Next: Naive QR algorithm

- Some variant QR algorithm is used in many commercial-grade eigenvalue computation routines.
- Algorithm: two part iteration:
 - QR decomposition: $A_n \rightarrow Q_n R_n$
 - Create next matrix: $A_{n+1} = R_n Q_n$
- Similar to simultaneous iteration because you re-orthogonalize at each step.
- Note difference between "QR decomposition" (matrix decomposition) and "QR algorithm" (finding eigenvalues)

Naive QR algorithm

- 1. Input: symmetric matrix A
- 2. Loop:
- 3. Compute $[Q, R] = qr(A_n)$
- **4.** Update $A_{n+1} = R^*Q$
- 5. Check for convergence: $norm(A_{n+1} A_n) < tol?$ If yes, eigenvalues lie on diagonal of A_{n+1} .

 If no, continue looping.

To get real eigenvalues for demo purposes.
Algorithm will also work on any square matrix after modifications.

Demonstration

```
>> A
A =
                                                    Start with
   -0.6412
                        -3.0582
                                  1.1469
              1.2549
                       1.1162
                                                    symmetric
    1.2549 -2.1334
                                 0.4487
   -3.0582
              1.1162
                        -3.1301
                                 -0.0432
                                                    matrix for real
    1.1469
              0.4487
                        -0.0432
                                  -1.4683
                                                    eigenvalues
>> my_eig_qr(A)_
                            Uses QR iteration to find
ans =
                            all eigenvalues
   -5.9322
   -2.1390
    1.8135
   -1.1153
>> eigs(A) ◄
                            Matlab built-in
ans =
   -5.9322
   -2.1390
    1.8135
```

-1.1153

Remarks on QR algorithm

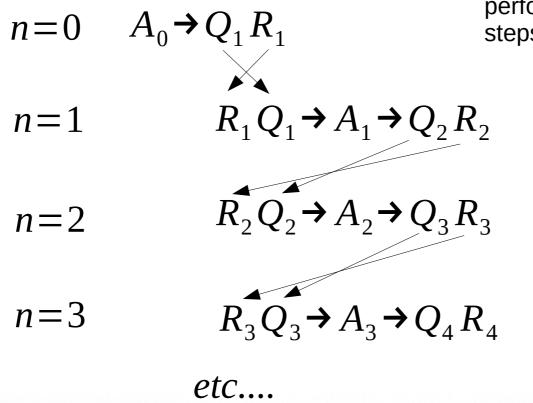
- Magical!
- Works for all square matrices
- Convergence is slow.
 - Can be improved using shifting (next)
- Dealing with complex eigenvalues requires special effort.
- Real implementations usually start by reducing input matrix to Hessenberg form.

 Triangular with additional set of

non-zeros on first off-diag.

Why does QR work?

- Start with matrix A₀
- Consider the iteration:



This is the calc we have performed written out in steps.

Powers of A

Define

$$\hat{Q}_k = Q_1 Q_2 Q_3 \cdots Q_k$$

$$\hat{R}_k = R_k R_{k-1} \cdots R_1$$

• Consider 3^{rd} power of A_0 :

$$A_{0}^{3} = (Q_{1}R_{1})(Q_{1}R_{1})(Q_{1}R_{1})$$

$$Q_{1} Q_{2}R_{2} Q_{2}R_{2} R_{1}$$

$$Q_{1} Q_{2} Q_{3}R_{3} R_{2} R_{1}$$

Therefore:

$$A_0^3 = Q_1 Q_2 Q_3 R_3 R_2 R_1 = \hat{Q}_3 \hat{R}_3$$

$$A_0 \rightarrow Q_1 R_1$$

$$A_1 = R_1 Q_1 \rightarrow Q_2 R_2$$

$$A_2 = R_2 Q_2 \rightarrow Q_3 R_3$$

$$A_3 = R_3 Q_3 \rightarrow Q_4 R_4$$
For reference – from last slide

QR decomposition of (input A)³

Iterates of A

• Consider 3^{rd} iterate of A_{α} :

$$A_3 = R_3 Q_3$$

$$A_2 = Q_3 R_3 \qquad \Rightarrow \qquad Q_3^T A_2 = R_3$$

- Therefore,
- Similarly,

Every time I iterate, I get back a new matrix with the same eigenvalues as the old one.

$$A_3 = Q_3^T Q_2^T A_1 Q_2 Q_3$$

 $A_3 = Q_3^T A_2 Q_3^T$

$$A_3 = Q_3^T A_2 = R_3$$
 $A_3 = Q_3^T A_2 Q_3$
 $A_3 = R_3 Q_3 \rightarrow Q_4 R_4$
For reference – from last slide
 $A_3 = Q_3^T Q_2^T A_1 Q_2 Q_3$
 $A_4 = \hat{Q}_3^T Q_2^T Q_1^T A_0 Q_1 Q_2 Q_3$
Similarity transform of $A_4 = P_1 P_2 P_2 P_2 P_3 P_4 P_4$

 $A_0 \rightarrow Q_1 R_1$

 $A_1 = R_1 Q_1 \rightarrow Q_2 R_2$

$$A_3 = \hat{Q}_3^T A_0 \hat{Q}_3$$

Similarity transform of A_0 – preserves eigenvalues

• Or,
$$A_0 = \hat{Q}_3 A_3 \hat{Q}_3^T$$

Interpretation

$$A_0^n = \hat{Q}_n \hat{R}_n$$

Statement about powers of A

$$A_0 = \hat{Q}_n A_n \hat{Q}_n^T$$

Statement about iterates of A

- $A_0^n = \hat{Q}_n \hat{R}_n$ says \hat{Q}_n is an orthonormal basis for A_0^n .
- Recall simultaneous iteration. In the limit, the cols of \hat{Q}_n converge to the similar to eigenvectors of A_0^n .
- $A_0 = \hat{Q}_n A_n \hat{Q}_n^T$ says A_0 and A_n have same eigenvalues

 Because this is a similarity transformation
- How do we know the eigenvalues are on the main diagonal?

