# More Linear Algebra<sup>1</sup> STA 302: Fall 2020

<sup>&</sup>lt;sup>1</sup>See Chapter 2 of *Linear models in statistics* for more detail. This slide show is an open-source document. See last slide for copyright information.

# Overview

- 1 Things you already know
- 2 Trace
- (3) Spectral decomposition
- 4 Positive definite
- **5** Square root matrices
- 6 Extras



# You already know about

- Matrices  $\mathbf{A} = (a_{ij})$
- Matrix addition and subtraction  $\mathbf{A} + \mathbf{B} = (a_{ij} + b_{ij})$
- Column vectors  $\mathbf{v} = (v_j)$
- Scalar multiplication  $a\mathbf{B} = (a b_{ij})$

• Matrix multiplication 
$$\mathbf{AB} = \left(\sum_{k} a_{ik} b_{kj}\right)$$

In words: The i, j element of **AB** is the inner product of row i of **A** with column j of **B**.

- Inverse  $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$
- Transpose  $\mathbf{A}' = (a_{ji})$
- Symmetric matrices  $\mathbf{A} = \mathbf{A}'$
- Determinants
- Linear independence

# Inverses: Proving $\mathbf{B} = \mathbf{A}^{-1}$

- $\mathbf{B} = \mathbf{A}^{-1}$  means  $\mathbf{A}\mathbf{B} = \mathbf{B}\mathbf{A} = \mathbf{I}$ .
- It looks like you have two things to show.
- But if **A** and **B** are square matrices of the same size, you only need to do it in one direction.

### Theorem

If **A** and **B** are square matrices and AB = I, then **A** and **B** are inverses.

**Proof**: Suppose AB = I

• A and B must both have inverses, for otherwise  $|AB| = |A| |B| = 0 \neq |I| = 1$ . Now,

•  $AB = I \Rightarrow ABB^{-1} = IB^{-1} \Rightarrow A = B^{-1}.$ 

•  $AB = I \Rightarrow A^{-1}AB = A^{-1}I \Rightarrow B = A^{-1}.$ 

# How to show $\mathbf{A}^{-1\prime} = \mathbf{A}^{\prime-1}$

- Let  $\mathbf{B} = \mathbf{A}^{-1}$ .
- Want to prove that **B**' is the inverse of **A**'.
- It is enough to show that  $\mathbf{B'A'} = \mathbf{I}$ .
- $AB = I \Rightarrow B'A' = I' = I$

# Three mistakes that will get you a zero Numbers are $1 \times 1$ matrices, but larger matrices are not just numbers.

You will get a zero if you

- Write AB = BA. It's not true in general.
- Write  $\mathbf{A}^{-1}$  when  $\mathbf{A}$  is not a square matrix. The inverse is not even defined.
- Represent the inverse of a matrix (even if it exists) by writing it in the denominator, like  $\mathbf{a'B^{-1}a} = \frac{\mathbf{a'a}}{\mathbf{B}}$ . Matrices are not just numbers.

If you commit one of these crimes, the mark for the question (or part of a question, like 3c) is zero, regardless of what else you write.

### Half marks off, at least

You will lose at least half marks for writing a product like AB when the number of colmns in A does not equal the number of rows in B.

### Linear combination of vectors

Let  $\mathbf{x}_1, \ldots, \mathbf{x}_p$  be  $n \times 1$  vectors and  $a_1, \ldots, a_p$  be scalars. A *linear combination* is



### Linear independence

A set of vectors  $\mathbf{x}_1, \ldots, \mathbf{x}_p$  is said to be *linearly dependent* if there is a set of scalars  $a_1, \ldots, a_p$ , not all zero, with

$$a_1 \begin{pmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n1} \end{pmatrix} + a_2 \begin{pmatrix} x_{12} \\ x_{22} \\ \vdots \\ x_{n2} \end{pmatrix} + \dots + a_p \begin{pmatrix} x_{1p} \\ x_{2p} \\ \vdots \\ x_{np} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

If no such constants  $a_1, \ldots, a_p$  exist, the vectors are linearly independent. That is,

If  $a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \cdots + a_p\mathbf{x}_p = \mathbf{0}$  implies  $a_1 = a_2 \cdots = a_p = 0$ , then the vectors are said to be *linearly independent*.

