Portfolios that Contain Risky Assets
1.2. Covariance Matrices

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Portfolios that Contain Risky Assets
Part I: Portfolio Models

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1. Preliminary Topics

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1.2. Covariance Matrices

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Introduction

Suppose that we are considering return histories $\{r_i(d)\}_{d=1}^{D}$ for assets $i = 1, \cdots, N$ over a period of D trading days and assign day d a weight $w(d) > 0$ such that the weights $\{w(d)\}_{d=1}^{D}$ satisfy

$$\sum_{d=1}^{D} w(d) = 1 \,.$$

Then the return means, variances, and covariances are given by

$$
\begin{aligned}
m_i &= \sum_{d=1}^{D} w(d)\, r_i(d) \,, \\
v_{ij} &= \sum_{d=1}^{D} w(d)\, (r_i(d) - m_i)(r_j(d) - m_j) \,.
\end{aligned}
\tag{1.1}
$$

Introduction

The return history can be expressed as $\{\mathbf{r}(d)\}_{d=1}^{D}$ where

$$\mathbf{r}(d) = \begin{pmatrix} r_1(d) \\ \vdots \\ r_N(d) \end{pmatrix}.$$

The N-vector of return means $\mathbf{m}$ and the $N \times N$-matrix of return variances and covariances $\mathbf{V}$ then can be expressed as

$$\mathbf{m} = \begin{pmatrix} m_1 \\ \vdots \\ m_N \end{pmatrix} = \sum_{d=1}^{D} w(d)\,\mathbf{r}(d),$$

$$\mathbf{V} = \begin{pmatrix} v_{11} & \cdots & v_{1N} \\ \vdots & \ddots & \vdots \\ v_{N1} & \cdots & v_{NN} \end{pmatrix} = \sum_{d=1}^{D} w(d)\,(\mathbf{r}(d) - \mathbf{m})\,(\mathbf{r}(d) - \mathbf{m})^{\mathrm{T}}.$$

Introduction

We call **V** the *covariance matrix*. It also is called the *variance/covariance matrix* or the *variance matrix*.

The most important properties of **V**:

- *it is always symmetric,*
- *it is almost always positive definite*.
- *it can be diagonalized*.

These properties are taught in most elementary linear algebra courses, but they are so important that they will be reviewed in the next two sections. In subsequent sections these properties will be used to extract statistical information from **V**.

Symmetry and Definiteness (Review)

Here we review the notions of symmetric and definite matrices.

Definition 1. A real $N \times N$-matrix $\mathbf{A}$ is said to be *symmetric* if $\mathbf{A}^{\mathrm{T}} = \mathbf{A}$, where $\mathbf{A}^{\mathrm{T}}$ is the transpose of $\mathbf{A}$. It is said to be *nonnegative definite* or *positive semidefinite* if

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} \geq 0 \quad \text{for every } \mathbf{x} \in \mathbb{R}^N.$$

It is said to be *positive definite* if

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} > 0 \quad \text{for every nonzero } \mathbf{x} \in \mathbb{R}^N.$$

Remarks. Clearly, every positive definite matrix is nonnegative definite. A nonnegative definite matrix is positive definite if and only if

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = 0 \quad \implies \quad \mathbf{x} = \mathbf{0}. \tag{2.2}$$

Symmetry and Definiteness ($\mathbf{V}$ Nonnegative Definite)

Fact 1. The covariance matrix $\mathbf{V}$ is symmetric.

Proof. It is clear from (1.1) that $v_{ij} = v_{ji}$, whereby $\mathbf{V} = \mathbf{V}^{\mathrm{T}}$. □

Fact 2. The covariance matrix $\mathbf{V}$ is nonegative definite.

Proof. Let $\mathbf{x} \in \mathbb{R}^N$ be arbitrary. Then

$$
\begin{aligned}
\mathbf{x}^{\mathrm{T}}\mathbf{V}\mathbf{x} &= \mathbf{x}^{\mathrm{T}} \left(\sum_{d=1}^{D} w(d) \left(\mathbf{r}(d) - \mathbf{m}\right) \left(\mathbf{r}(d) - \mathbf{m}\right)^{\mathrm{T}} \right) \mathbf{x} \\
&= \sum_{d=1}^{D} w(d) \, \mathbf{x}^{\mathrm{T}} (\mathbf{r}(d) - \mathbf{m}) \left(\mathbf{r}(d) - \mathbf{m}\right)^{\mathrm{T}} \mathbf{x} \\
&= \sum_{d=1}^{D} w(d) \left((\mathbf{r}(d) - \mathbf{m})^{\mathrm{T}} \mathbf{x} \right)^2 \geq 0 \,.
\end{aligned}
$$

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Symmetry and Definiteness ($\mathbf{V}$ Positive Definite)

Fact 3. The covariance matrix $\mathbf{V}$ is positive definite if and only if the vectors $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ span $\mathbb{R}^N$.