• Consider focusing on one column of \hat{Q}_n

$$A_n = \hat{Q}_n^T A_0 \hat{Q}_n$$
 Columns are eigenvectors or A_0
$$= \hat{Q}_n^T A_0 \hat{Q}_n$$
 A_0
$$\hat{Q}_n$$
 Columns are eigenvectors or A_0

Diagonals

$$a_{ii} = \hat{q}_i^T A_0 \hat{q}_i^T$$
 q is eigenvector

$$a_{ii} = \hat{q}_i^T \lambda_i \hat{q}_i$$

$$a_{ii} = \lambda_i$$
 Because q is unit vector (Q is orthonormal)

Off-diagonals

$$a_{ji} = \hat{q}_j^T A_0 \hat{q}_i$$

$$a_{ji} = \hat{q}_{j}^{T} \lambda_{i} \hat{q}_{i}$$

$$a_{ii}=0$$

 Therefore, diagonals converge to eigenvalues of original matrix A_ο, off diags go to zero.

Improving convergence

Recall power method convergence:

$$A^{n}\vec{b}_{0} = \lambda_{1}^{n} \left(\beta_{1}\vec{q}_{1} + \beta_{2} \left(\frac{\lambda_{2}}{\lambda_{1}} \right)^{n} \vec{q}_{2} + \beta_{3} \left(\frac{\lambda_{3}}{\lambda_{1}} \right)^{n} \vec{q}_{3} + \dots + \beta_{k} \left(\frac{\lambda_{k}}{\lambda_{1}} \right)^{n} \vec{q}_{k} \right)$$

- Power method converges as: $(\lambda_2/\lambda_1)^n$
- Recall simultaneous iteration converges as:

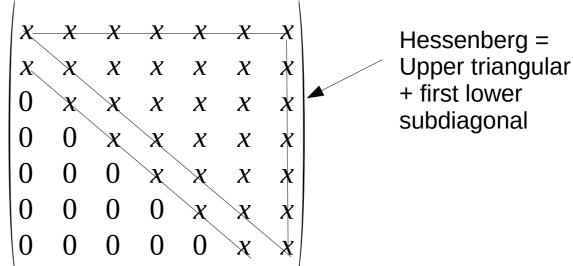
$$max(\lambda_{j+1}/\lambda_j)^n$$

Analogously, QR algorithm converges as

$$\max(\lambda_{j+1}/\lambda_j)^n$$
 Can converge slowly if eigenvalues are close in magnitude

Practical QR algorithm

- Improve convergence: Use "shifting" to make smallest eigenvalue converge extra fast.
- Also use "deflation" to shrink matrix as eigenvalues are found.
- Finally, most QR implementations first reduce input matrix to upper Hessenberg or other convenient form.



Shifting

Naive QR:

$$[Q,R] \leftarrow qr(A^{(n)})$$
$$A^{(n+1)} \leftarrow RQ$$

QR with shifting:

$$\sigma \leftarrow A_{end,end}^{(n)}$$

"Tail" of A – Move this element to zero to speed convergence of next eigenvalue

$$[Q,R] \leftarrow qr(A^{(n)} - \sigma I)$$
 Take away smallest value before doing qr

$$A^{(n+1)} \leftarrow R Q + \sigma I$$
 Then put it back to generate next A matrix.

Theorem

• If u = eigenvector & λ = eigenvalue of matrix A, we have:

$$Au = \lambda u$$

Consider adding in scalar p on the digaonal:

$$(A+pI)u = \lambda u + pIu$$

$$(A+pI)u = (\lambda + p)u$$

Therefore, eigenvalue of matrix (A + p I) is
 λ+p

 This fact can be useful when dealing with singular matrices, etc.

Why shift?

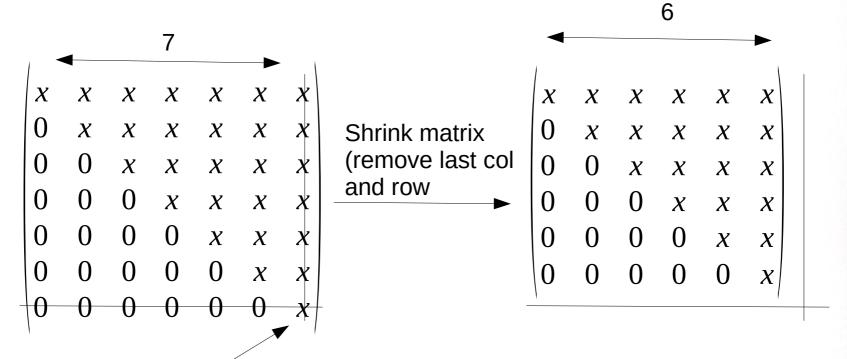
- Each eigenvalue converges like $(\lambda_{j+1}/\lambda_j)^n$
- Idea: the shift at each step moves the end λ_{j+1}/λ_j close to zero, thereby accelerating convergence.

$$\sigma \leftarrow A_{end,end}^{(n)} \qquad \qquad \text{Move diagonal element on tail close to zero} \\ [Q,R] \leftarrow qr(A^{(n)} - \sigma I) \\ A^{(n+1)} \leftarrow RQ + \sigma I \qquad \qquad \text{Recover original eigenvalues}$$

 Then recover matrix A's eigenvalues before next iteration

Deflation

 Once the bottom right "tail" eigenvalue has converged, add it to a list of eigenvalues, then shrink matrix.



This value converged.