### Bind the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_p$ into a matrix

$$a_{1}\mathbf{x}_{1} + a_{2}\mathbf{x}_{2} + \cdots + a_{p}\mathbf{x}_{p}$$

$$= \begin{pmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n1} \end{pmatrix} a_{1} + \begin{pmatrix} x_{12} \\ x_{22} \\ \vdots \\ x_{n2} \end{pmatrix} a_{2} + \cdots + \begin{pmatrix} x_{1p} \\ x_{2p} \\ \vdots \\ x_{np} \end{pmatrix} a_{p}$$

$$= \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & n_{np} \end{pmatrix} \begin{pmatrix} a_{1} \\ a_{2} \\ \vdots \\ a_{p} \end{pmatrix}$$

= Xa

A more convenient definition of linear independence  $a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \cdots + a_p\mathbf{x}_p = \mathbf{X}\mathbf{a}$ 

Let **X** be an  $n \times p$  matrix of constants. The columns of **X** are said to be *linearly dependent* if there exists  $\mathbf{a} \neq \mathbf{0}$  with  $\mathbf{X}\mathbf{a} = \mathbf{0}$ . We will say that the columns of **X** are linearly *independent* if  $\mathbf{X}\mathbf{a} = \mathbf{0}$  implies  $\mathbf{a} = \mathbf{0}$ .

For example, show that  $\mathbf{B}^{-1}$  exists implies that the columns of  $\mathbf{B}$  are linearly independent.

$$\mathbf{B}\mathbf{a} = \mathbf{0} \Rightarrow \mathbf{B}^{-1}\mathbf{B}\mathbf{a} = \mathbf{B}^{-1}\mathbf{0} \Rightarrow \mathbf{a} = \mathbf{0}.$$

### Trace of a square matrix: Sum of the diagonal elements

$$tr(\mathbf{A}) = \sum_{i=1}^{n} a_{i,i}.$$

- Obvious:  $tr(\mathbf{A} + \mathbf{B}) = tr(\mathbf{A}) + tr(\mathbf{B})$ .
- Not obvious:  $tr(\mathbf{AB}) = tr(\mathbf{BA})$
- Even though  $AB \neq BA$

### $tr(\mathbf{AB}) = tr(\mathbf{BA})$ Let $\mathbf{A}$ be $p \times q$ and $\mathbf{B}$ be $q \times p$ , so that $\mathbf{AB}$ is $p \times p$ and $\mathbf{BA}$ is $q \times q$ .

First, agree that  $\sum_{i=1}^{n} x_i = \sum_{j=1}^{n} x_j$ .

$$tr(\mathbf{AB}) = tr(\left(\sum_{k=1}^{q} a_{ik} b_{kj}\right))$$
$$= \sum_{i=1}^{p} \sum_{k=1}^{q} \frac{a_{ik} b_{ki}}{\sum_{k=1}^{q} \sum_{i=1}^{p} b_{ki} a_{ik}}$$
$$= \sum_{i=1}^{q} \sum_{k=1}^{p} b_{ik} a_{ki}$$
$$= tr(\left(\sum_{k=1}^{p} b_{ik} a_{kj}\right))$$
$$= tr(\mathbf{BA})$$

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### Example

Let 
$$\mathbf{A} = \begin{pmatrix} 2 & 1 & 0 \\ 5 & -4 & 3 \end{pmatrix}$$
 and  $\mathbf{B} = \begin{pmatrix} 1 & 0 \\ 2 & 3 \\ -1 & 3 \end{pmatrix}$ 

$$\mathbf{AB} = \begin{pmatrix} 4 & 3 \\ -6 & -3 \end{pmatrix}$$
$$\mathbf{BA} = \begin{pmatrix} 2 & 1 & 0 \\ 19 & -10 & 9 \\ 13 & -13 & 9 \end{pmatrix}$$

And  $tr(\mathbf{AB}) = tr(\mathbf{BA})$ .

### Eigenvalues and eigenvectors

Let  $\mathbf{A} = (a_{i,j})$  be an  $n \times n$  matrix, so that the following applies to square matrices.  $\mathbf{A}$  is said to have an *eigenvalue*  $\lambda$  and (non-zero) *eigenvector*  $\mathbf{x}$  corresponding to  $\lambda$  if

$$\mathbf{A}\mathbf{x} = \lambda \mathbf{x}.$$

- Eigenvalues are the  $\lambda$  values that solve the determinantal equation  $|\mathbf{A} \lambda \mathbf{I}| = 0$ .
- The determinant is the product of the eigenvalues:  $|\mathbf{A}| = \prod_{i=1}^{n} \lambda_i$

### Spectral decomposition of symmetric matrices

The Spectral decomposition theorem says that every square and symmetric matrix  $\mathbf{A} = (a_{i,j})$  may be written

$$\mathbf{A} = \mathbf{C}\mathbf{D}\mathbf{C}',$$

where the columns of **C** (which may also be denoted  $\mathbf{x}_1, \ldots, \mathbf{x}_n$ ) are the eigenvectors of **A**, and the diagonal matrix **D** contains the corresponding eigenvalues.