Proof. Because $w(d) > 0$, the calculation in the previous proof shows that $\mathbf{x}^{\mathrm{T}}\mathbf{V}\mathbf{x} = 0$ if and only if

$$(\mathbf{r}(d) - \mathbf{m})^{\mathrm{T}}\mathbf{x} = 0 \quad \text{for every } d = 1, \cdots, D. \tag{2.3}$$

First, suppose that $\mathbf{V}$ is not positive definite. Then by (2.2) there exists an $\mathbf{x} \in \mathbb{R}^N$ such that $\mathbf{x}^{\mathrm{T}}\mathbf{V}\mathbf{x} = 0$ and $\mathbf{x} \neq \mathbf{0}$. This implies by (2.3) that the vectors $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ lie in the hyperplane orthogonal (normal) to $\mathbf{x}$. Therefore the vectors $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ do not span $\mathbb{R}^N$.

Conversely, suppose that the vectors $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ do not span $\mathbb{R}^N$. Then there must be a nonzero vector $\mathbf{x}$ that is orthogonal to their span. This implies that $\mathbf{x}$ satisfies (2.3), whereby $\mathbf{x}^{\mathrm{T}}\mathbf{V}\mathbf{x} = 0$. Therefore $\mathbf{V}$ is not positive definite by (2.2). ☐

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Symmetry and Definiteness (Need $D > N$)

Remark. The set of vectors $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ is linearly dependent because

$$\sum_{d=1}^{D} w(d)(\mathbf{r}(d) - \mathbf{m}) = \sum_{d=1}^{D} w(d)\mathbf{r}(d) - \mathbf{m} \sum_{d=1}^{D} w(d) = \mathbf{0}\,.$$

Therefore it can span $\mathbb{R}^N$ only if $D > N$. Hence, we require that $D > N$.

Remark. In practice D will be much larger than N. In the homework and projects for this course usually $N \leq 10$ while $D \geq 42$ (often $D = 252$). When D is so much greater than N the covariance matrix $\mathbf{V}$ will almost always be positive definite.

Symmetry and Definiteness (Two Spanning Conditions)

Remark. If $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ spans $\mathbb{R}^{N}$ then $\{\mathbf{r}(d)\}_{d=1}^{D}$ also spans $\mathbb{R}^{N}$. Indeed, if $\mathbf{x} \in \mathrm{Span}\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ then for some $\{a(d)\}_{d=1}^{D}$ we have

$$\mathbf{x} = \sum_{d=1}^{D} a(d)(\mathbf{r}(d) - \mathbf{m}) = \sum_{d=1}^{D} \left(a(d) - w(d) \sum_{d'=1}^{D} a(d') \right) \mathbf{r}(d).$$

Therefore $\mathbf{x} \in \mathrm{Span}\{\mathbf{r}(d)\}_{d=1}^{D}$. However, the converse need not hold. A counterexample for $N = 2$ and any $D > 2$ can be constructed as follows. Let $\{\mathbf{m}, \mathbf{n}\}$ span $\mathbb{R}^{2}$. Let $\mathbf{r}(d) = \mathbf{m} + h(d)\mathbf{n}$ where $h(d) \neq 0$ and

$$\sum_{d=1}^{D} w(d)h(d) = 0.$$

Then $\{\mathbf{r}(d)\}_{d=1}^{D}$ spans $\mathbb{R}^{2}$ while $\{\mathbf{r}(d) - \mathbf{m}\}_{d=1}^{D}$ does not span $\mathbb{R}^{2}$ because every $\mathbf{r}(d) - \mathbf{m}$ is proportional to $\mathbf{n}$.

Eigenpairs and Diagonalization (Eigenpairs)

Recall from linear algebra that an *eigenpair* $(\kappa, \mathbf{q})$ of a real $N \times N$ matrix $\mathbf{A}$ is a scalar κ (possibly complex) and a nonzero vector $\mathbf{q}$ (possibly with complex entries) such that

$$\mathbf{Aq} = \kappa \mathbf{q}. \tag{3.4}$$

An eigenpair is called a real eigenpair when κ and every entry of $\mathbf{q}$ is real.

