Scientific Computation

Spring, 2019

Lecture 11

Imperial College
London

Notes

- HW2: Posted online today ~7pm, due by end of next Friday (1/3)
- HW1 solutions will be posted on Friday, feedback, early next week
- Today's office hour is in 6M20
- Anonymous online feedback: https://goo.gl/forms/K5YEXbxZFTbUdfda2

Overview of time-marching methods

- **Discussed: implicit/explicit, fixed time-step and variable time-step methods**

- **Fixed time-step methods:**
  - **Accuracy characterized by truncation error**
  - **Also considered stability (model equation,** dy/dt = ay, Real(a)<=0)

- **Variable time-step methods**
  - **Time step automatically reduced to reach error**
  - ***Stiffness* rather than stability is main concern**

Overview of time-marching methods

- **Discussed: implicit/explicit, fixed time-step and variable time-step methods**

- **Fixed time-step methods:**
  - **Accuracy characterized by truncation error**
  - **Also considered stability (model equation,** $dy/dt = ay$, $\text{Real}(a) <= 0$)

  ❑ **Explicit Euler: truncation error ~** Δt, ***unconditionally unstable*** **for model eqn.**

  ❑ **RK4: truncation error ~** Δt^4, ***conditionally stable*** **for model eqn.**

  ❑ **Implicit Euler: truncation error ~** Δt, ***unconditionally stable*** **for model eqn.**

Overview of time-marching methods

- Discussed: implicit/explicit, fixed time-step and variable time-step methods

- Variable time-step methods
  - Time step automatically reduced to reach error
  - *Stiffness* rather than stability is main concern

  ❑ Explicit variable time-step (e.g. RK45): Good for linear dynamics (single time scale)

  ❑ Implicit variable time-step (e.g. odeint, BDF): Good for *stiff* systems with multiple time scales – problems with strong nonlinearity

Overview of time-marching methods

- Discussed: implicit/explicit, fixed time-step and variable time-step methods

- Variable time-step methods
  - Time step automatically reduced to reach error
  - *Stiffness* rather than stability is main concern

  - ❑ Explicit variable time-step (e.g. RK45): Good for linear dynamics (single time scale)

  - ❑ Implicit variable time-step (e.g. odeint, BDF): Good for *stiff* systems with multiple time scales – problems with strong nonlinearity

- How do these models select their time steps?
  - By computing the solution y_{i+1} from y_i with 2 (or more) different time steps, they can estimate the *error* for y_{i+1}, E_{i+1}
  - Then, this error is compared to tolerance for the *absolute* and *relative* errors: ε_{abs} and ε_{rel}
  - The solution is accepted if $E_{i+1} < |y_{i+1}| \, \varepsilon_{rel} + \varepsilon_{abs}$

Overview of time-marching methods

- **Discussed: implicit/explicit, fixed time-step and variable time-step methods**

- **Fixed time-step methods:**
  - **Accuracy characterized by truncation error**
  - **Also considered stability (model equation,** dy/dt = ay, Real(a)<=0**)**

- **Variable time-step methods**
  - **Time step automatically reduced to reach error**
  - ***Stiffness* rather than stability is main concern**

- **How do you choose one method vs. another?**
  - **Generally: Fastest method that provides a desired level of accuracy**
    - **Desired accuracy is context-dependent**
    - **The best we can hope for with double-precision arithmetic is ~1e-13**
  - **My (idiosyncratic) approach:**
    - **Use** odeint **(or something similar) for systems of ODEs, and single PDEs**
    - **Use something like RK4 for systems of PDEs**

Data science

- No particularly standard definition
- Combination of analysis, processing, and machine learning
  - Analysis and processing – “shape” or simplify data to facilitate understanding of underlying dynamics and trends
  - Learning – train models to classify data and/or predict trends
  - Often requires use of optimization methods (or ideas)
- Method 1: Principal Component Analysis (PCA)
- But first, let’s take a detour through an optimization problem

Matrix operators

- **How can we interpret:** $Ax = b \qquad x \in \mathbb{R}^N,\ b \in \mathbb{R}^M$
  - **If** A **and** b **are known: system of equations**
  - **If** A **and** x **are known: transformation of** x **to** b
- **Let's think about the general case where *neither* x nor b are known**

