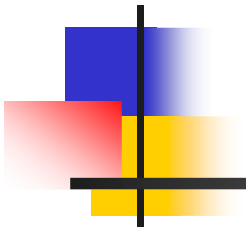
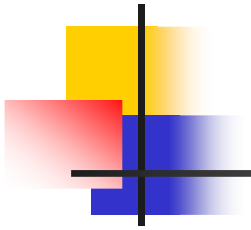


Algorithms 2005

Ramesh Hariharan

Algebraic Methods

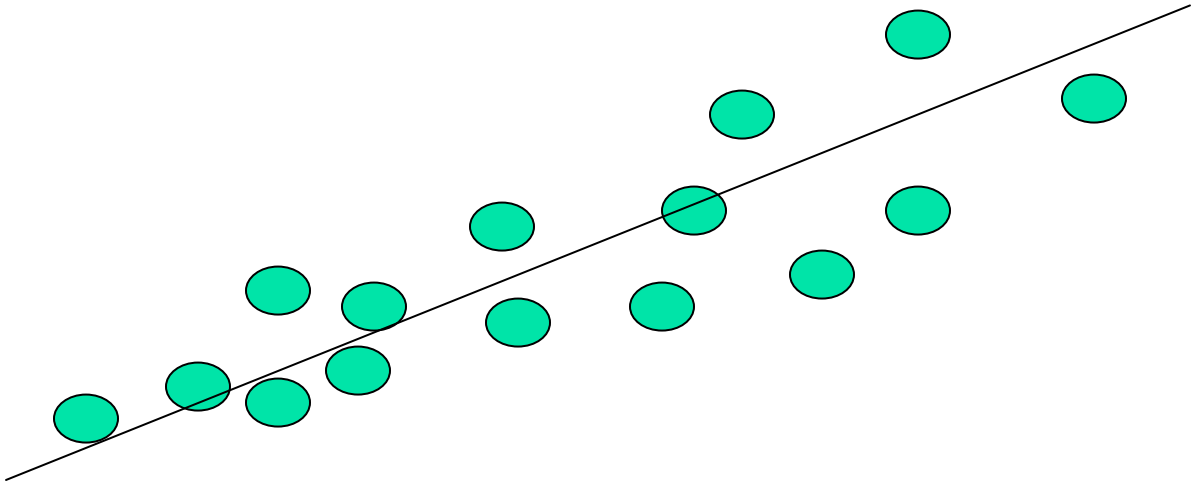


Principal Component Analysis

- Given m points in a n dimensional space, for large n, how does one project on to a 2 or 3 dimensional space while preserving broad trends in the data and allowing it to be visualized?

Principal Component Analysis

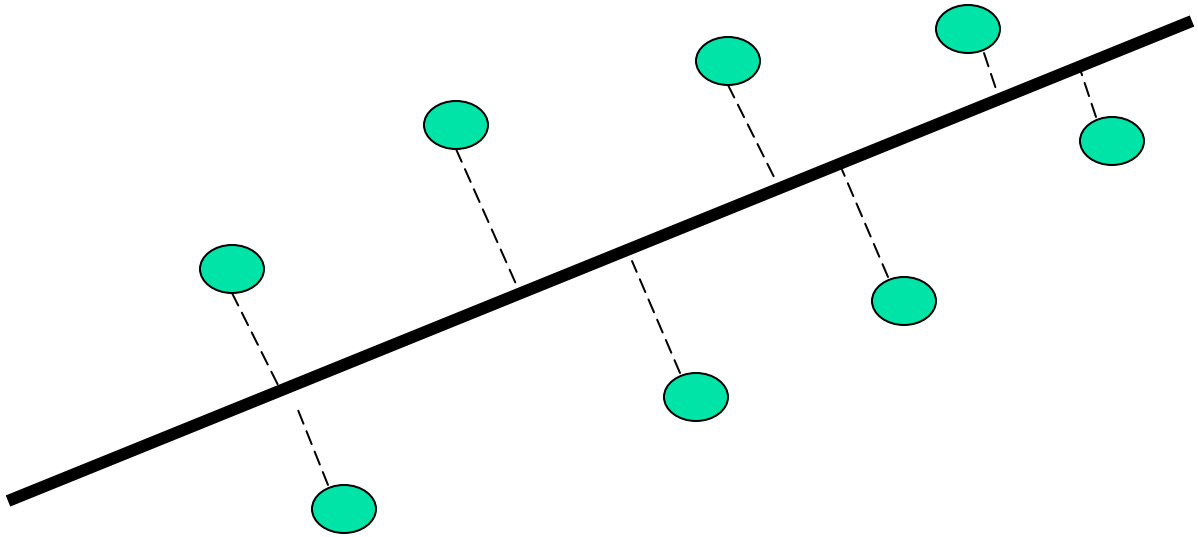
- Given m points in a n dimensional space, for large n, how does one project on to a 1 dimensional space?