Recall too that if $\mathbf{A}$ is real and symmetric then it has N real eigenpairs

$$(\kappa_1, \mathbf{q}_1), \quad (\kappa_2, \mathbf{q}_2), \quad \cdots \quad (\kappa_N, \mathbf{q}_N), \tag{3.5}$$

such that the eigenvectors $\{\mathbf{q}_i\}_{i=1}^N$ are an orthonormal set. This means that they satisfy the orthonormality conditions

$$\mathbf{q}_i^{\mathrm{T}} \mathbf{q}_j = \delta_{ij} \equiv \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \tag{3.6}$$

Eigenpairs and Diagonalization (Orthonormal Basis)

Because the $\{\mathbf{q}_i\}_{i=1}^N$ satisfy the orthonormality conditions (3.6), they form an orthonormal basis of $\mathbb{R}^N$. Every $\mathbf{x} \in \mathbb{R}^N$ can be expanded as

$$\mathbf{x} = \mathbf{q}_1 \, \mathbf{q}_1^{\mathrm{T}} \mathbf{x} + \mathbf{q}_2 \, \mathbf{q}_2^{\mathrm{T}} \mathbf{x} + \cdots + \mathbf{q}_N \, \mathbf{q}_N^{\mathrm{T}} \mathbf{x} \,. \tag{3.7}$$

The numbers $\{\mathbf{q}_i^{\mathrm{T}} \mathbf{x}\}_{i=1}^N$ are called the coordinates of $\mathbf{x}$ for the orthonormal basis $\{\mathbf{q}_i\}_{i=1}^N$. By multiplying (3.7) on the left by $\mathbf{x}^{\mathrm{T}}$ we see that the square of the Euclidean norm of $\mathbf{x}$ is given by

$$\|\mathbf{x}\|^2 = \mathbf{x}^{\mathrm{T}} \mathbf{x} = \left(\mathbf{q}_1^{\mathrm{T}} \mathbf{x}\right)^2 + \left(\mathbf{q}_2^{\mathrm{T}} \mathbf{x}\right)^2 + \cdots + \left(\mathbf{q}_N^{\mathrm{T}} \mathbf{x}\right)^2 \,. \tag{3.8}$$

Eigenpairs and Diagonalization (Orthonormal Basis)

Because the $\{\mathbf{q}_i\}_{i=1}^N$ are eigenvectors of $\mathbf{A}$, we see from (3.7) that

$$
\begin{aligned}
\mathbf{Ax} &= \mathbf{Aq}_1\,\mathbf{q}_1^{\mathrm{T}}\mathbf{x} + \mathbf{Aq}_2\,\mathbf{q}_2^{\mathrm{T}}\mathbf{x} + \cdots + \mathbf{Aq}_N\,\mathbf{q}_N^{\mathrm{T}}\mathbf{x} \\
&= \kappa_1\,\mathbf{q}_1\,\mathbf{q}_1^{\mathrm{T}}\mathbf{x} + \kappa_2\,\mathbf{q}_2\,\mathbf{q}_2^{\mathrm{T}}\mathbf{x} + \cdots + \kappa_N\,\mathbf{q}_N\,\mathbf{q}_N^{\mathrm{T}}\mathbf{x}\,.
\end{aligned}
\tag{3.9}
$$

Hence, the $\{\kappa_i\,\mathbf{q}_i^{\mathrm{T}}\mathbf{x}\}_{i=1}^N$ are the coordinates of $\mathbf{Ax}$ for the orthonormal basis $\{\mathbf{q}_i\}_{i=1}^N$. Therefore by (3.8) we have

$$
\|\mathbf{Ax}\|^2 = \kappa_1^2(\mathbf{q}_1^{\mathrm{T}}\mathbf{x})^2 + \kappa_2^2(\mathbf{q}_2^{\mathrm{T}}\mathbf{x})^2 + \cdots + \kappa_N^2(\mathbf{q}_N^{\mathrm{T}}\mathbf{x})^2\,.
\tag{3.10}
$$

Eigenpairs and Diagonalization (Definiteness)

Fact 4. If $\mathbf{A}$ is a real symmetric matrix then the properties of nonnegative definite and positive definite can be characterized as follows.

- $\mathbf{A}$ is nonnegative definite if and only if its eigenvalues are all nonnegative.

- $\mathbf{A}$ is positive definite if and only if its eigenvalues are all positive.