Deflation

Example: run_myeig_qr_shifted

```
After iteration 3, W = 5, matrix =
   -2.0663
            -1.5073
                      -0.1273
                                         0.0000
                                0.0272
   -1.5073 4.6719 0.6218
                               -0.0402
                                         -0.0000
   -0.1273 0.6218
                     -1.4940
                              0.6710
                                         -0.0000
   0.0272 - 0.0402
                     0.6710
                               -0.2151
                                         -0.0000
   0.0000
            -0.0000
                      -0.0000
                               -0.0000
                                          1.6376
After iteration 4, W = 4, matrix =
   1.0400
            -3.7089
                      -0.0730
                                0.0245
   -3.7089 1.6249 0.1008
                                0.0057
                                              Element
   -0.0730 0.1008
                     -1.1270
                                0.9171
                                              converged
   0.0245
           0.0057
                     0.9171
                               -0.6413
                                             Matrix deflated
                                             at next iteration
```

QR algorithm convergence much faster with shift and deflate

- Example 5x5 matrix using naive QR:
 - --- We converged after 1356 iterations! ---
- Same matrix using QR with shift and deflate:
 - --- We converged after 11 iterations! ---
- Why so different?
 - Naive QR converges as $(\lambda_{j+1}/\lambda_j)^n$
 - If two eigenvalues are close to each other, convergence can be very slow.

Extreme

but real

case

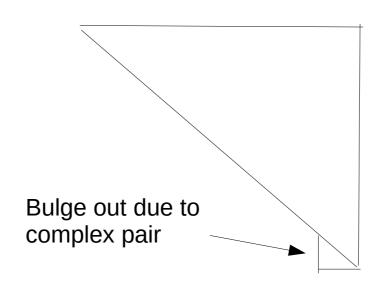
Shifting fixes this problem.

Next problem: complex eigenvalues

- QR iteration on arbitrary square matrix gives:
 - Upper triangular
 - 2x2 blocks on main diagonal which correspond to complex eigenvalues.

```
Matrix after iteration
                         90 =
               1.0151
                                                0.0693
    1.0008
                         -0.2210
                                    -2.8003
                                                          -0.3408
   -2.1101
               1.8797
                         -0.2943
                                                1.5698
                                     0.7947
                                                          -1.5082
   -0.0000
              -0.0000
                         -0.2707
                                     1.6899
                                                1.5577
                                                           0.5418
    0.0000
               0.0000
                         -1.2961
                                    -0.2603
                                                           0.9187
                                               -1.1709
   -0.0000
               0.0000
                          0.0000
                                    -0.0000
                                               -1.2889
                                                          -0.5015
   -0.0000
              -0.0000
                          0.0000
                                     0.0000
                                               -0.0000
                                                           0.7922
```

Francis's double-shift algorithm



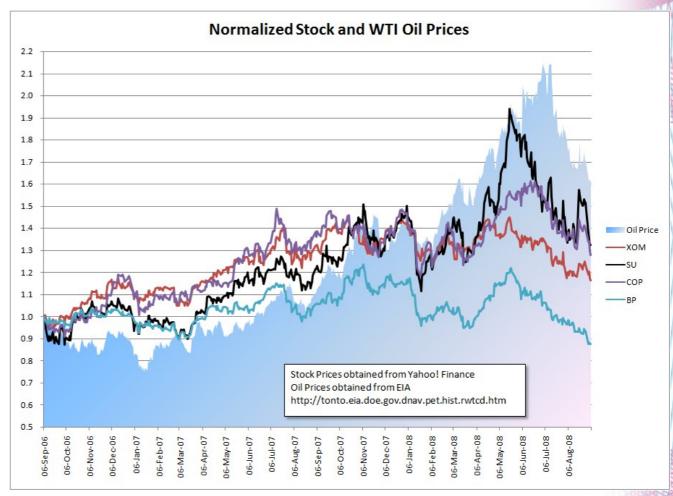
Mini-project for somebody?

New topic: PCA Principal Component Analysis

- Traditionally uses EVD.
 - Modern method uses SVD.
- Very useful data analysis technique.
- Looks for correlations between data sets, recommends way to convert correlated data sets into smaller set of uncorrelated data.
- Identifies "underlying dynamics".
- Often first step in dimensionality reduction.

Example: Stock prices

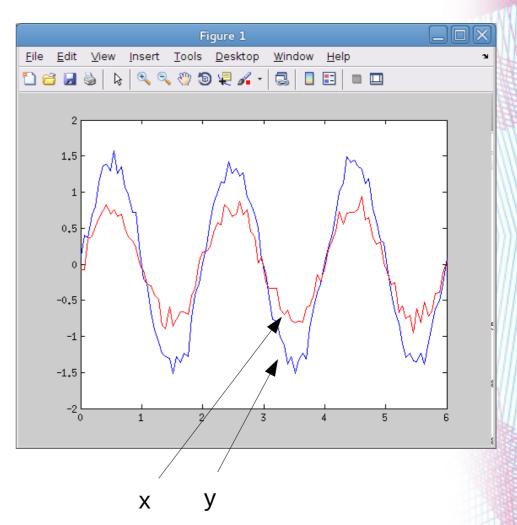
 Stock prices seem to move together, but also have some component of individual behavior.



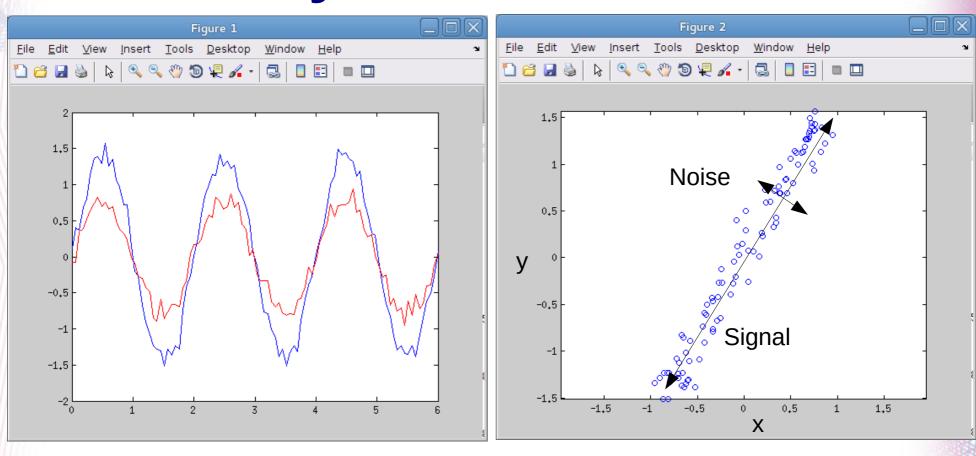
Can we separate the common motions from the individual behaviors?

