Kernel PCA
&
Isomap + TSNE
LINEAR PROJECTIONS

Works when data lies in a low dimensional linear sub-space
We have nice methods for linear dimensionality reduction.

Can we use this beyond the linear realm?

Kernel function measures similarity between points.
• Lift to higher dimensions (introduces non-linearity)

• Perform linear dimensionality reduction in this high dimensional space

Kernel function measures similarity between points.
Example

Original Data in 2D

\[(x, y)\]

Data Lifted to 3D

\[(x, y, x^2 + y^2)\]
Given $x_t \in \mathbb{R}^d$, the feature space vector is given by mapping

$$\Phi(x_t) = (x_t[1], \ldots, x_t[d], x_t[1] \cdot x_t[1], x_t[1] \cdot x_t[2], \ldots, x_t[d] \cdot x_t[d], \ldots)^\top$$

Enumerating products up to order $K$ (ie. products of at most $K$ coordinates) we can get degree $K$ polynomials.

However dimension blows up as $d^K$

Is there a way to do this without enumerating $\Phi$?
**Kernel Trick**

- **Essence of Kernel trick:**
  - If we can write down an algorithm only in terms of $\Phi(x_t)^\top \Phi(x_s)$ for data points $x_t$ and $x_s$
  - Then we don’t need to explicitly enumerate $\Phi(x_t)$’s but instead, compute $k(x_t, x_s) = \Phi(x_t)^\top \Phi(x_s)$ (even if $\Phi$ maps to infinite dimensional space)

- Example: RBF kernel $k(x_t, x_s) = \exp(-\sigma \|x_t - x_s\|_2^2)$, polynomial kernel $k(x_t, x_s) = (x_t^\top y_t)^p$

- Kernel function measures similarity between points.
\[(x_t^\top y_t)^p = \sum_{k_1+k_2+\ldots+k_d=p} \left( \binom{p}{k_1, k_2, \ldots, k_d} \prod_{j=1}^{d} (x_t[j]^p y_t[j])^{k_j} \right)\]

\[= \sum_{k_1+k_2+\ldots+k_d=p} \left( \sqrt{\binom{p}{k_1, k_2, \ldots, k_d}} \prod_{j=1}^{d} x_t[j]^{k_j} \right) \cdot \left( \sqrt{\binom{p}{k_1, k_2, \ldots, k_d}} \prod_{j=1}^{d} y_t[j]^{k_j} \right)\]

\[\Phi(x)^\top = \left( \ldots, \sqrt{\binom{p}{k_1, k_2, \ldots, k_d}} \prod_{j=1}^{d} x_t[j]^{k_t}, \ldots \right)_{k_1+k_2+\ldots+k_d=p}\]
If an algorithm only depends on inner products, we can simply replace inner product in $x$ space by inner product in $\phi(x)$ space.
Can we write PCA so it only depends on inner products?
L E T S  R E W R I T E  P C A

Let's start with the assumption that Data is centered! (i.e. Sum of \( x_t \)'s is 0)

- \( k^{th} \) column of \( W \) is eigenvector of covariance matrix
  That is, \( \lambda_k W_k = \Sigma W_k \). Rewriting, for centered \( X \)

\[
\lambda_k W_k = \frac{1}{n} \left( \sum_{t=1}^{n} x_t x_t^\top \right) W_k = \frac{1}{n} \sum_{t=1}^{n} (x_t^\top W_k) x_t
\]

But \( x_t^\top W_k = y_t[k] \)

\[
\lambda_k W_k = \frac{1}{n} \sum_{t=1}^{n} y_t[k] x_t
\]
Let's rewrite PCA

\[ y_s[k] = W_k^\top x_s \]

\[ = \frac{1}{\lambda_k} \left( \frac{1}{n} \sum_{t=1}^{n} y_t[k] x_t \right)^\top x_s \]

\[ = \frac{1}{n \lambda_k} \sum_{t=1}^{n} y_t[k] x_t^\top x_s \]

\[ = \frac{1}{n \lambda_k} \sum_{t=1}^{n} y_t[k] \tilde{K}_{s,t} \]

