Analyzing functional data with Direct Functional PCA in Functional Data Explorer

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JMP

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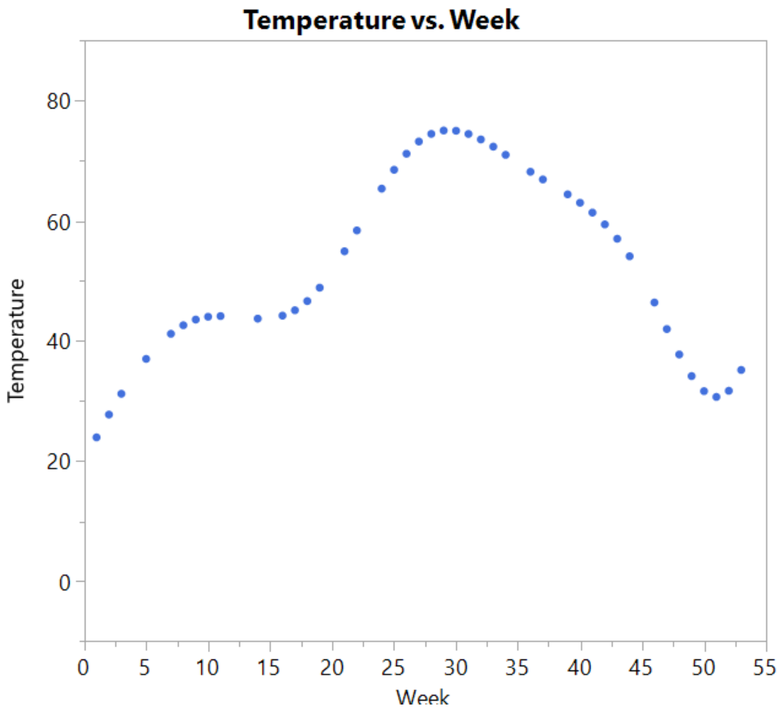
Functional Data



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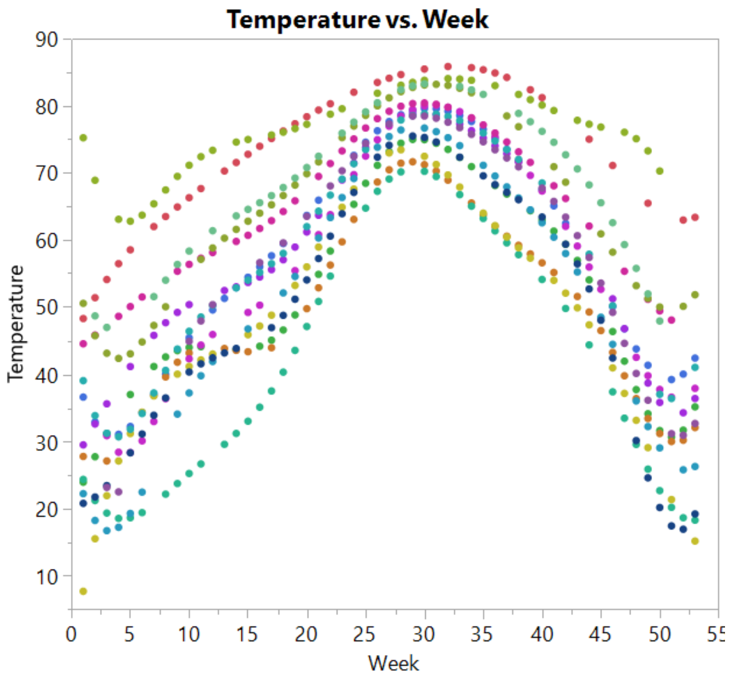