Proof. The ($\Longrightarrow$) directions of these characterizations follow from the fact that if $(\kappa, \mathbf{q})$ is an eigenpair of $\mathbf{A}$ that is normalized so that $\mathbf{q}^{\mathrm{T}}\mathbf{q} = 1$ then

$$\kappa = \kappa\,\mathbf{q}^{\mathrm{T}}\mathbf{q} = \mathbf{q}^{\mathrm{T}}(\kappa\mathbf{q}) = \mathbf{q}^{\mathrm{T}}(\mathbf{A}\mathbf{q}) = \mathbf{q}^{\mathrm{T}}\mathbf{A}\mathbf{q}\,.$$

Hence, if $\mathbf{A}$ is nonnegative definite then $\kappa \geq 0$ and if $\mathbf{A}$ is positive definite then $\kappa > 0$.

Eigenpairs and Diagonalization (Definiteness)

The ($\Longleftarrow$) directions of these characterizations use the full power of the orthonormality conditions (3.6) as embodied by expansion (3.9),

$$\mathbf{A}\mathbf{x} = \kappa_1 \mathbf{q}_1 \mathbf{q}_1^{\mathrm{T}}\mathbf{x} + \kappa_2 \mathbf{q}_2 \mathbf{q}_2^{\mathrm{T}}\mathbf{x} + \cdots + \kappa_N \mathbf{q}_N \mathbf{q}_N^{\mathrm{T}}\mathbf{x}.$$

By taking the scalar product of this expansion with $\mathbf{x}$ we obtain

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \kappa_1 (\mathbf{q}_1^{\mathrm{T}}\mathbf{x})^2 + \kappa_2 (\mathbf{q}_2^{\mathrm{T}}\mathbf{x})^2 + \cdots + \kappa_N (\mathbf{q}_N^{\mathrm{T}}\mathbf{x})^2.$$

It is thereby clear that:
- if $\kappa_i \geq 0$ for every $i = 1, \cdots, N$ then $\mathbf{A}$ is nonnegative definite;
- if $\kappa_i > 0$ for every $i = 1, \cdots, N$ then $\mathbf{A}$ is positive definite.

This proves the ($\Longleftarrow$) directions of the characterizations. □

Eigenpairs and Diagonalization (Diagonalization)

Fact 5. Expansion (3.9) shows that if **A** is a real symmetric $N \times N$ matrix then it can be expressed in the factored form

$$\mathbf{A} = \mathbf{Q}\mathbf{D}\mathbf{Q}^{\mathrm{T}}, \tag{3.11}$$

where **D** and **Q** are the real $N \times N$ matrices constructed from the real eigenpairs (3.5) as

$$\mathbf{D} = \begin{pmatrix} \kappa_1 & 0 & \cdots & 0 \\ 0 & \kappa_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \kappa_N \end{pmatrix}, \qquad \mathbf{Q} = \begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_N \end{pmatrix}. \tag{3.12}$$

This factorization is called a diagonalization of **A** because **D** is a diagonal.

Eigenpairs and Diagonalization ($\mathbf{Q}$ is Orthogonal)

The matrix $\mathbf{Q}$ constructed from the eigenvectors $\{\mathbf{q}_i\}_{i=1}^N$ by (3.12) satisfies the relations

$$\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I} = \mathbf{Q}\mathbf{Q}^{\mathrm{T}}. \tag{3.13}$$

- $\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I}$ is a recasting of the orthonormality conditions (3.6).
- $\mathbf{I} = \mathbf{Q}\mathbf{Q}^{\mathrm{T}}$ is equivalent to $\mathbf{x} = \mathbf{Q}\mathbf{Q}^{\mathrm{T}}\mathbf{x}$, which is a recasting of expansion (3.7).
- Relations (3.13) show that $\mathbf{Q}$ and $\mathbf{Q}^{\mathrm{T}}$ are inverses of each other — i.e. that $\mathbf{Q}^{-1} = \mathbf{Q}^{\mathrm{T}}$ and that $\mathbf{Q}^{-\mathrm{T}} = \mathbf{Q}$.
- They imply that the factored form (3.11) is equivalent to $\mathbf{AQ} = \mathbf{QD}$.

Any matrix $\mathbf{Q}$ satisfying relations (3.13) is called an orthogonal matrix.

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Eigenpairs and Diagonalization (By Matlab)

The eigenpairs of a matrix **A** can be approximated numerically with the Matlab command "eig". Specifically, if the $N \times N$ matrix **A** is stored as A then the command line

$$> [Q,D] = eig(A);$$

will return a diagonal matrix D of eigenvalues and an orthogonal matrix Q whose columns are corresponding eigenvectors — i.e. so that AQ = QD.