Matrix operators

- **How can we interpret:** $Ax = b \qquad x \in \mathbb{R}^N,\ b \in \mathbb{R}^M$
  - **If** A **and** b **are known: system of equations**
  - **If** A **and** x **are known: transformation of** x **to** b
- **Let's think about the general case where *neither* x nor b are known**

Given a matrix A**, find** x **so that** |b| **is maximized**

Application: system of linear ODEs: $\frac{dx}{dt} = Mx$

$$x(t) = A(t)x_0,\ A = exp(Mt)$$

(here, *exp* is the *matrix exponential*)

More generally, a broad range of dynamical process can be stated (sometimes approximately) in an iterative form: $x_{i+1} = Ax_i$

And the optimization problem aims to find the maximum possible "growth"

Maximum growth

- **We need to be more careful with our problem statement:**

Given a matrix A, find x so that |b| is maximized with |x|=1

1. **We first set an upper bound for the growth**
2. **Then, we see if we can reach that upper bound**

Maximum growth

- We need to be more careful with our problem statement:

Given a matrix A, find x so that |b| is maximized with |x|=1

1. We first set an upper bound for the growth
2. Then, we see if we can reach that upper bound

Task 1:

We have: $Ax = b$ which implies, $x^T A^T A x = b^T b$

Note that $A^T A$ is symmetric and thus can be orthogonally diagonalized:

$$A^T A = V S V^T$$

Here, V is the orthogonal eigenvector matrix and S is a diagonal matrix with the eigenvalues of $A^T A$ on the diagonal.

Maximum growth

Task 1:

We have: $Ax = b$ **which implies,** $x^T A^T A x = b^T b$ **(1)**

Note that $A^T A$ **is symmetric and thus can be orthogonally diagonalized:**

$$A^T A = V S V^T$$

Here, V **is the orthogonal eigenvector matrix and** S **is a diagonal matrix with the eigenvalues of** $A^T A$ **on the diagonal.**

- **Note that the eigenvalues of** $A^T A$ **are real and non-negative, and we construct** S **so that the eigenvalues appear in descending order,**

$$S_{i,i} = \lambda_i, \;\; \lambda_1 \geq \lambda_2 ... \geq \lambda_N$$

- **So (1) can be re-written as:** $x^T V S V^T x = b^T b$
- **Now, if we take** $x = V z$**, we have:** $z^T S z = b^T b$

Maximum growth

Task 1:

- **So (1) can be re-written as:** $x^T V S V^T x = b^T b$
- **Now, if we take x = V z, we have:** $z^T S z = b^T b$ **which can be rearrange as:** $b^T b = \lambda_1 z_1^T z_1 + \lambda_2 z_2^T z_2 + ... + \lambda_N z_N^T z_N$ **and z_i is the i^{th} element of z**

Then: $b^T b \leq \lambda_1 \left(z_1^T z_1 + z_2^T z_2 + ... + z_N^T z_N \right)$

$$b^T b \leq \lambda_1 z^T z$$

$$x^T x = z^T z$$

$$b^T b \leq \lambda_1 x^T x$$

Task 2: Find x such that $x^T x = 1$ and $b^T b = \lambda_1$

Maximum growth

Task 2: Find x such that $x^T x = 1$ and $b^T b = \lambda_1$

This is easier!

We know $A^T A v_1 = \lambda_1 v_1$

and $v^T v = 1$, so if $x = v_1$, $|Ax| = |Av_1| = v_1^T \lambda_1 v_1 = \lambda_1$

The 'most dangerous' x is the "first" eigenvector of $A^T A$

Computational cost

- **Eigenvalues and eigenvectors of $F = A^T A$ are needed**

- **Implementations typically use variations of QR algorithm**
  - **Basic idea: iteratively obtain a matrix *similar* to F which is nearly triangular**
  - **$F_k = Q^{-1} F Q$ after k iterations with approximations of the eigenvalues of F_k on its diagonal**
  - **Cost is generally estimated to be $O(N^3)$, though this depends on rate of convergence of iterations**
  - **Can we do better?**