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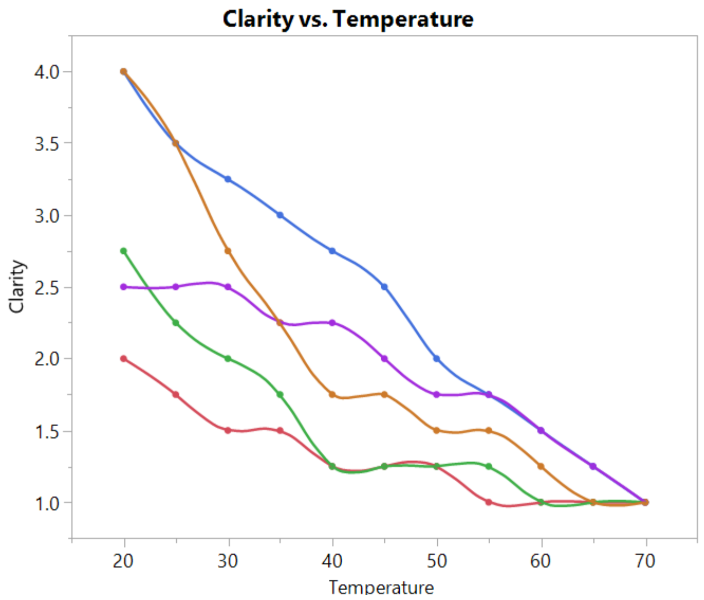

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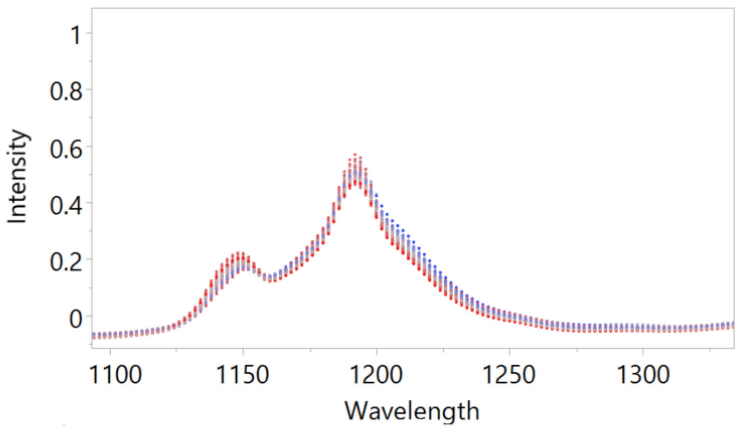

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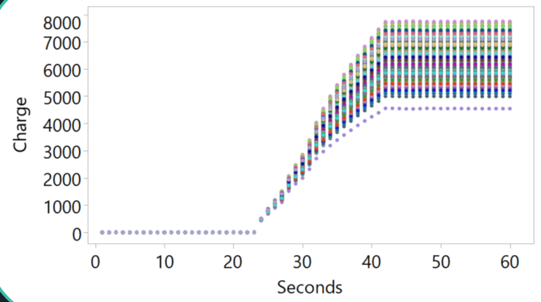

