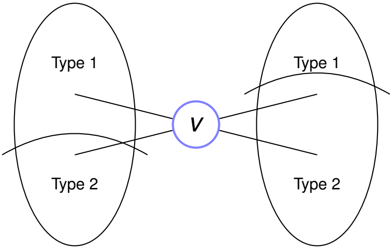

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Generic clustering algorithm is rounded version of power method.

See you on Tuesday.