Remark. The Matlab command "eig" computes eigenpairs of positive definite matrices using the QR algorithm. This algorithm is often covered in graduate courses on numerical methods. It will not be presented here. However, significant errors in the smaller eigenvalues can arise when the ratio of the largest to the smallest eigenvalue is large. This ratio is the *condition number* of **A**.

Remark. The R command "eigen" is similar.

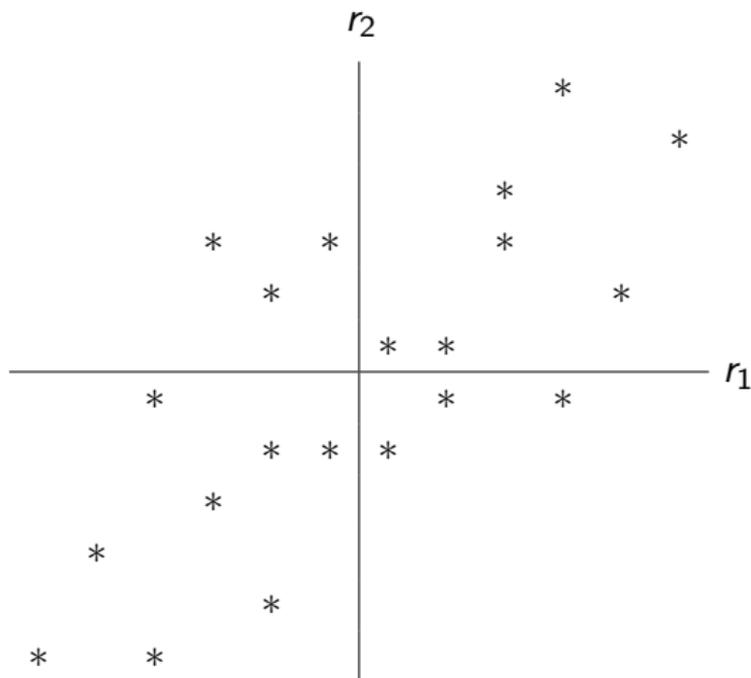## Statistical Interpretation ($N = 2$ Examples)

In order to illustrate the statistical information contained in the return mean vector $\mathbf{m}$ and return covariance matrix $\mathbf{V}$, we consider the case $N = 2$ and $D = 21$. Given the return history $\{(r_1(d), r_2(d))\}_{d=1}^{21}$, the vector $\mathbf{m}$ and matrix $\mathbf{V}$ computed with uniform weights are

$$\mathbf{m} = \begin{pmatrix} m_1 \\ m_2 \end{pmatrix} = \frac{1}{21} \sum_{d=1}^{21} \begin{pmatrix} r_1(d) \\ r_2(d) \end{pmatrix} \,,$$

$$\mathbf{V} = \begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} = \frac{1}{21} \sum_{d=1}^{21} \begin{pmatrix} \tilde{r}_1(d)^2 & \tilde{r}_1(d)\tilde{r}_2(d) \\ \tilde{r}_2(d)\tilde{r}_1(d) & \tilde{r}_2(d)^2 \end{pmatrix} \,,$$

where $\tilde{r}_1(d) = r_1(d) - m_1$ and $\tilde{r}_2(d) = r_2(d) - m_2$.

Example 1. Suppose that when the return history $\{(r_1(d), r_2(d))\}_{d=1}^{21}$ is plotted as points in the $r_1 r_2$-plane we obtain the plot on the next slide.

Statistical Interpretation ($N = 2$ Examples)

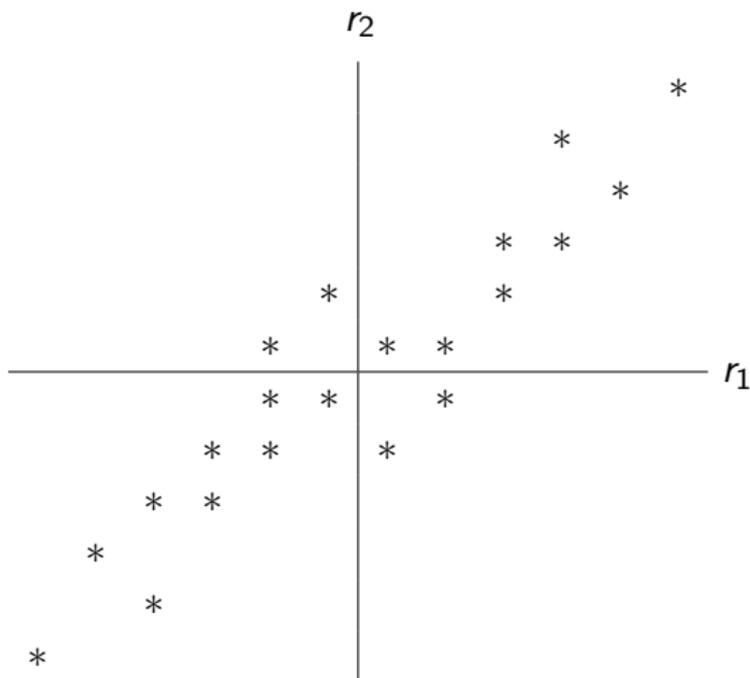## Statistical Interpretation ($N = 2$ Examples)