- Choose a line that fits the data so the points are spread out well along the line

Principal Component Analysis

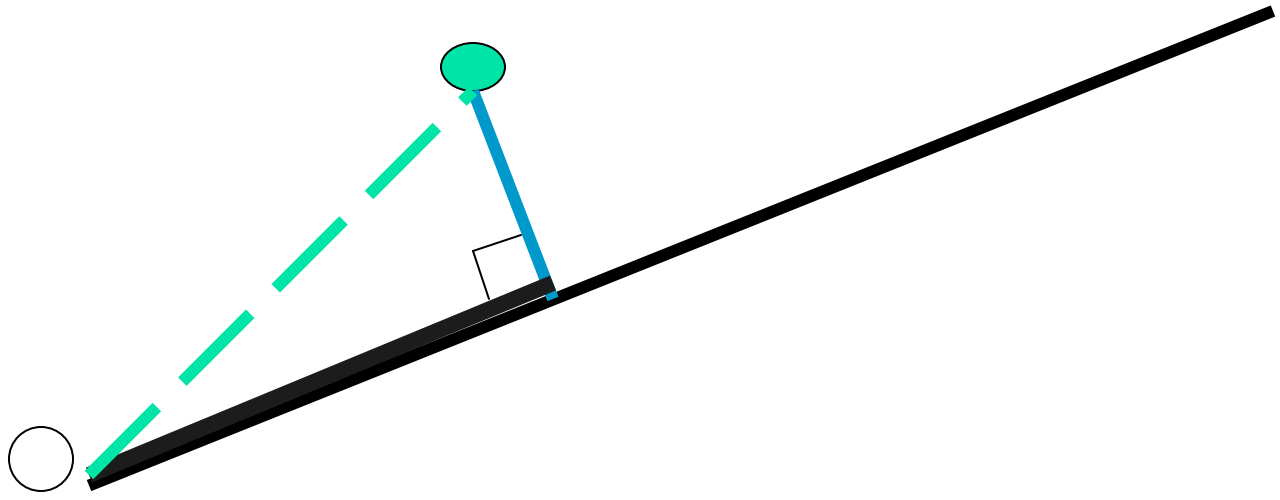
- Formally, minimize sum of squares of distances to the line.



- Why sum of squares? Because it allows fast minimization, assuming the line passes thru 0

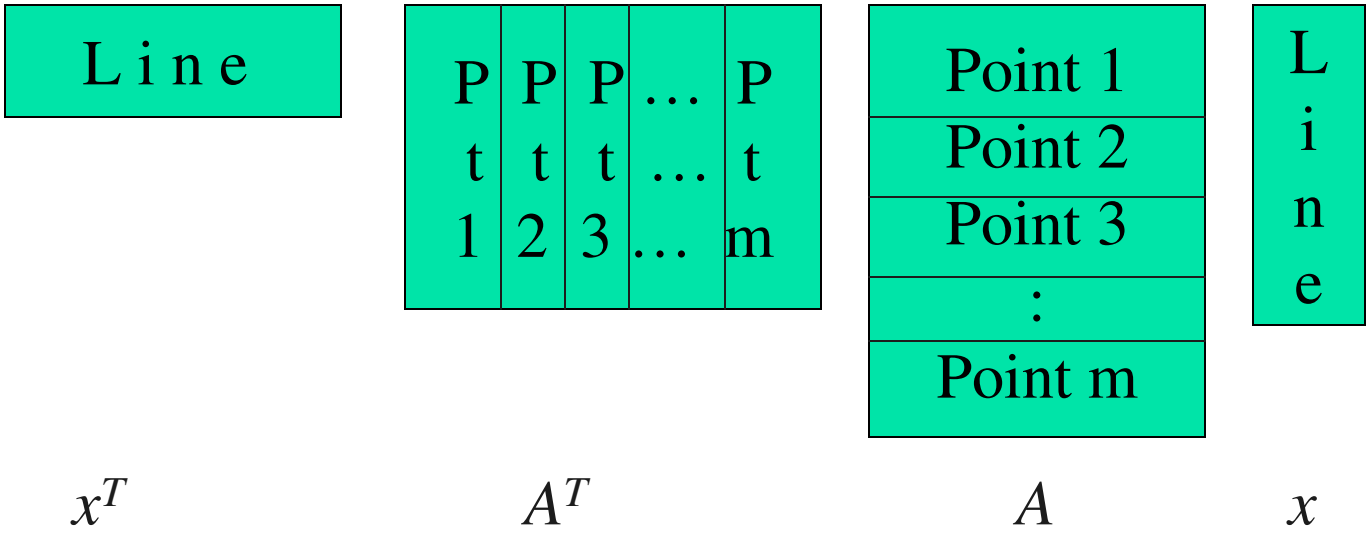
Principal Component Analysis

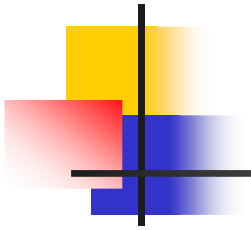
- Minimizing sum of squares of distances to the line is the same as maximizing the sum of squares of the projections on that line, thanks to Pythagoras.