Singular value decomposition

- **The eigenvalues and eigenvectors of F can be found from the singular value decomposition (SVD) of A:**

$$A = U\Sigma W^T$$

- **Recall that** $F = A^T A = VSV^T$

- **From the SVD:** $A^T A = W\Sigma^2 W^T$ **(U and W are orthogonal – as they are left and right eigenvectors of F which is symmetric)**

- **Comparing:** $\Sigma^2 = S$

$$W = V$$

- **The key point here is that variants of QR have been developed specifically to compute the SVD (avoids explicitly constructing A^TA)**

- **Asymptotic cost is similar to QR: $O(M^2N) + O(N^3)$ for A with size M x N**

QR vs SVD

- **Approximate costs are similar, what do we see in practice?**

```
In [9]: A = np.random.randn(800,800)

In [10]: A.shape
Out[10]: (800, 800)

In [11]: C = np.dot(A.T,A)

In [12]: timeit l,v = np.linalg.eig(C)
543 ms ± 13.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

In [13]: timeit u,s,vh = np.linalg.svd(A)
300 ms ± 1.62 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

QR vs SVD

- **Approximate costs are similar, what do we see in practice?**

```
In [9]: A = np.random.randn(800,800)

In [10]: A.shape
Out[10]: (800, 800)

In [11]: C = np.dot(A.T,A)

In [12]: timeit l,v = np.linalg.eig(C)
543 ms ± 13.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

In [13]: timeit u,s,vh = np.linalg.svd(A)
300 ms ± 1.62 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

```
In [22]: l[0]
Out[22]: 3195.472688027676

In [23]: s[0]**2
Out[23]: 3195.4726880276557
```

Note: Should use scipy.sparse.linalg **when working with large sparse matrices**

Data science

- No particularly standard definition

- Combination of analysis, processing, and machine learning
  - Analysis and processing – “shape” or simplify data to facilitate understanding of underlying dynamics and trends
  - Learning – train models to classify data and/or predict trends
  - Often requires use of optimization methods

Data science

- No particularly standard definition

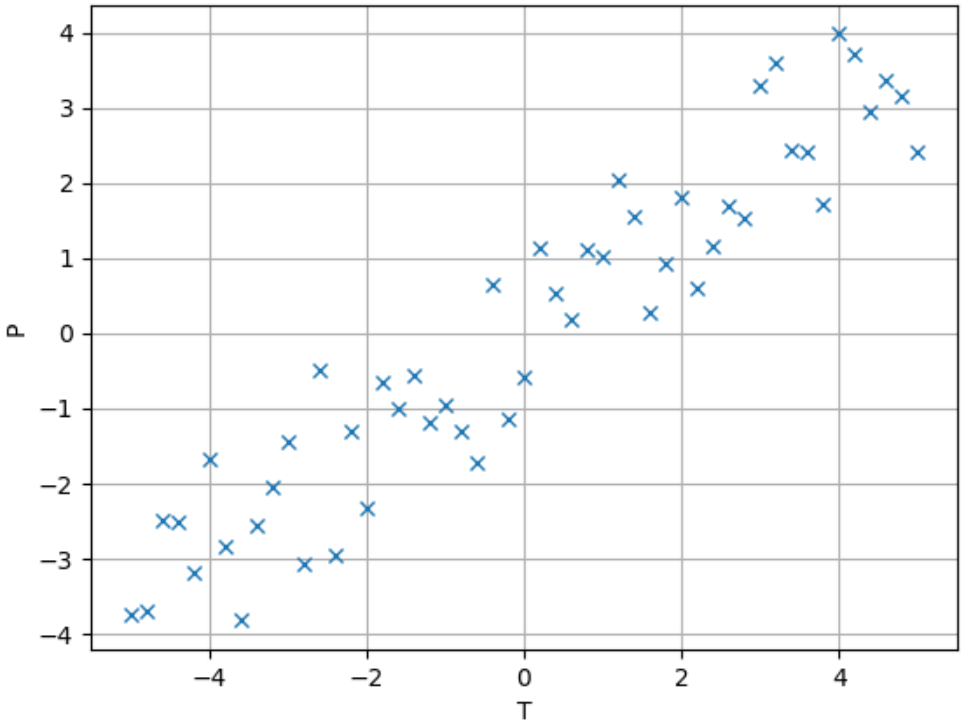
- Combination of analysis, processing, and machine learning
  - Analysis and processing – "shape" or simplify data to facilitate understanding of underlying dynamics and trends
  - Learning – train models to classify data and/or predict trends
  - Often requires use of optimization methods