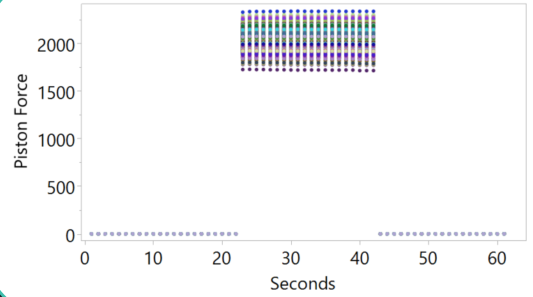

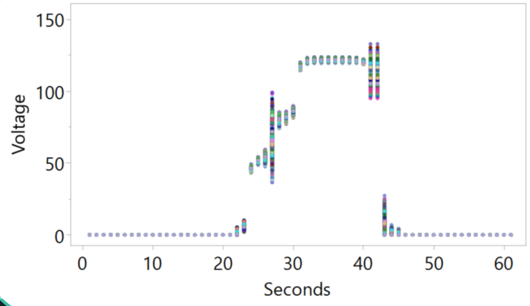

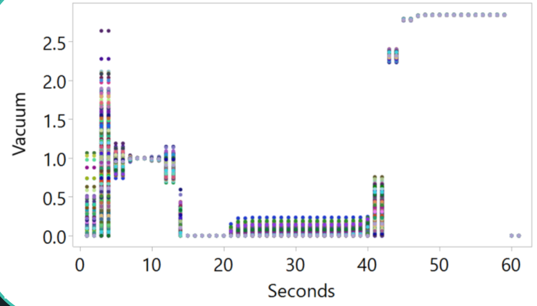

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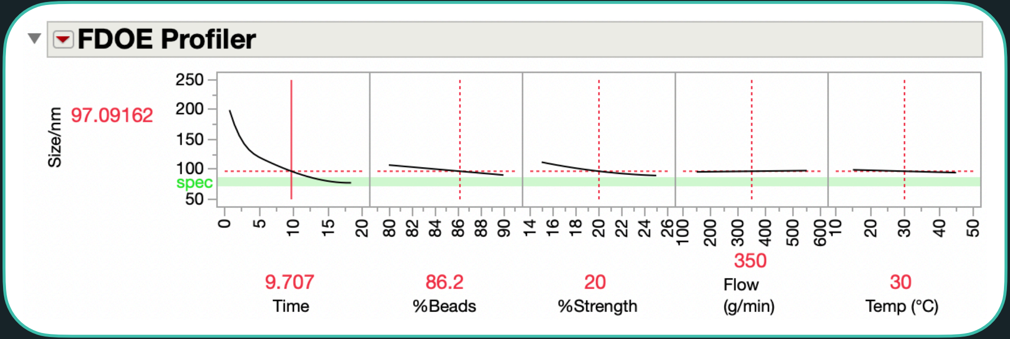
Functional Data Explorer

Functional DOE

- How can we use DOE factors to predict a response function?

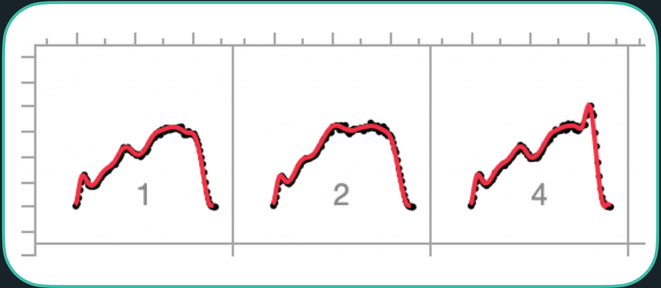


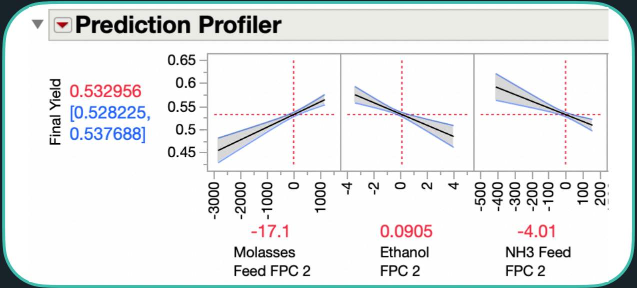
- Want our process to remain in specification as long as possible.

Functional Data Explorer

Functional Machine Learning

- How can we predict the outcome of a process using functions as inputs?





- Predict ***Final Yield*** of a fermentation process using sensor streams.

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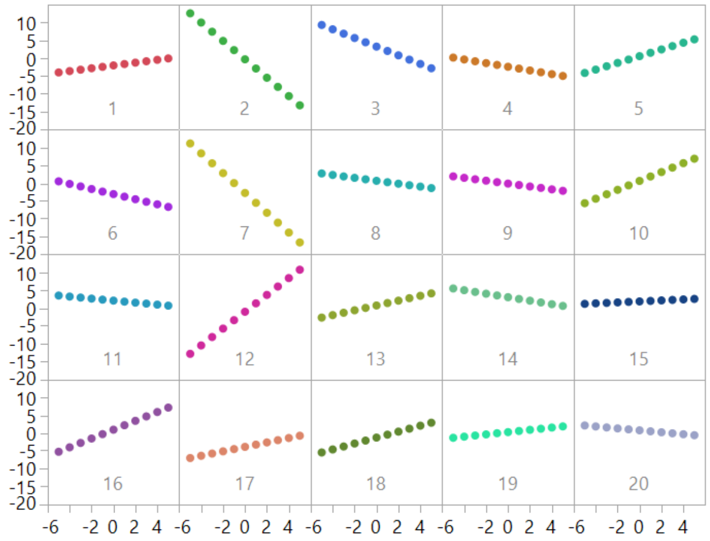
Functional Data Explorer