Concept: Covariance

- Consider two random variables, x and y.
 - Imagine they correspond to two different time series
- Suppose x and y track each other (statistically dependent).

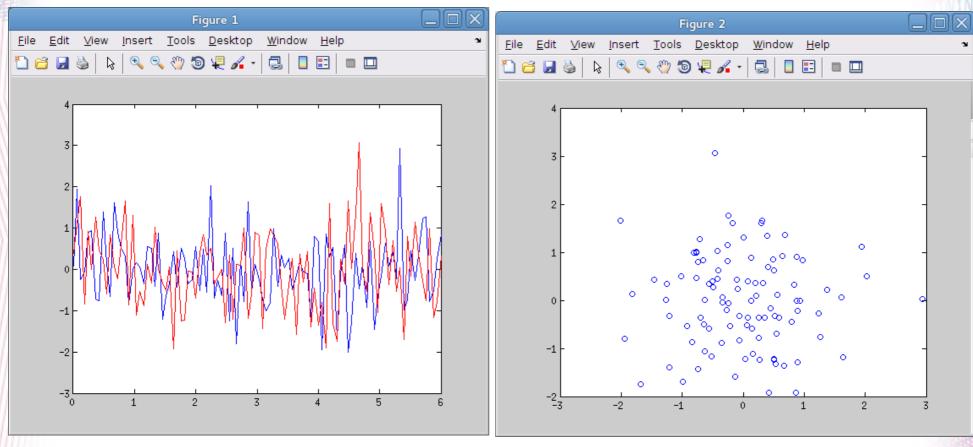


One way to see covariance



- Plot x vs. y scatterplot
- Correlation between signals shows up as closely grouped points in scatterplot

Another signal – uncorrelated noise



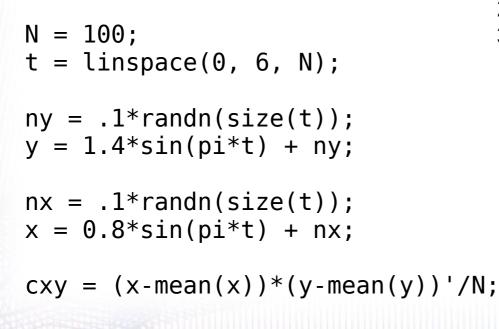
Uncorrelated noise signals show up as round scatterplot.

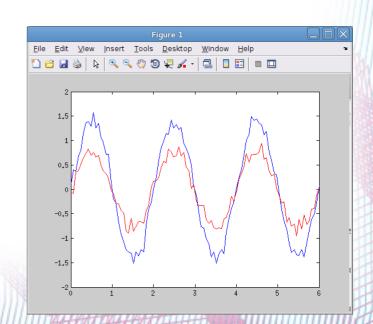
Convariance (scalar)

 We can calculate the degree to which the two variables track each other using covariance:

$$cov(x,y)=E((x-E(x))(y-E(y)))$$

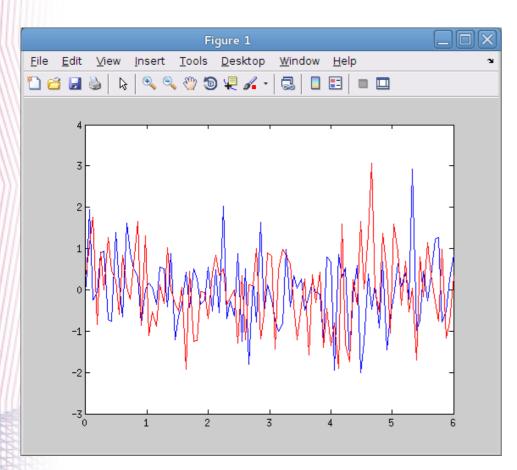
- 1. Subtract off mean
- 2. Multiply pairwise
- 3. Take mean of series

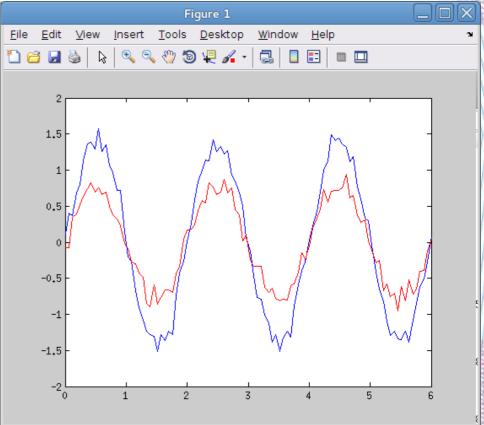




Consider two signals

$$cov(x,y) = E((x-E(x))(y-E(y)))$$





Covariance cxy = -0.026734

Covariance cxy = 0.546910

Variance and covariance

Variance if same signal is used

$$var(x) = E((x-E(x))(x-E(x)))$$

Covariance if different signals are used

$$cov(x,y) = E((x-E(x))(y-E(y)))$$

Covariance matrix

We have 2 signals:

$$X_{1}, X_{2}$$

Create matrix whose elements are

$$c_{ij} = cov(x_i, x_j)$$

= $E((x_i - E(x_i))(x_i - E(x_i)))$

Matrix will be

$$S = \begin{pmatrix} var(x_1, x_1) & cov(x_1, x_2) \\ cov(x_2, x_1) & var(x_2, x_2) \end{pmatrix}$$

Three covariance trials

- Covariance of noise signals is small -> statistically independent. Off-diag terms small.
- Covariance of sine waves is large -> statistically related. Off-diag terms large.

What if we have multiple signals?