- Step 1: Data collection/acquisition
  - Lab measurements
  - Online databases (e.g. Kaggle)
  - Simulation results
- Typically have data corresponding to multiple variables
  - Temperature, pressure, humidity, wind speed and direction
  - IP address, location, duration of visit, number of visits, pages visited

- But often don't know in advance if all of these variables are "important" – how many variables do we actually need to capture the essential trends or dynamics?

Data analysis

- **Example: Consider the data in the figure corresponding to measurements of temperature and pressure**
  - **Before looking at the data, we might conjecture that the underlying dynamics are connected to a general function of these two variables,** $f(T,P)=c$ **with** c **some constant**
  - **But do we really need two independent variables?**

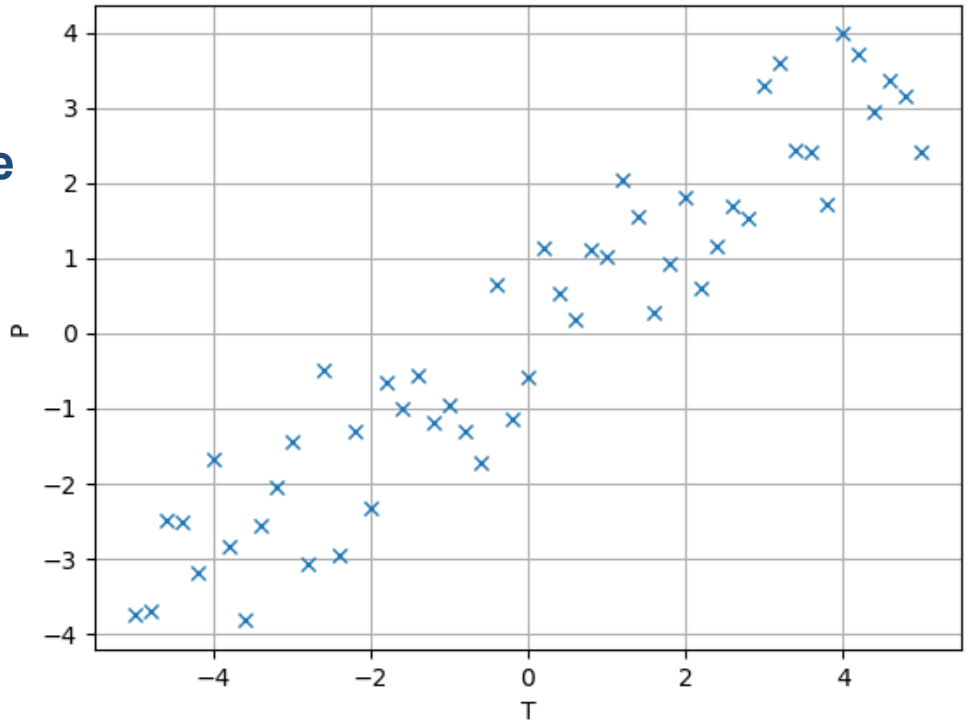


Data analysis

- **Example: Consider the data in the figure corresponding to measurements of temperature and pressure**
  - **Before looking at the data, we might conjecture that the underlying dynamics are connected to a general function of these two variables,** $f(T,P)=c$ **with** c **some constant**
  - **But do we really need two independent variables?**

Basic ideas:
Interesting/important dynamics are large-variance dynamics

The less correlation between independent variables, the better



Data analysis

- **Example 2: Say you are tracking a meteor heading towards Earth**
  - **How many variables do you need?**
  - **Three position coordinates?** x(t), y(t), z(t)
  - **Maybe three velocity components as well?** u(t), v(t), w(t)

But what if the meteor is just moving in a circular orbit?