Principal Component Analysis

- How is the sum of squares of projection lengths expressed in algebraic terms?





Principal Component Analysis

- How is the sum of squares of projection lengths expressed in algebraic terms?

$$\max(x^T A^T Ax), \text{ subject to } x^T x = 1$$

Principal Component Analysis

- Rewriting this:

$$x^T A^T A x = e = e\, x^T x = x^T (ex)$$

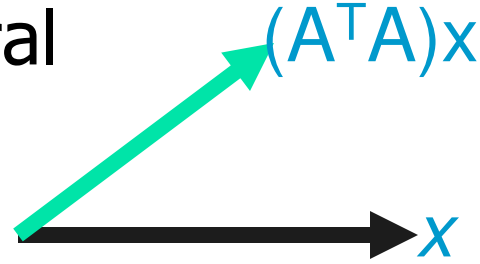
$$<=> \quad x^T (A^T A x - ex) = 0$$

- Show that the maximum value of $x^T A^T A x$ is obtained for x satisfying $A^T A x = ex$

- So, find the largest e and associated x such that the matrix $A^T A$ when applied to x yields a new vector which is in the same direction as x, only scaled by a factor e.

Principal Component Analysis

- $(A^TA)x$ points in some other direction in general



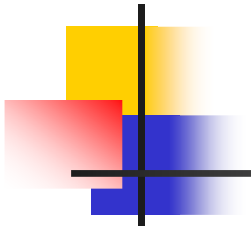
x is an eigenvector and e an eigenvalue if

Principal Component Analysis

- How many eigenvectors are there?
- For Real Symmetric Matrices
  - except in degenerate cases when eigenvalues repeat, there are n eigenvectors

    $x_1 \ldots x_n$ are the eigenvectors

    $e_1 \ldots e_n$ are the eigenvalues
  - all eigenvectors are mutually orthogonal and therefore form a new basis
    - Eigenvectors for distinct eigenvalues are mutually orthogonal
    - Eigenvectors corresponding to the same eigenvalue have the property that any linear combination is also an eigenvector with the same eigenvalue; one can then find as many orthogonal eigenvectors as the number of repeats of the eigenvalue.
  - Show the above properties



Principal Component Analysis

- For matrices of the form $A^T A$
  - All eigenvalues are non-negative (show this)

Principal Component Analysis

- How are the eigenvectors computed?

  Since the eigenvectors form a basis:

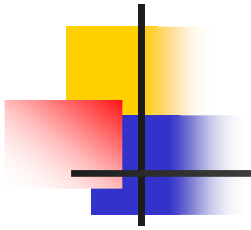
  $(A^T A)\, y = (A^T A)\,(a_1 x_1 + a_2 x_2 \ldots\ldots + a_n x_n)$

  $= a_1 e_1 x_1 + \ldots + a_n e_n x_n$

  $(A^T A)(A^T A)\, y = a_1 e_1 e_1 x_1 + \ldots + a_n e_n e_n\, x_n$

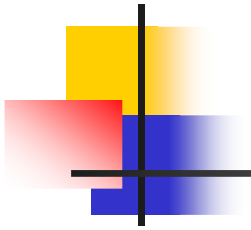
- Repeated application of $A^T A$ on almost any vector y converges to a scaled version of the eigenvector x_1 corresponding to the largest eigenvalue e_1.
- y should satisfy $a_1 != 0$

What happens if e_1 is a repeated eigen value?



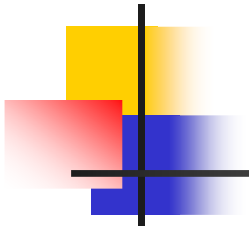
Principal Component Analysis

- Algorithm for computing the fitting line
  - Compute A^TA
  - Start with (almost) any vector y
  - Repeatedly multiply A^TA with y and rescale until convergence (in practice, a fixed number of times)
  - The resulting direction is the fitting line direction!!