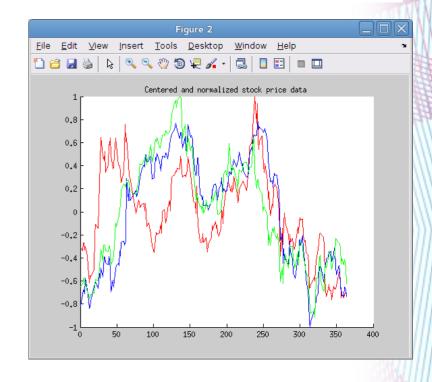
Consider 3 signals:

$$X_{1}, X_{2}, X_{3}$$

 Consider computing covariances for all signal pairs:

$$c_{ij} = cov(x_i, x_j)$$

= $E((x_i - E(x_i))(x_j - E(x_j)))$



Arrange into matrix:

$$S = \begin{vmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{vmatrix}$$
 Covariance matrix

How to calculate covariance matrix?

1. Start with time series data arranged in rows in a data matrix M.

$$M = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & \cdots \\ y_1 & y_2 & y_3 & y_4 & y_5 & \cdots \\ z_1 & z_2 & z_3 & z_4 & z_5 & \cdots \end{pmatrix}$$

2. Subtract off mean for each row. (Zero-center the data) for idx = 1:N

```
r = M(idx, :);

r = r-mean(r);

M(idx, :) = r;

end
```

3. Compute matrix product (performs sums along rows)

$$S = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & \cdots \\ y_1 & y_2 & y_3 & y_4 & y_5 & \cdots \\ z_1 & z_2 & z_3 & z_4 & z_5 & \cdots \end{pmatrix} \begin{pmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \\ x_4 & y_4 & z_4 \\ x_5 & y_5 & z_5 \\ \vdots & \vdots & \vdots \end{pmatrix}$$

4. Normalize:

$$S = \frac{1}{N} M M^{T}$$

$$N = \text{number of } S = \frac{1}{N} M M^{T}$$

Covariance matrix S

Use this expression when data is placed in rows of matrix M.

N = number of rows

Covariance matrix properties

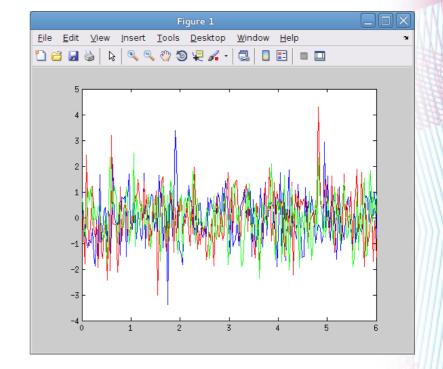
- On-diagonal elements are variances of each individual data series.
- Off-diagonal elements are covariances between dataset i and j.

$$S = \begin{vmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{vmatrix}$$

- Covariance matrix is symmetric.
- Covariance matrix is positive semi-definite.
 - Eigenvalues are non-negative.

Covariance matrix properties....

- Consider three uncorrelated random processes.
- On-diagonal elements of covariance matrix are large



 Off-diagonal elements of covariance matrix are small

Covariance matrix C = 0.9308 **→** 0.0027 -0.0903

>> three noise series

0.0027

-0.0903

1.0858

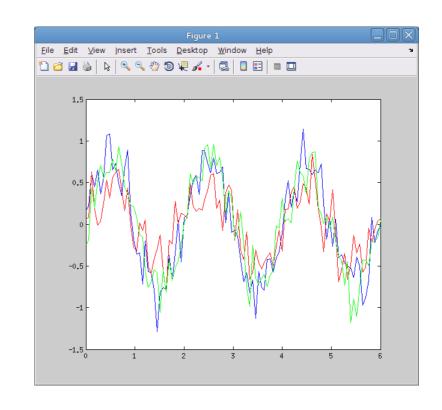
0.0709

0.0709

0.8793

Covariance matrix properties...

- Consider three correlated random processes
- Off diagonal elements of covariance matrix are not small. This says that the processes are correlated.



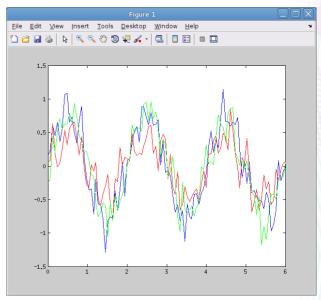
```
>> three_time_series

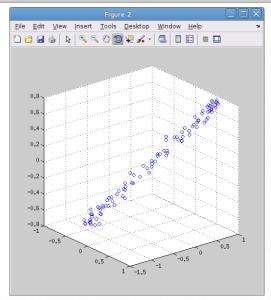
Covariance matrix C =
    0.3352    0.1703    0.2759
    0.1703    0.1404    0.1631
    0.2759    0.1631    0.3114
```

Symptoms of correlated signals

- Three time-varying signals evince correlated behavior
- Structure of scatterplot suggests signals are not independent.
- Off-diagonal terms in covariance matrix suggest correlation between signals

```
Covariance matrix C = 0.3352 0.1703 0.2759 0.1631 0.2759 0.1631
```

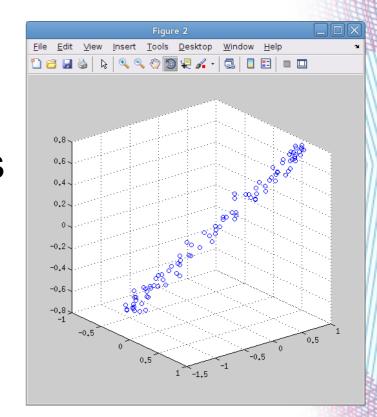




Correlated signals suggest underlying dynamics

Goal: find principal axes of correlation

- Can we find dominant axis of scatterplot?
- Yes by finding eigenvectors of covariance matrix.
- This technique is called "principal component analysis" or PCA.



 PCA can be useful for identifying underlying dynamics of a signal or data source.