Let's translate ideas of extracting "important" variables into the language of linear algebra

PCA

- **We measure the meteor coordinates at:** N **times and store them in a** 3 x N **array:**
- **Data:** $A = \begin{bmatrix} x_1 & x_2 & \dots & x_N \\ y_1 & y_2 & \dots & y_N \\ z_1 & z_2 & \dots & z_N \end{bmatrix}$

- x, y, z **are each N-element column vectors, so:** $A = \begin{bmatrix} \mathrm{x}^T \\ \mathrm{y}^T \\ \mathrm{z}^T \end{bmatrix}$

We assume that each has been scaled to have zero mean, e.g. $\sum_{i=1}^{N} x_i = 0$

Then, $C = AA^T$ **is the *covariance matrix* (technically, it should be scaled with** N**)**

The diagonal elements are the variances of x, y, **and** z**. The off-diagonal elements contain covariances such as:** $\mathrm{x}^t\mathrm{z} = \sum_{i=1}^{N} x_i z_i$

PCA

- **Method: Project data onto new variables so covariance matrix is diagonalized**
  - **With zero covariance – the new variables will be "independent"**
  - **The variable with the larger variance is more "important"**

- **Let** F A = G **-- need to find a "projection matrix",** F, **so that** GG^T=D **is diagonal**

- A **contains projection weights**
  - **The first row transforms** $\mathrm{x} \rightarrow \tilde{\mathrm{x}}$ **:** $\alpha_1 \mathrm{x} + \alpha_2 \mathrm{y} + \alpha_3 \mathrm{z} = \tilde{\mathrm{x}}$
  - **And the full projection matrix is:** $F = \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{bmatrix}$

- **We need** $D = FAA^TF^T = FCF^T$

- **Note: if** A **has zero-mean, so does** G

PCA

- **We need** $D = FAA^TF^T = FCF^T$
- **The covariance matrix is symmetric and orthogonally diagonalizable…**

$$AA^T = VSV^T$$

- **And by inspection, we see that** $F = V^T$ **gives** $D = S$

Notes:

1. V **and** S **contain the eigenvectors and eigenvalues of** AA^T
2. **Eigenvalues of** AA^T **and** A^TA **are the same (but one may have more zeros)**
3. **Here,** V **corresponds to** U **in the SVD of** A: $A = U\Sigma W^T$
4. **Our transformed data is** $G = V^T A$ **and the eigenvalues of** S **indicate the "importance" of each row of** G
5. **Since** F **is orthogonal,** G **and** A **have the same variance (they have the same trace)**

Data analysis

- **Python implementation (2 variables):**

1. **Set up, solve eigenvalue problem:**

Data analysis

- **Python implementation:**

1. Set up, solve eigenvalue problem:

```
In [45]: A.shape
Out[45]: (2, 51)

In [46]: A.mean(axis=1)
Out[46]: array([-6.26949473e-16,
5.22457894e-17])

In [47]: U,S,VT = svd(A)
```

2. Compute transformed data:

```
In [48]: F = U.T

In [49]: G = np.dot(F,A)

In [50]: np.dot(G,G.T)
Out[50]:
array([[ 8.33602821e+02,
-1.18785463e-13],
       [-1.18785463e-13,
1.50729071e+01]])
```