Functional PCA

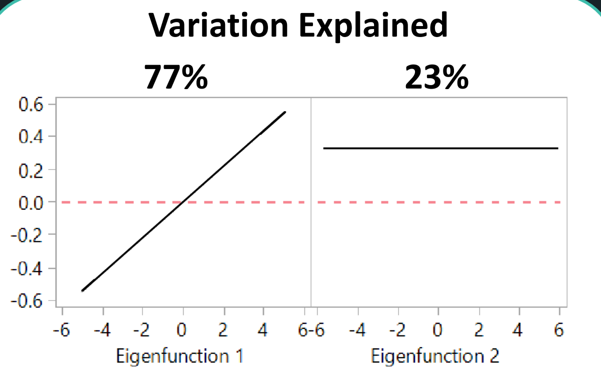
- FPCA decomposes data into orthogonal eigenfunctions
- Explains as much function-to-function variation as possible
- Allows us to extract summaries for predictive modeling

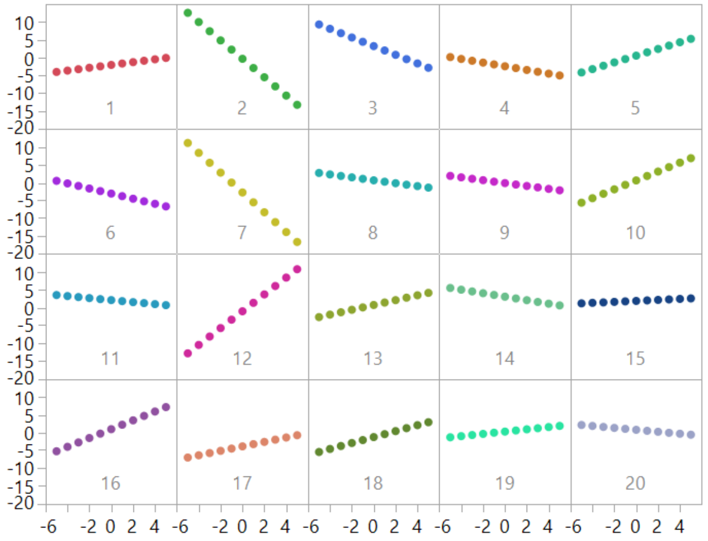


Functional PCA

Eigenfunctions

- Eigenfunction plots highlight features in the functional data

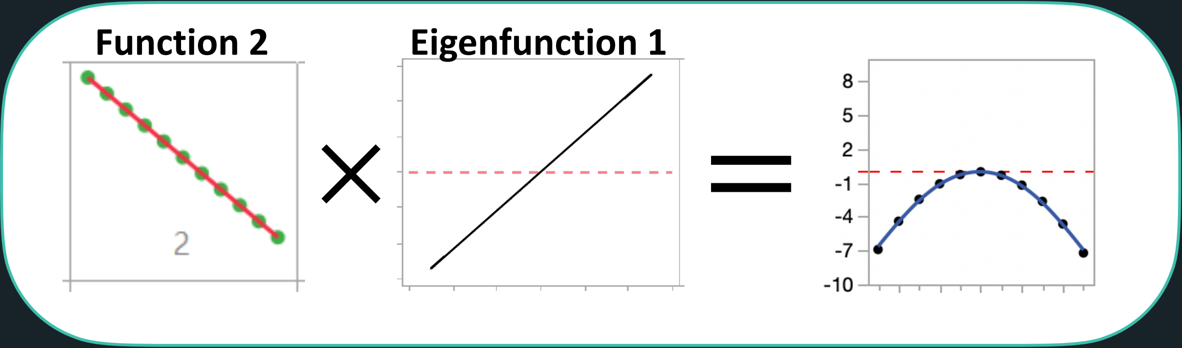




Functional PCA

Functional Principal Components

- FPCs summarize differences between functions



ID	FPC 1	FPC 2
1	3.63	-6.41
2	-23.5	-1.14
3	-11.1	10.15
4	-4.64	-7.63
5	8.58	1.81
6	-6.48	-9.73
7	-25.2	-8.81
8	-3.74	2.08
9	-3.68	-0.41
10	11.35	2.03