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

The eigenvectors may be chosen to be orthonormal, so that  $\mathbf{C}$  is an orthogonal matrix. That is,  $\mathbf{CC}' = \mathbf{C}'\mathbf{C} = \mathbf{I}$ .

# Positive definite matrices

### The $n \times n$ matrix **A** is said to be *positive definite* if

### $\mathbf{y}'\mathbf{A}\mathbf{y} > 0$

for all  $n \times 1$  vectors  $\mathbf{y} \neq \mathbf{0}$ . It is called *non-negative definite* (or sometimes positive semi-definite) if  $\mathbf{y}' \mathbf{A} \mathbf{y} \ge 0$ .

### Example: Show $\mathbf{X}'\mathbf{X}$ non-negative definite

Let **X** be an  $n \times p$  matrix of real constants and let **y** be  $p \times 1$ . Then  $\mathbf{z} = \mathbf{X}\mathbf{y}$  is  $n \times 1$ , and

$$\mathbf{y}' (\mathbf{X}'\mathbf{X}) \mathbf{y}$$

$$= (\mathbf{X}\mathbf{y})' (\mathbf{X}\mathbf{y})$$

$$= \mathbf{z}' \mathbf{z}$$

$$= \sum_{i=1}^{n} z_i^2 \ge 0 \quad \blacksquare$$

Some properties of symmetric positive definite matrices Variance-covariance matrices are often assumed positive definite.

For a symmetric matrix,

```
Positive definite

\downarrow

All eigenvalues positive

\downarrow

Inverse exists \Leftrightarrow Columns (rows) linearly independent.
```

If a real symmetric matrix is also non-negative definite, as a variance-covariance matrix *must* be, Inverse exists  $\Rightarrow$  Positive definite

### Showing Positive definite $\Rightarrow$ Eigenvalues positive

Let the  $p \times p$  matrix **A** be positive definite, so that  $\mathbf{y}' \mathbf{A} \mathbf{y} > 0$  for all  $\mathbf{y} \neq \mathbf{0}$ .

 $\lambda$  an eigenvalue means  $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ , with  $\mathbf{x}'\mathbf{x} = 1$ .

 $\Rightarrow 0 < \mathbf{x}' \mathbf{A} \mathbf{x} = \mathbf{x}' \lambda \mathbf{x} = \lambda \mathbf{x}' \mathbf{x} = \lambda.$ 

# Inverse of a diagonal matrix To set things up

Suppose  $\mathbf{D} = (d_{i,j})$  is a diagonal matrix with non-zero diagonal elements. It is easy to verify that

$$\begin{pmatrix} d_{1,1} & 0 & \cdots & 0 \\ 0 & d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_{n,n} \end{pmatrix} \begin{pmatrix} 1/d_{1,1} & 0 & \cdots & 0 \\ 0 & 1/d_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/d_{n,n} \end{pmatrix} = \mathbf{I}$$

So  $\mathbf{D}^{-1}$  exists.

### Showing Eigenvalues positive $\Rightarrow$ Inverse exists For a symmetric, positive definite matrix

Let  $\mathbf{A}$  be symmetric and positive definite. Then  $\mathbf{A} = \mathbf{CDC'}$ , and its eigenvalues are positive.

Let  $\mathbf{B} = \mathbf{C}\mathbf{D}^{-1}\mathbf{C}'$ . Show  $\mathbf{B} = \mathbf{A}^{-1}$ .

 $\mathbf{AB} = \mathbf{CDC}' \mathbf{CD}^{-1}\mathbf{C}' = \mathbf{I}$ 

 $\operatorname{So}$ 

$$\mathbf{A}^{-1} = \mathbf{C}\mathbf{D}^{-1}\mathbf{C}'$$

### Square root matrices For symmetric, non-negative definite matrices

To set things up, define

$$\mathbf{D}^{1/2} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0\\ 0 & \sqrt{\lambda_2} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix}$$

So that

$$\mathbf{D}^{1/2}\mathbf{D}^{1/2} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix} \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \end{pmatrix}$$
$$= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \mathbf{D}$$