This so-called *scatter plot* shows a distribution of points clustered about the origin in a way that favors the first and third quadrants.

- The vector $\mathbf{m}$ gives the center of the cluster. It lies in the third quadrant close to the origin.
- The matrix $\mathbf{V}$ will have eigenvectors that are roughly parallel to $\nearrow$ and to $\nwarrow$. The eigenvalue associated with $\nearrow$ will be greater than the one associated with $\nwarrow$. Their square roots give the spread of the data from $\mathbf{m}$ in their respective eigendirections.

This is how $\mathbf{m}$ and $\mathbf{V}$ tell us that the points are clustered about the origin in a way that favors the first and third quadrants.

Example 2. Now suppose that when the return history $\{(r_1(d), r_2(d))\}_{d=1}^{21}$ is plotted as points in the $r_1 r_2$-plane we instead obtain the scatter plot on the next slide.

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Statistical Interpretation ($N = 2$ Examples)

Statistical Interpretation ($N = 2$ Examples)

In this scatter plot r_1 and r_2 are more highly correlated than in the first.

- The vector **m** is almost the same as it was for the first scatter plot. It lies in the third quadrant close to the origin.

- The matrix **V** again has eigenvectors that are roughly parallel to $\nearrow$ and to $\nwarrow$. However now the eigenvalue associated with $\nearrow$ is *very much greater* than the one associated with $\nwarrow$. Their square roots give the spread of the data from **m** in their respective eigendirections.

Both the scatter plot and the analysis of **m** and **V** suggest that the points $\{(r_1(d), r_2(d))\}_{d=1}^{21}$ cluster along a line.

Statistical Interpretation (One Dimensional Behavior)

If eigenvectors associated with the largest eigenvalue of $\mathbf{V}$ are proportional to $(1, b)$ then the points in the $r_1 r_2$-plane are clustered along the line

$$r_2 - m_2 = b(r_1 - m_1).$$

This suggests $r_2(d)$ could be modeled as

$$r_2(d) - m_2 = b(r_1(d) - m_1) + z(d),$$

where $z(d)$ are small random numbers that on average sum to zero.

Remark. Scatter plots become harder to visualize as N grows beyond 3. However the eigenpair analysis of $\mathbf{V}$ can be carried out easily for much larger N.

Principal Component Analysis (Eigenpairs of **V**)

In statistics the eigenpair analysis of the covariance matrix **V** is called *Principal Component Analysis (PCA)*.

A principal component analysis of **V** yields N eigenpairs

$$(\kappa_1, \mathbf{q}_1), \quad (\kappa_2, \mathbf{q}_2), \quad \cdots, \quad (\kappa_N, \mathbf{q}_N). \qquad (5.14)$$

The eigenvalues will almost always be distinct, in which case we will order them as

$$\kappa_1 > \kappa_2 > \cdots > \kappa_N > 0. \qquad (5.15)$$

In this case the eigenvectors will be unique up to a nonzero factor. If they are normalized so that $\|\mathbf{q}_i\| = 1$ then they are unique up to a factor of ± 1 and $\{\mathbf{q}_i\}_{i=1}^{N}$ will be an orthonormal basis of $\mathbb{R}^N$.

Principal Component Analysis (Components)

Let $\mathbf{D}$ and $\mathbf{Q}$ be the diagonal and orthogonal matrices constructed from the eigenpairs (5.14) as in (3.12). Then $\mathbf{V} = \mathbf{Q}\mathbf{D}\mathbf{Q}^{\mathrm{T}}$ and $\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{Q}\mathbf{Q}^{\mathrm{T}} = \mathbf{I}$.