$$FPC_{ij} = \int_X Y_i(x) \times E_j(x)$$

Functional PCA

Function Approximation

ID	FPC 1	FPC 2
1	3.63	-6.41
2	-23.5	-1.14
3	-11.1	10.15
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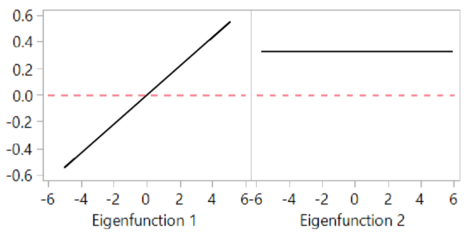
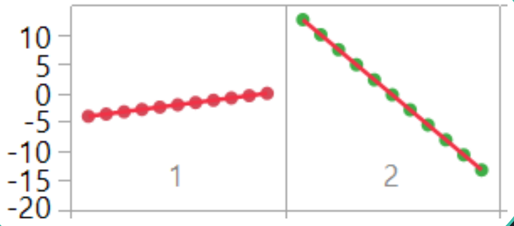




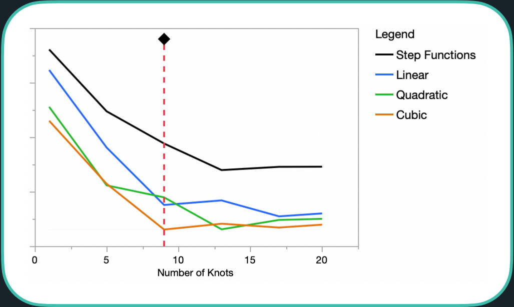
$$Y_1(x) \approx \mu(x) + 3.63 \times E_1(x) - 6.41 \times E_2(x)$$

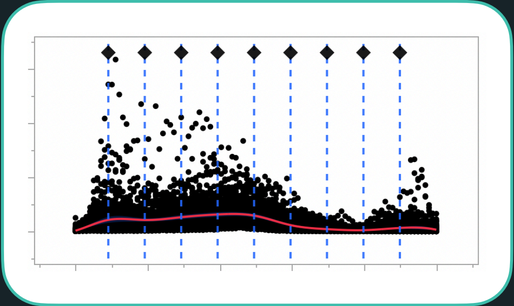
$$Y_2(x) \approx \mu(x) - 23.5 \times E_1(x) - 1.14 \times E_2(x)$$

Direct Functional PCA

Why DFPCA?

- FDE fits basis function models
  - B-splines, P-splines, Fourier
- FPCA on the model coefficients
- For large problems:
  - Unfeasible parameter tuning
  - Computing can be costly