### For a non-negative definite, symmetric matrix $\mathbf{A}$ So that $\mathbf{A} = \mathbf{CDC'}$

### Define

$$\mathbf{A}^{1/2} = \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}'$$

So that

$$\begin{aligned} \mathbf{A}^{1/2} \mathbf{A}^{1/2} &= \mathbf{C} \mathbf{D}^{1/2} \mathbf{C}' \mathbf{C} \mathbf{D}^{1/2} \mathbf{C}' \\ &= \mathbf{C} \mathbf{D}^{1/2} \mathbf{I} \mathbf{D}^{1/2} \mathbf{C}' \\ &= \mathbf{C} \mathbf{D}^{1/2} \mathbf{D}^{1/2} \mathbf{C}' \\ &= \mathbf{C} \mathbf{D} \mathbf{C}' \\ &= \mathbf{A} \end{aligned}$$

# The square root of the inverse is the inverse of the square root

Let **A** be symmetric and positive definite, with  $\mathbf{A} = \mathbf{CDC'}$ . Let  $\mathbf{B} = \mathbf{CD}^{-1/2}\mathbf{C'}$ . What is  $\mathbf{D}^{-1/2}$ ? Show  $\mathbf{B} = (\mathbf{A}^{-1})^{1/2}$ .  $\mathbf{BB} = \mathbf{CD}^{-1/2}\mathbf{C'}\mathbf{CD}^{-1/2}\mathbf{C'}$  $= \mathbf{CD}^{-1}\mathbf{C'} = \mathbf{A}^{-1}$ 

Show 
$$\mathbf{B} = (\mathbf{A}^{1/2})^{-1}$$
  
 $\mathbf{A}^{1/2}\mathbf{B} = \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}' \mathbf{C}\mathbf{D}^{-1/2}\mathbf{C}' = \mathbf{I}$ 

Just write  $\mathbf{A}^{-1/2} = \mathbf{C}\mathbf{D}^{-1/2}\mathbf{C}'$ 

Extras You may not know about these, and we may use them occasionally

- Rank
- Partitioned matrices

# Rank

- Row rank is the number of linearly independent rows.
- Column rank is the number of linearly independent columns.
- Rank of a matrix is the minimum of row rank and column rank.
- $rank(\mathbf{AB}) = \min(rank(\mathbf{A}), rank(\mathbf{B})).$

### Partitioned matrix

### • A matrix of matrices

# $\left[ \begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{C} & \mathbf{D} \end{array} \right]$

• Row by column (matrix) multiplication works, provided the matrices are the right sizes.

### Matrix calculation with R

> is.matrix(3) # Is the number 3 a 1x1 matrix?

[1] FALSE

#### > treecorr = cor(trees); treecorr

Girth Height Volume Girth 1.000000 0.5192801 0.9671194 Height 0.5192801 1.000000 0.5982497 Volume 0.9671194 0.5982497 1.000000

> is.matrix(treecorr)

[1] TRUE

### Creating matrices Bind rows into a matrix

```
> # Bind rows of a matrix together
> A = rbind(c(3, 2, 6, 8)),
            c(2,10,-7,4),
+
+
            c(6, 6, 9,1) ); A
    [,1] [,2] [,3] [,4]
[1,]
    3 2 6
                    8
[2,] 2 10 -7 4
                    1
[3,]
      6
           6 9
> # Transpose
> t(A)
    [,1] [,2] [,3]
[1,]
      3 2
               6
[2,]
      2 10
               6
[3,] 6
               9
        -7
               1
[4,]
       8
           4
```

# Matrix multiplication Remember, $\mathbf{A}$ is $3 \times 4$

```
> # U = AA' (3x3), V = A'A (4x4)
> U = A % * % t(A)
> V = t(A) %*% A; V
     [,1] [,2] [,3] [,4]
[1,]
       49
            62
                 58
                       38
[2,]
               -4
       62
           140
                       62
[3,]
       58
           -4
                166
                      29
[4,]
       38
            62
                 29
                       81
```

### Determinants

[1] 1490273 [1] -3.622862e-09

Inverse of  $\mathbf{U}$  exists, but inverse of  $\mathbf{V}$  does not.