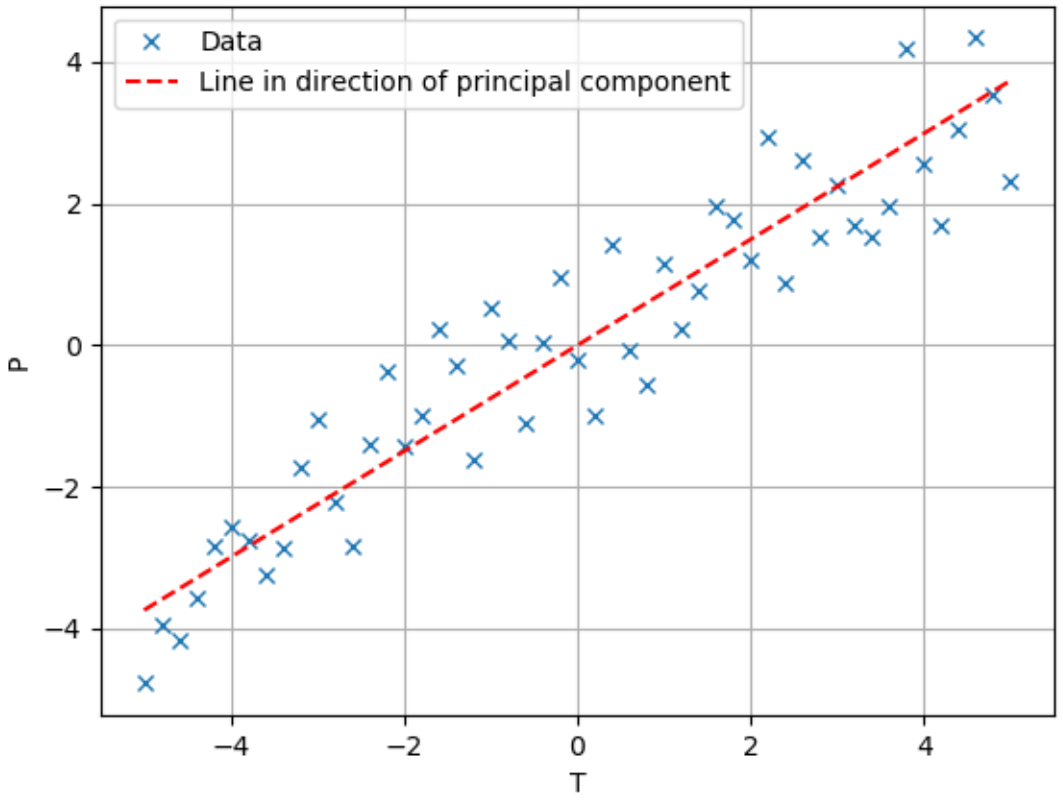
Data analysis

- **Python implementation:**

3. Compare first eigenvector (corresponding to largest eigenvalue) to data:

```
In [51]: plot(t,U[1,0]*t/U[0,0]-5,'r--')
```

- **The eigenvectors of C are the *principal components***
- **The 1st component points in the direction of maximum variance**
- **What is the direction of the 2nd component?**



Dimension reduction

- **The eigenvalues tell us how much of the variance is associated with the principal component:**

```
In [52]: S
Out[52]: array([28.87218075,  3.8823842 ])
```

- **Dimension reduction: discard variables (row of G) associated with low variance For this example, discard 2nd row of G and retain 1st row**

- **How do we express reduced data in original variables? Recall:**

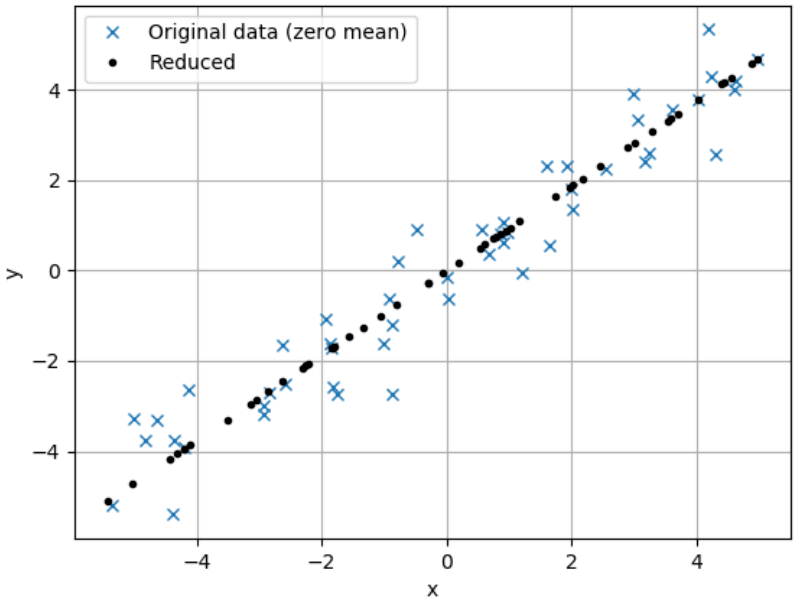
$$U^T A = G \text{ or } A = UG$$

The *reduced* data, in our original variables, is then the outer product of the 1st eigenvector of U with the 1st row of G:

```
In [64]: A2=np.outer(U[:,0],G[0,:])

In [65]: A2.shape
Out[65]: (2, 51)

In [66]: plot(A2[0,:],A2[1,:],'k.')
```