Principal Component Analysis

- Time taken for convergence
  - How many iterations i before
    - $[a_1(e_1)^i] / [\Sigma a_k(e_k)^i] > 1-\varepsilon$
    - $a_1(e_1)^i \varepsilon > \Sigma a_{k>1}(e_{k>1})^i$
    - $a_1(e_1)^i \varepsilon > n\, a_{max}\, (e_2)^i$
    - $a_1 / a_{max}\, (e_1/e_2)^i > n/\varepsilon$
    - $i > \log(n/\varepsilon\ a_{max}/a_1) / \log(e_1/e_2)$



Principal Component Analysis

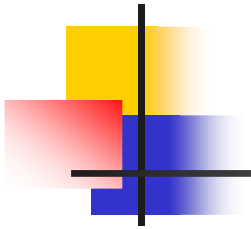
- Optimization
  - if A is mxn and m<<n then A^TA is nxn >> mxm
  - use AA^T instead, eigenvector of AA^T is easily converted to that of A^TA

$(AA^T)y=e'y$

$=>A^T(AA^T)y=e'(A^Ty)$

$=>(A^TA)(A^Ty)=e'(A^Ty)$

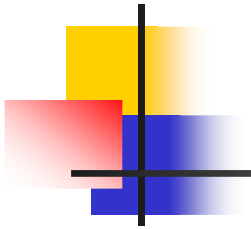
$=>A^Ty$ is the eigenvector of A^TA



Principal Component Analysis

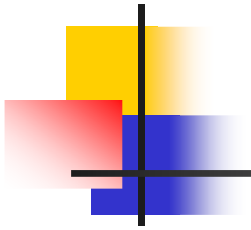
- New algorithm for computing the fitting line

  - Compute $B = A^T A$ or AA^T whichever is smaller
  - Start with (almost) any vector y
  - Repeatedly multiply B with y and rescale until convergence
  - If $B=A^T A$ then the resulting direction is the fitting line direction
  - If $B=AA^T$ then A^T times the resulting direction is the fitting line direction



Principal Component Analysis

- Complexity
  - Compute $B = A^TA$ or AA^T : (cols x rows x cols) or (rows x cols x rows), whichever is smaller
  - Iterations: cols x cols x numInterations or rows x rows x numIterations, whichever is smaller
  - If $B=AA^T$ then multiplication with A^T takes cols x rows



Principal Component Analysis

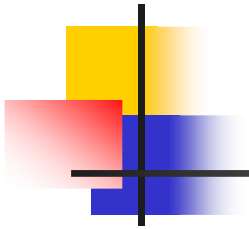
- The Conundrum in Practice
  - For 9000x2000, $B = A^T A$ takes 2000x9000x2000
  - For 2000x9000, $B = AA^T$ takes 2000x9000x2000
  - Iterations: 2000x2000xnumIterations in both cases
  - For 2000x9000, $B = AA^T$ and multiplication with A^T takes 2000x9000

Yet, 9000x2000 takes 100 times what 2000x9000 takes!!!!

Principal Component Analysis

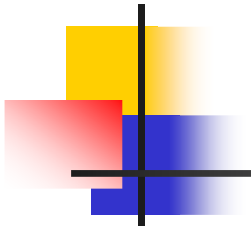
- A careful look at the code

```
for i=0 to min(rows,cols)
   for j=0 to min(rows,cols)
       if  rows<cols
           {for k=0 to cols
                B[i,j]=A[i,k]*A[j,k]
           }
        else
           {for k=0 to rows
                B[i,j]=A[k,i]*A[k,j]
           }
```



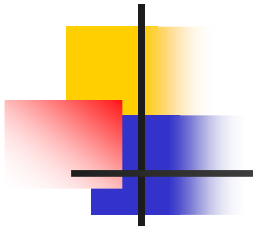
Principal Component Analysis

- A careful look at the code
  - The AA^T option shows strong locality of reference
  - The A^TA option shows strong non-locality of reference
  - Caching misses cause a greater than 100 fold slowdown in the latter cache



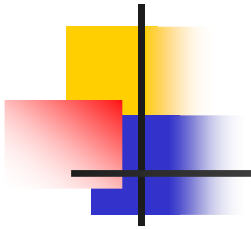
Principal Component Analysis

- The solution
  - Prior to doing A^TA, move A into a linear array stored in column major order.
  - Currently done using an extra array, can one save an array? More space usage is bad. How does one convert row major to col major order in place for a rectangular matrix?
  - With this, both A^TA and AA^T take the same amount of time.



Principal Component Analysis

- Further dimensions
  - Once the line along which projections are made is found, all points are projected to the space orthogonal to this line to find further dimensions, recursively.
  - These dimensions are called principal components; usually only a few are computed.
  - The strength associated with a dimension is the corresponding eigenvalue = the sum of squares of projection lengths
  - The total sum of all eigenvalues over all eigenvectors is equal to the squares of the lengths of the point vectors themselves; the strength of an eigenvalue is expressed as a fraction of this quantity.



Principal Component Analysis

- Why normalize points?
  - Assumption: Fitting line passes through the origin.
  - This assumption is necessary for fast computation.
  - If data is skewed along any dimension then good fitting lines need not pass through the origin; mean centering helps reduce this skew.