Then the underlying return history $\{\mathbf{r}(d)\}_{d=1}^{D}$ can be transformed into the history $\{\mathbf{p}(d)\}_{d=1}^{D}$ where

$$\mathbf{p}(d) = \mathbf{Q}^{\mathrm{T}}\mathbf{r}(d) \,.$$

The entries of $\mathbf{p}(d)$ are called the *principle components* of $\mathbf{r}(d)$.

Their mean vector is given by

$$\sum_{d=1}^{D} w(d)\mathbf{p}(d) = \sum_{d=1}^{D} w(d)\mathbf{Q}^{\mathrm{T}}\mathbf{r}(d) = \mathbf{Q}^{\mathrm{T}}\left(\sum_{d=1}^{D} w(d)\mathbf{r}(d)\right) = \mathbf{Q}^{\mathrm{T}}\mathbf{m} \,.$$

Principal Component Analysis (Diagonal Covariance)

Similarly, their covariance matrix is given by

$$\sum_{d=1}^{D} w(d)(\mathbf{p}(d) - \mathbf{Q}^{\mathrm{T}}\mathbf{m})(\mathbf{p}(d) - \mathbf{Q}^{\mathrm{T}}\mathbf{m})^{\mathrm{T}}$$

$$= \mathbf{Q}^{\mathrm{T}}\left(\sum_{d=1}^{D} w(d)(\mathbf{r}(d) - \mathbf{m})(\mathbf{r}(d) - \mathbf{m})^{\mathrm{T}}\right)\mathbf{Q}$$

$$= \mathbf{Q}^{\mathrm{T}}\mathbf{V}\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}(\mathbf{Q}\mathbf{D}\mathbf{Q}^{\mathrm{T}})\mathbf{Q} = (\mathbf{Q}^{\mathrm{T}}\mathbf{Q})\mathbf{D}(\mathbf{Q}^{\mathrm{T}}\mathbf{Q}) = \mathbf{D}\,.$$

Because the ith entry of $\mathbf{p}(d)$ is $\mathbf{q}_i^{\mathrm{T}}\mathbf{r}(d)$, its variance is κ_i. Because $\mathbf{D}$ is a diagonal matrix, the covariance of distinct entries of $\mathbf{p}(d)$ vanishes. Thus, distinct principle components of the data are uncorrelated.

Principal Component Analysis (Summary)

Therefore PCA can be viewed as an orthogonal coordinate transformation that maps the data into new coordinates (the principal components) that are uncorrelated and such that the first entry has the largest variance, the second entry has the second largest variance, and so on.

Remark. The vectors $\mathbf{q}_i$ are called the *principal component coefficients* because they are the vectors whose scalar product with the data $\mathbf{r}(d)$ gives the principle components. They are also called *loadings*.

Remark. Principal component analysis is related to a weighted singular value decomposition (SVD) of the $N \times D$ matrix

$$\mathbf{R} = \begin{pmatrix} \mathbf{r}(1) - \mathbf{m} & \mathbf{r}(2) - \mathbf{m} & \cdots & \mathbf{r}(D) - \mathbf{m} \end{pmatrix}.$$

This is because $\mathbf{V} = \mathbf{R}\mathbf{W}\mathbf{R}^{\mathrm{T}}$ where $\mathbf{W}$ is the $D \times D$ diagonal matrix with the weights $w(d)$ on the diagonal.

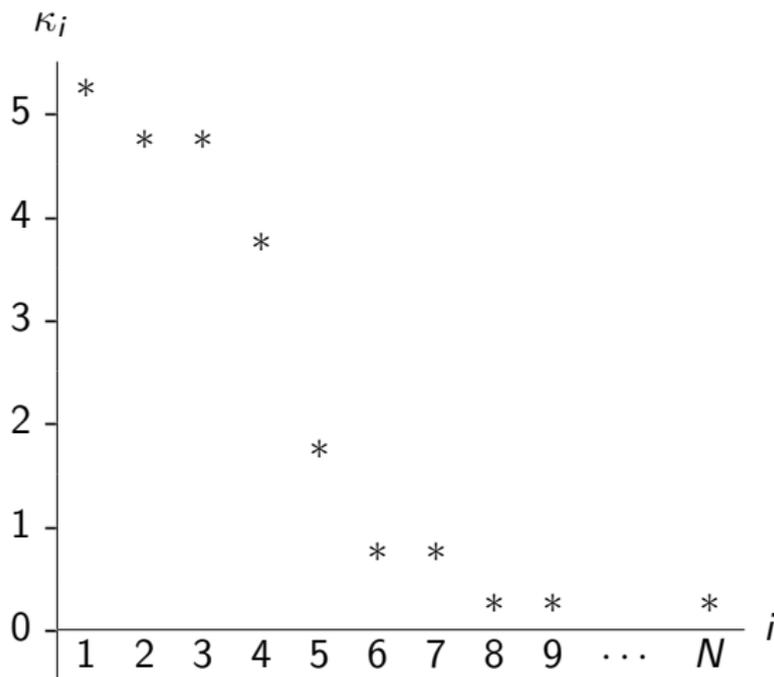## Dimension of the Data (Introduction)