Dimension reduction

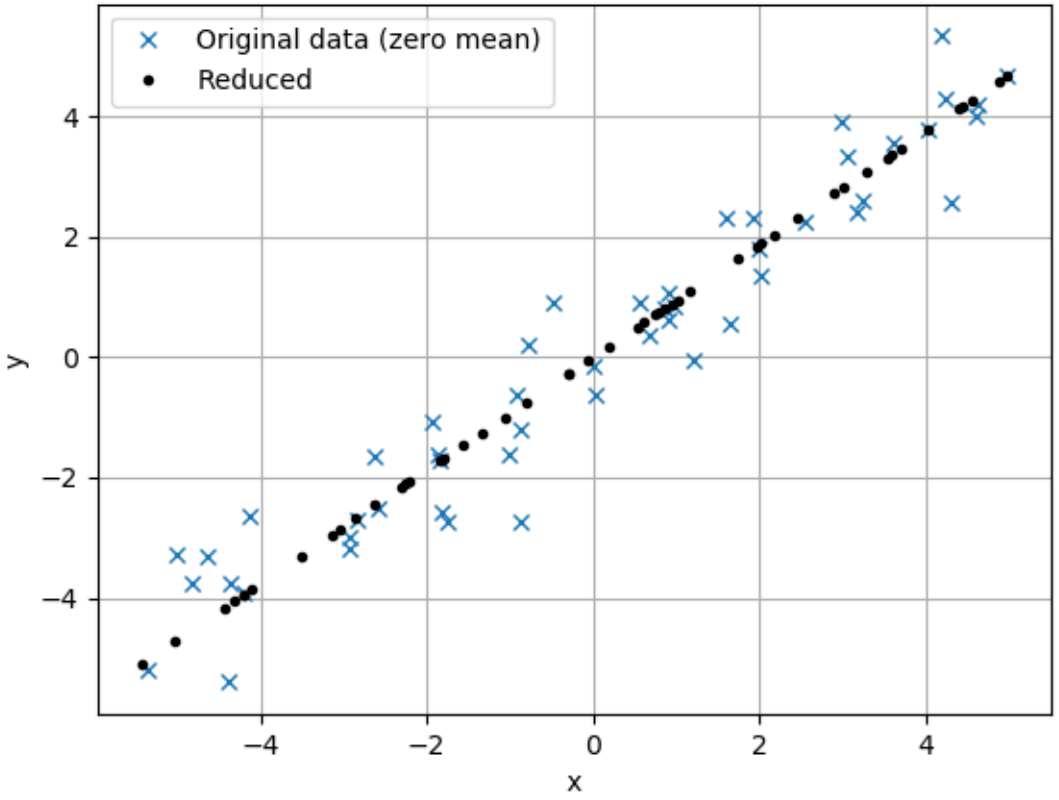
The eigenvalues tell us how much of the variance is associated with the principal component:

```
In [52]: S
Out[52]: array([28.87218075,  3.8823842 ])
```

Dimension reduction: discard variables (columns of G) associated with low variance

For this example, discard 2nd row of G and retain 1st row

- **Can reduce redundancy and simplify models for underlying dynamics**
- **This example with just two variables is not a practical application**
- **Many problems have 10s, 100s, or even 1000s of variables**



Notes

- The presented procedure for PCA then is:

1) Arrange data into a matrix (subtracting means if needed)

2) Compute eigenvalues and eigenvectors of covariance matrix

3) Order eigenvalues and corresponding eigenvectors (if needed)

4) “Focus” on the components corresponding to the largest eigenvalues

- What is the cost of PCA?