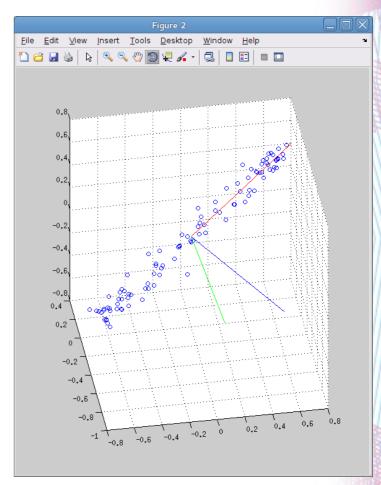
PCA algorithm

Data matrix

- 1. Put time series data into rows M
- Subtract off mean from each row (zero-center data)
- 3. Form covariance matrix $S = M M^T$
- **4.** Do eigenvalue decomposition of S: $S \rightarrow Q^T \wedge Q$
- Sort eigenvalues and eigenvectors from high to low.
- 6. Eigenvectors point along principal directions variance.

Example PCA run

```
C = M*M'/N;
% Do eigenvalue decomposition
[V,D] = eig(C);
% Sort eigenvalues in decreasing order
[Ds, idx]=sort(diag(D), 1, 'descend');
% Rearrange eigenvectors to
% match eigenvalues.
for cnt=1:length(Ds)
  Vs(:,cnt)=V(:,idx(cnt));
end
% Now plot eigenaxes
e1 = horzcat([0;0;0], Vs(:,1))';
plot3(e1(:,1), e1(:,2), e1(:,3), 'r')
e2 = horzcat([0;0;0], Vs(:,2))';
plot3(e2(:,1), e2(:,2), e2(:,3), 'b')
e3 = horzcat([0;0;0], Vs(:,3))';
plot3(e3(:,1), e3(:,2), e3(:,3), 'g')
```

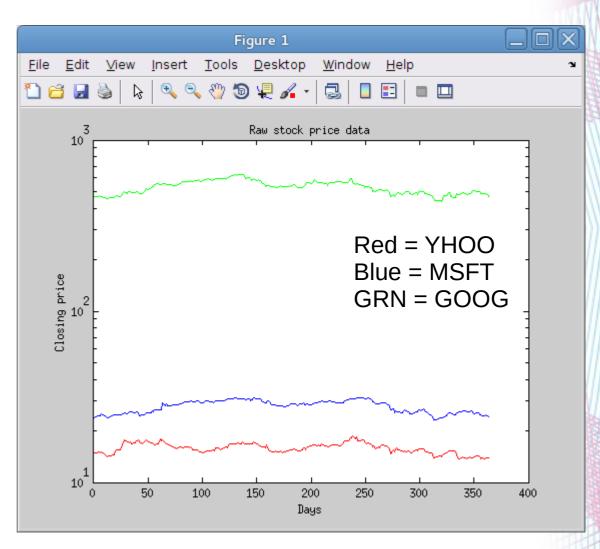


Remarks

- First eigenvector points in direction of maximum variance.
- Next eigenvector points in next direction of max variance, etc.
- These are the "principal components" of your data.
- If you have redundancy in your data (different measurements are correlated), PCA will show it to you.

Another example

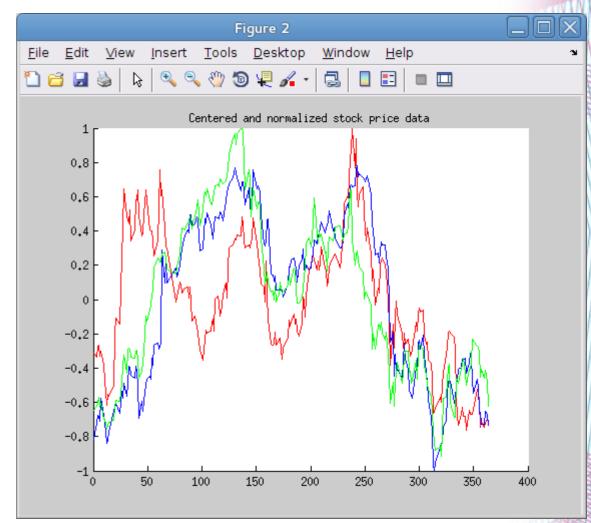
- One year of real stock market data
- Time series starts on 8.21.2009
- Ends on 8.20.2010



Source: http://pages.swcp.com/stocks/

Preprocessing

- Clean data
- Zero-center all data (i.e. subtract off mean)
- Normalize all data so abs(max(data)) = 1



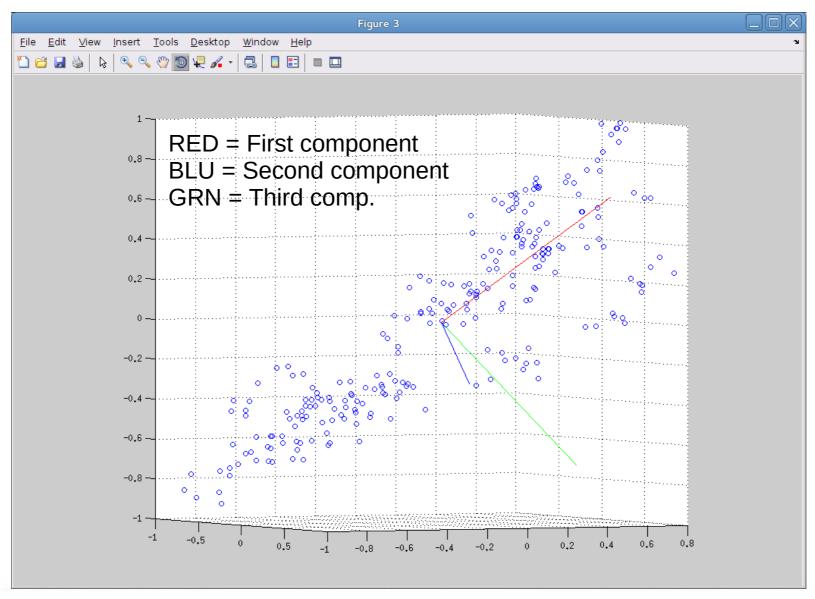
Covariance of different stocks is very evident

Preprocessing

```
% Normalize price data and make it zero-centered
% i.e. subtract off mean and normalize it.
for idx = 1:num_stocks
   S = A(idx, :);
   S = S-mean(S);
   peak = max(abs(S));
   S = S/peak;
   A(idx, :) = S;
end
```

- PCA requires zero-centered data.
- If you don't zero-center the data, then covariance matrix has large off-diagonal elements, and eigenvalue decomposition doesn't identify axes of variation.
- Normalizing data is optional but often recommended.