### Inverses

- The solve function is for solving systems of linear equations like Mx = b.
- Just typing solve(M) gives  $M^{-1}$ .

```
> # Recall U = AA' (3x3), V = A'A (4x4)
> solve(U)
```

	[,1]	[,2]	[,3]
[1,]	0.0173505123	-8.508508e-04	-1.029342e-02
[2,]	-0.0008508508	5.997559e-03	2.013054e-06
[3,]	-0.0102934160	2.013054e-06	1.264265e-02

### > solve(V)

```
Error in solve.default(V) :
    system is computationally singular: reciprocal condition
    number = 6.64193e-18
```

### Eigenvalues and eigenvectors

```
> # Recall U = AA' (3x3), V = A'A (4x4)
```

```
> eigen(U)
```

\$values
[1] 234.01162 162.89294 39.09544

#### \$vectors

	[,1]	[,2]	[,3]
[1,]	-0.6025375	0.1592598	0.78203893
[2,]	-0.2964610	-0.9544379	-0.03404605
[3,]	-0.7409854	0.2523581	-0.62229894

V should have at least one zero eigenvalue Because A is  $3 \times 4$ ,  $\mathbf{V} = \mathbf{A}'\mathbf{A}$ , and the rank of a product is the minimum rank of the matrices.

#### > eigen(V)

\$values

[1] 2.340116e+02 1.628929e+02 3.909544e+01 -1.012719e-14

#### \$vectors

	[,1]	[,2]	[,3]	[,4]
[1,]	-0.4475551	0.006507269	-0.2328249	0.863391352
[2,]	-0.5632053	-0.604226296	-0.4014589	-0.395652773
[3,]	-0.5366171	0.776297432	-0.1071763	-0.312917928
[4,]	-0.4410627	-0.179528649	0.8792818	0.009829883

# Spectral decomposition $\mathbf{V} = \mathbf{CDC'}$

```
> eigenV = eigen(V)
> C = eigenV$vectors; D = diag(eigenV$values); D
```

	[,1]	[,2]	[,3]	[,4]
[1,]	234.0116	0.0000	0.00000	0.000000e+00
[2,]	0.0000	162.8929	0.00000	0.000000e+00
[3,]	0.0000	0.0000	39.09544	0.000000e+00
[4,]	0.0000	0.0000	0.00000	-1.012719e-14

```
> # C is an orthoganal matrix
> C %*% t(C)
```

[,1] [,2] [,3] [,4] [1,] 1.00000e+00 5.551115e-17 0.000000e+00 -3.989864e-17 [2,] 5.551115e-17 1.000000e+00 2.636780e-16 3.556183e-17 [3,] 0.00000e+00 2.636780e-16 1.000000e+00 2.558717e-16 [4,] -3.989864e-17 3.556183e-17 2.558717e-16 1.000000e+00

# Verify $\mathbf{V} = \mathbf{CDC}'$

### > V; C %\*% D %\*% t(C)

[1,] [2,] [3,] [4,]	[,1] 49 62 58 38	[,2] 62 140 -4 62	[,3] 58 -4 166 29	[,4] 38 62 29 81
[1,]	[,1] 49	[,2] 62	[,3] 58	[,4] 38
[2,]	62	140	-4	62
[3,]	58	-4	166	29
[4,]	38	62	29	81

# Square root matrix $\mathbf{V}^{1/2} = \mathbf{C}\mathbf{D}^{1/2}\mathbf{C}'$

```
> sqrtV = C %*% sqrt(D) %*% t(C)
```

```
Warning message:
In sqrt(D) : NaNs produced
```

```
> # Multiply to get V
> sqrtV %*% sqrtV; V
```

	[,1]	[,2]	[,3]	[,4]
[1,]	NaN	NaN	NaN	NaN
[2,]	NaN	NaN	NaN	NaN
[3,]	NaN	NaN	NaN	NaN
[4,]	NaN	NaN	NaN	NaN
	[,1]	[,2]	[,3]	[,4]
[1,]	49	62	58	38
[2,]	62	140	-4	62
[3,]	58	-4	166	29

# What happened?

### > D; sqrt(D)

[,1]	[,2]	[,3]	[,4]
234.0116	0.0000	0.00000	0.000000e+00
0.0000	162.8929	0.00000	0.000000e+00
0.0000	0.0000	39.09544	0.000000e+00
0.0000	0.0000	0.00000	-1.012719e-14
	234.0116 0.0000 0.0000 0.0000	234.0116 0.0000 0.0000 162.8929 0.0000 0.0000 0.0000 0.0000	[,1] [,2] [,3] 234.0116 0.0000 0.00000 0.0000 162.8929 0.00000 0.0000 0.0000 39.09544 0.0000 0.0000 0.00000

	[,1]	[,2]	[,3]	[,4]
[1,]	15.29744	0.00000	0.000000	0
[2,]	0.00000	12.76295	0.000000	0
[3,]	0.00000	0.00000	6.252635	0
[4,]	0.00000	0.00000	0.000000	NaN

Warning message: In sqrt(D) : NaNs produced

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http://www.utstat.toronto.edu/~brunner/oldclass/302f20