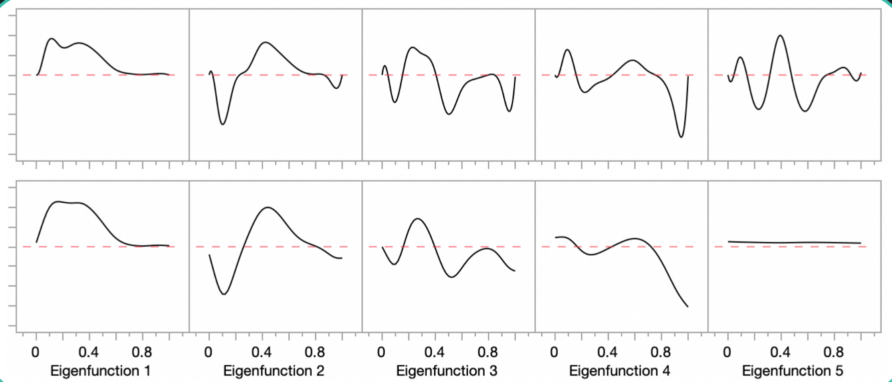




Direct Functional PCA

B-splines

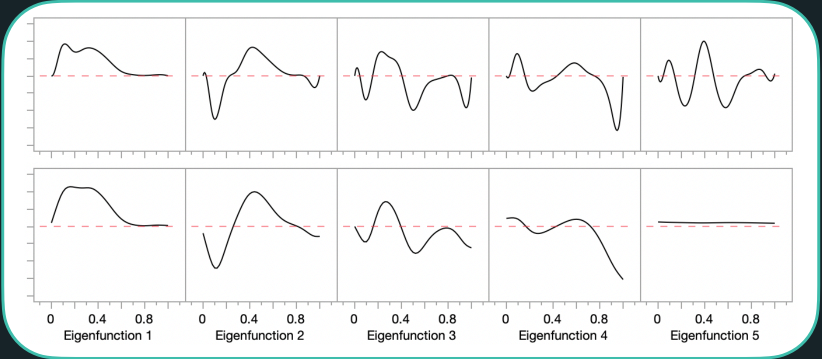
DFPCA

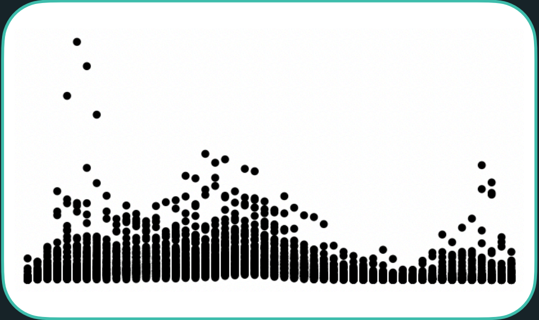


- Operates directly on the data
- Smooths the eigenfunctions

Direct Functional PCA

- Iterative algorithm that identifies one eigenfunction at a time
  - Similar in spirit to Rice and Silverman (1991)
- Data must be on a regular grid
  - We interpolate it for you
  - Can control this with ***Reduce***
- Smoothing simpler eigenfunctions makes DFPCA very fast!

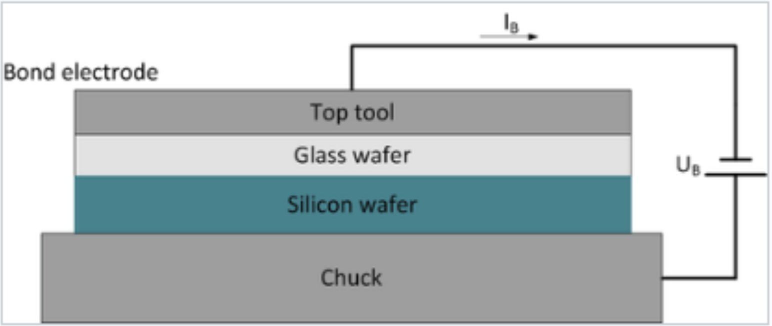




Example

Anodic Bonding

- Semiconductor manufacturing process where glass is bonded to the devices
- Process destroys $\approx 10\,\%$ of wafers, but they are not identified until production process is complete
- **Goal**: use sensor stream functional data to identify wafers to discard early



Scheme of anodic bonding procedure. The top tool works as a cathode and the chuck as anode.

Source: *https://en.wikipedia.org/wiki/Anodic_bonding*

Demo

Direct Functional PCA

Tips on using DFPCA

- Fast computing makes it ideal for larger data sets.
- Data must be gridded
  - Use ***Reduce*** to control the grid
- Diagnostics provided to help identify issues.
  - As with any statistical model, check to make sure it is working well!

Thank you!

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References

- Rice, J.A. and Silverman, B.W. (1991). Estimating the mean and covariance structure non parametrically when the data are curves. *Journal of the Royal Statistical Society*, Series B, 53, 233-243.

- Ramsay, J.O and Silverman, B.W. (2005). Functional data analysis, second edition (Springer series in statistics).

Direct Functional PCA

Algorithm

- Direct FPCA algorithm on data matrix M:

  1. Perform Lanczos SVD to capture the i^{th} eigenfunction
  2. Smooth the eigenfunction using penalized splines
  3. Normalize the eigenfunction to have unit norm
  4. Orthogonalize the eigenfunction
  5. Subtract the component from M and go back to step 1