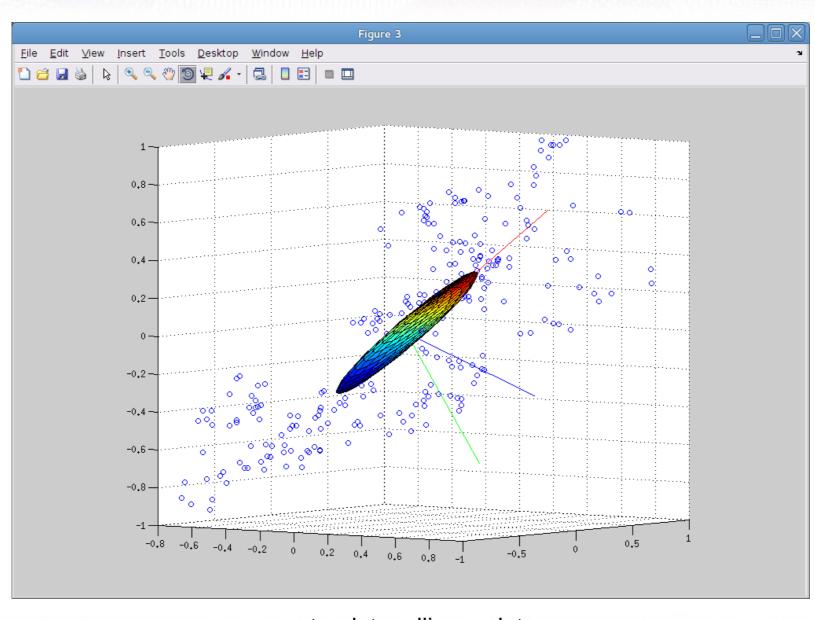
Perform PCA



First component corresponds to overall move of three stocks together

Why does PCA work?

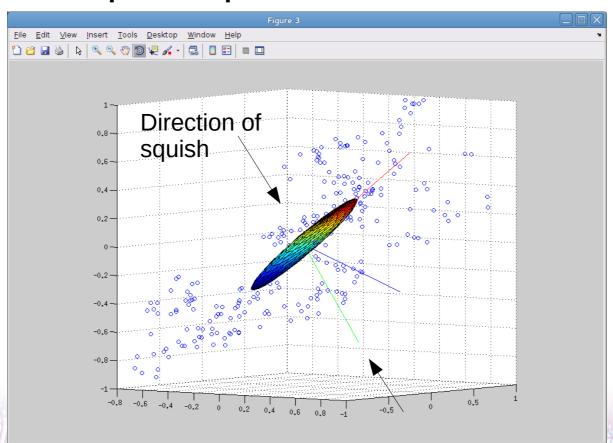
- Recall covariance matrix symmetric, positive semi-definite.
- Recall how we visualized any matrix by looking at its action on a unit ball.
- In this case, the covariance matrix induces a 3D ellipse whose axes are aligned with the principal axes of the data's variation.
- The lengths of the axes correspond to the variance in each direction.



generate_data_ellipse_plot.m

Next: Projecting to new basis

- The eigenvectors define a new basis set.
- We can project data to this new basis set.
- In this example, squish out third dimension



Projection onto subspace

Project datapoints into new (reduced) basis.

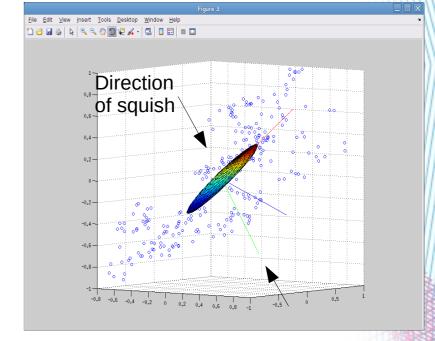
 Only project onto first two axes – drop dependence on third (green) axis. This is dimensionality reduction.

 Projection is derived from eigenvectors.

 Projection operator is 2x3 matrix (dimensionality reduction)

$$\begin{pmatrix} b_{1i} \\ b_{2i} \end{pmatrix} = \begin{pmatrix} \cdots \hat{e}_1 \cdots \\ \cdots \hat{e}_2 \cdots \end{pmatrix} \begin{pmatrix} a_{1i} \\ a_{2i} \\ a_{3i} \end{pmatrix}$$

Projected First 2 Input data data (2D) eigenvectors (3D)

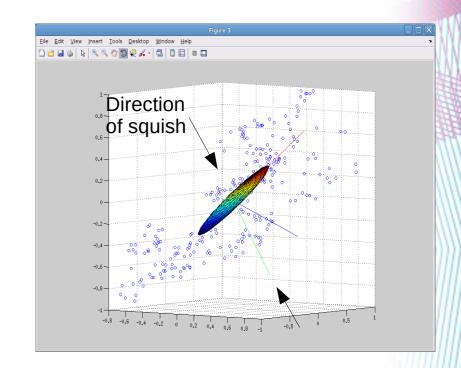


Projection matrix

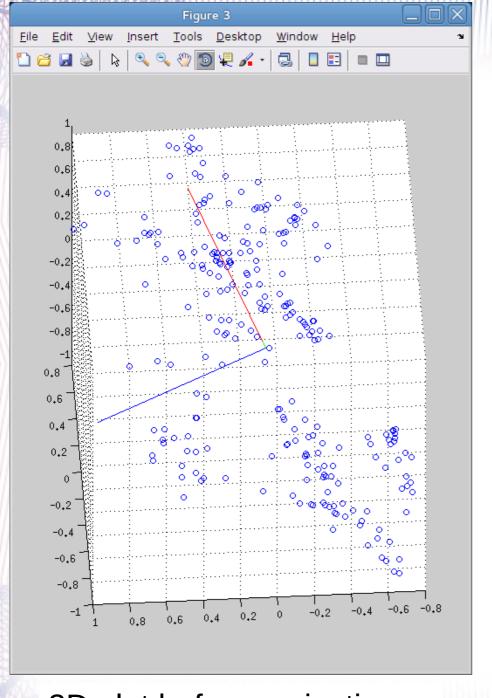
Consider what this does:

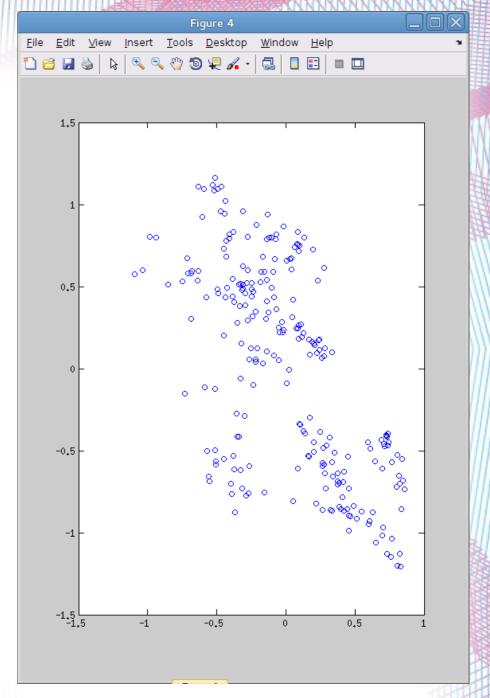
$$\begin{pmatrix} b_{1i} \\ b_{2i} \end{pmatrix} = \begin{pmatrix} \cdots \hat{e}_1 \cdots \\ \cdots \hat{e}_2 \cdots \end{pmatrix} \begin{pmatrix} a_{1i} \\ a_{2i} \\ a_{3i} \end{pmatrix}$$

Projected First 2 Input data data (2D) eigenvectors (3D)



- Starts with data point [a₁ a₂ a₃].
- Finds amount of a pointing in direction $\hat{e_1}^T a \Rightarrow b_1$
- Finds amount of a pointing in direction $\hat{e}_2^T a \Rightarrow b_2$
- Discards anything pointing in direction \hat{e}_3





3D plot before projection

2D plot after projection

run_analysis.m

Sounds like the SVD?

- Classical PCA was framed in terms of doing an eigenvalue decomposition of the covariance matrix.
 - Perhaps because it was invented long before the SVD became well known.
- Dimensionality reduction and projection onto new bases are also associated with SVD analyses.
- You can also (almost) think of PCA as simply doing an SVD on the data matrix itself.

Relationship between PCA and SVD

Recall relation of SVD to eigendecomposition:

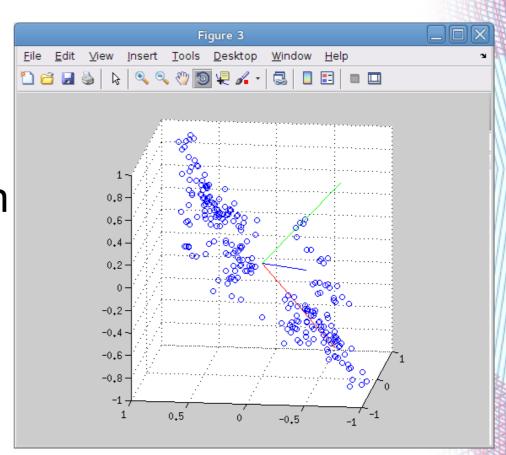
$$svd(A) \Leftrightarrow eig(A^T A) = eig(A A^T)$$
 Homework problem

- Doing eigendecomposition of covariance matrix A^τA is almost same as doing SVD on original matrix A.
- One difference: Covariance matrix is zerocentered (subtract means from rows).
 - Therefore, subtract mean from each row prior to SVD.
- Otherwise, PCA using eigenvalue decomposition and SVD are equivalent.

PCA using SVD

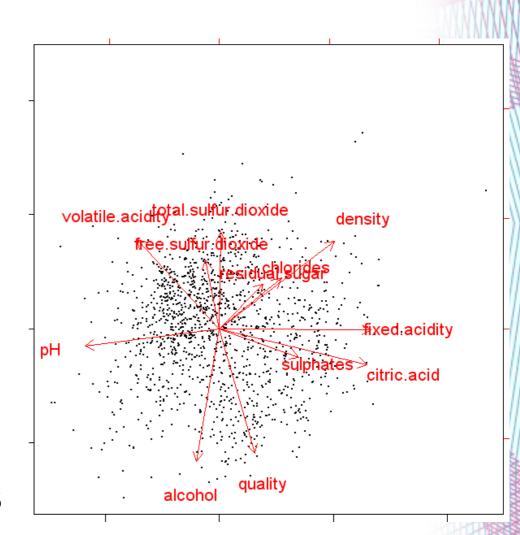
$A \rightarrow U S V^T$

- Since my data are in rows, the eigenvectors of the principal components show up in columns of U.
- Note that the axes may change sign (flip directions) between PCA runs using eigenvectors and svd.



Example PCA applications

- Examine and separate tastes in wine.
- Dimensions of manufactured parts.
 - Are more errors along certain dimensions?
- Epidemiology
- Genetics/bioinformatics



Session topics

- QR algorithm for eigenvalues
- Covariance matrix
 - Matrix is PSD
 - Zero off-diagonals indicate statistically independent data series.
 - Non-zero elements indicate correlation between corresponding data series.
- PCA
- Finds main axes of interesting dynamics
- Computed using eigenvalue decomposition.
- Or computed using SVD.