Where \( \tilde{K}_{s,t} = x_t^\top x_s \) is the kernel matrix for centered data.
Hence, the $k$'th column on $Y$ matrix is such that

$$y[k] = \frac{1}{n\lambda_k} y[k] \tilde{K}$$

Also we have, 

$$1 = \|W_k\|^2 = \frac{1}{\lambda_k^2 n^2} \left( \sum_{t=1}^{n} y_t[k] x_t \right) \left( \sum_{s=1}^{n} y_s[k] x_s \right)$$

$$= \frac{1}{\lambda_k^2 n^2} \sum_{t=1}^{n} \sum_{s=1}^{n} y_s[k] x_s^\top x_t y_t[k]$$

$$= \frac{1}{\lambda_k^2 n^2} y[k] \tilde{K} y[k]^\top = \frac{1}{n\lambda_k} \|y[k]\|^2$$

Hence $P_k = y[k]/\sqrt{n\lambda_k}$ is an eigenvector of $\tilde{K}$ with eigen value $\gamma_k = n\lambda_k$
We assumed centered data, what if it's not,

\[
\tilde{K}_{s,t} = \left( x_t - \frac{1}{n} \sum_{u=1}^{n} x_u \right)^\top \left( x_s - \frac{1}{n} \sum_{u=1}^{n} x_u \right) \\
= x_t^\top x_s - \left( \frac{1}{n} \sum_{u=1}^{n} x_u \right)^\top x_s - \left( \frac{1}{n} \sum_{u=1}^{n} x_u \right)^\top x_t \\
+ \frac{1}{n^2} \left( \sum_{u=1}^{n} x_u \right)^\top \left( \sum_{v=1}^{n} x_v \right) \\
= x_t^\top x_s - \frac{1}{n} \sum_{u=1}^{n} x_u^\top x_s - \frac{1}{n} \sum_{u=1}^{n} x_u^\top x_t + \frac{1}{n^2} \sum_{u=1}^{n} \sum_{v=1}^{n} x_u^\top x_v
\]
Equivalently, if \( \text{Kern} \) is the matrix \( \text{Kern}_{t,s} = x_t^T x_s \),

\[
\tilde{K} = \text{Kern} - \frac{(\mathbf{1}_{n \times n} \times \text{Kern})}{n} - \frac{(\text{Kern} \times \mathbf{1}_{n \times n})}{n} + \frac{(\mathbf{1}_{n \times n} \times \text{Kern} \times \mathbf{1}_{n \times n})}{n^2}
\]
Kernel PCA

1. \[ \tilde{K} = \text{Kern} - \frac{1}{n} (\mathbf{1} \text{ Kern} + \text{Kern} \mathbf{1}) + \frac{1}{n^2} \mathbf{1} \text{ Kern} \mathbf{1} \]

2. \[ \text{Kern} = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_n) \\
 k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_n) \\
 \vdots & \vdots & \ddots & \vdots \\
 k(x_{n-1}, x_1) & k(x_{n-1}, x_2) & \cdots & k(x_{n-1}, x_n) \\
 k(x_n, x_1) & k(x_n, x_2) & \cdots & k(x_n, x_n) \end{bmatrix} \]
Kernel PCA

3. \[
\begin{bmatrix}
    P & \gamma \\
    K & K
\end{bmatrix}
= \text{eigs}\left(\begin{bmatrix}
    \tilde{K} \\
    K
\end{bmatrix}\right)
\]

4. \[
\begin{bmatrix}
    Y \\
    K
\end{bmatrix}
= \begin{bmatrix}
    P_{1\sqrt{\gamma}} & P_{K\sqrt{\gamma}} \\
    K & K
\end{bmatrix}
\]
Demo
Kernel Methods: A note

• We can kernelize CCA and any other linear dimensionality reduction method.

• For any linear method, solution lies within linear span of data.

• Hence y’s can be computed only based on inner products.
Key Assumption: Points live on a low dimensional manifold

Manifold: subspace that looks locally Euclidean

Given data, can we uncover this manifold?

Can we unfold this?
Method I: Isomap

1. For every point, find its \((k-)\) Nearest Neighbors
**Method I: Isomap**

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2. Form the Nearest Neighbor graph
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3. For every pair of points $A$ and $B$, distance between point $A$ to $B$ is shortest distance between $A$ and $B$ on graph
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2. Form the Nearest Neighbor graph

3. For every pair of points \(A\) and \(B\), distance between point \(A\) to \(B\) is shortest distance between \(A\) and \(B\) on graph.