One application of PCA is to explore possible lower dimensional models
that capture the bulk of the variation in the data. The dimension of such
a model can be found by selecting a subset of the larger eigenvalues of **V**.
There are many ways in which this can be done.

For example, suppose that the eigenvalues of **V** are ordered as

$$\kappa_1 \geq \kappa_2 \geq \cdots \geq \kappa_{N-1} \geq \kappa_N > 0\,,$$

and that a plot of κ_i versus i looks like the figure on the next slide.

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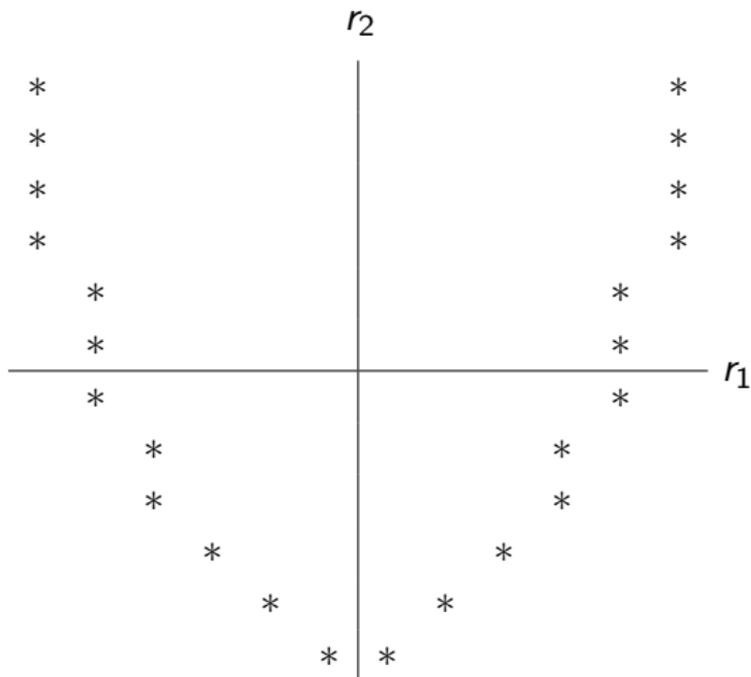## Dimension of the Data (Example Graph)

Dimension of the Data (Example Discussion)

This figure shows that the underlying data has four major dimensions and that eigenvalues are negligible for $i \geq 8$. It suggests that the data might be captured well with a 4, 5, or 7 dimensional model.

- A 4 dimensional model is suggested by the fact that the gap $\kappa_4 - \kappa_5$ is larger than the gap between any other pair of adjacent eigenvalues.
- A 7 dimension model is suggested by the fact that the ratio κ_7/κ_8 is larger than the ratio between any other pair of adjacent eigenvalues.
- A 5 or 7 dimension model might be suggested by the fact that the ratio κ_6/κ_1 is below .2 or the fact that the ratio κ_8/κ_1 is below .1. The threshold chosen is arbitrary, but should be small.

Remark. Dimensions obtained by these methods may not be the actual dimension of the data, which can be much lower when the data satisfies an approximate nonlinear relationship. Such a relationship is illustrated on the next slide for two dimensional data.

Intro
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Sym and Def
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Eigen and Diag
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Stat Interp
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PCA
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Data Dim
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Dimension of the Data (Nonlinear Dependence Example)

Intro
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Sym and Def
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Eigen and Diag
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Stat Interp
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PCA
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Data Dim
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Dimension of the Data (Summary)

This figure shows that the underlying data lies along a parabola-like curve, whereby it is one dimensional. However, principle component analysis does not see this because the 2×2 matrix **V** has two comparable eigenvalues.

Remark. This use of PCA is called *exploritory analysis.* While it can show that data behaves like its dimension is lower than N, it typically does not give a unique value for the lower dimension. However, it usually does give a small set of candidates for the lower dimension that can be evaluated by other criteria.