4. Find points in low dimensional space such that distances between points in this space is equal to distance on graph.

Pair-wise Distance Matrix
ISOMAP: Pitfalls

1. If we don’t take enough nearest neighbors, then graph may not be connected

2. If we connect points too far away, points that should not be connected can get connected

3. There may not be a right number of nearest neighbors we should consider!
Use a probabilistic notion of which points are neighbors.

Probability that points \( s \) and \( t \) are connected

\[
P_{s,t} = P_{t,s} = \exp(-\frac{\|x_s - x_t\|^2}{2})
\]

\[
\sum_{u \neq t} \exp(-\frac{\|x_u - x_t\|^2}{2})
\]

Goal: Find \( y_1, \ldots, y_n \) with stochastic neighborhood distribution \( Q \) such that "\( P \) and \( Q \) are similar"

\[
\text{minimize: } \text{KL}(P \| Q) = \sum_{s,t} P_{s,t} \log \left( \frac{P_{s,t}}{Q_{s,t}} \right) - \sum_{s,t} P_{s,t} \log \left( P_{s,t} \right)
\]
Use a probabilistic notion of which points are neighbors.

Close by points are neighbors with high probability, ... Eg: For point \( x_t \), point \( x_s \) is picked as neighbor with probability

\[
p_{t \rightarrow s} = \frac{\exp\left(-\frac{\|x_s-x_t\|^2}{2\sigma^2}\right)}{\sum_{u \neq t} \exp\left(-\frac{\|x_u-x_t\|^2}{2\sigma^2}\right)}
\]

Probability that points \( s \) and \( t \) are connected \( P_{s,t} = P_{t,s} = \frac{p_{t \rightarrow s} + p_{s \rightarrow t}}{2n} \)
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**Stochastic Neighborhood Embedding**

- Use a probabilistic notion of which points are neighbors.

  Close by points are neighbors with high probability, ... 
  Eg: For point $x_t$, point $x_s$ is picked as neighbor with probability

  $$p_{t \rightarrow s} = \frac{\exp(-\frac{\|x_s - x_t\|^2}{2\sigma^2})}{\sum_{u \neq t} \exp(-\frac{\|x_u - x_t\|^2}{2\sigma^2})}$$

  Probability that points $s$ and $t$ are connected $P_{s,t} = P_{t,s} = \frac{p_{t \rightarrow s} + p_{s \rightarrow t}}{2n}$

- Goal: Find $y_1, \ldots, y_n$ with stochastic neighborhood distribution $Q$ such that “$P$ and $Q$ are similar”

  i.e. minimize:

  $$\text{KL}(P \| Q) = \sum_{s,t} P_{s,t} \log \left( \frac{P_{s,t}}{Q_{s,t}} \right) = \sum_{s,t} P_{s,t} \log (P_{s,t}) - \sum_{s,t} P_{s,t} \log (Q_{s,t})$$
Choice for $Q$

Just like we defined $P$, we can define $Q$ for a given $y_1, \ldots, y_n$ by

$$q_{t \to s} = \frac{\exp\left(-\frac{\|y_s - y_t\|^2}{2\sigma^2}\right)}{\sum_{u \neq t} \exp\left(-\frac{\|y_u - y_t\|^2}{2\sigma^2}\right)}$$

and then set $Q_{s,t} = \frac{q_{t \to s} + q_{s \to t}}{2n}$
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- However we are faced with the crowding problem:
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  - For \( d \) dimensional gaussians, most points are found at distance \( \sqrt{d} \) from mean!
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  - In high dimension we have a lot of space, Eg. in \( d \) dimension we have \( d + 1 \) equidistant point
  - For \( d \) dimensional gaussians, most points are found at distance \( \sqrt{d} \) from mean!
  - If we use gaussians in both high and low dimensional space, all the points are squished in to a small space
  - Too many points crowd the center!
Method II: t-SNE

- Instead for $Q$ we use, student $t$ distribution which is heavy tailed:

$$q_{t \rightarrow s} = \frac{(1 + \|y_s - y_t\|^2)^{-1}}{\sum_{u \neq t} (1 + \|y_u - y_t\|^2)^{-1}}$$

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- It can be verified that

$$\nabla_{y_t} KL(P || Q) = 4 \sum_{s=1}^{n} (P_{s,t} - Q_{s,t})(y_t - y_s) \left(1 + \|y_s - y_t\|^2\right)^{-1}$$
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- Algorithm: Find $y_1, \ldots, y_n$ by performing gradient descent
Demo