Teaching Statistics using 3D Graphics in R

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Outline

Statistical Programming Course

- Introductory programming course for 50–80 statistical and actuarial students.
- Starts with programming; uses R.
- Continues with Monte Carlo simulation, computational linear algebra, and numerical optimization.
- Uses both "classic" S graphics and `rgl` for debugging and understanding theory and algorithms.
- Today: singular value decompositions and Nelder-Mead optimization.

The Singular Value Decomposition

For a square $n \times n$ matrix A, the SVD is

$$A = UDV^T \tag{1}$$

where

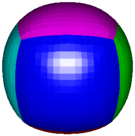
- U and V are $n \times n$ orthogonal matrices (i.e. $U^T U = V^T V = I$)
- D is an $n \times n$ diagonal matrix with non-negative entries
- the superscript T indicates matrix transposition.

Displaying a Matrix Graphically

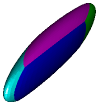
- Matrices are representations of linear operators on vector spaces.
- The matrix A is characterized by the behaviour of $y = Ax$ as we vary x.
- Use the `rgl` package to develop a graphical representation of 3×3 matrices.
- While the action on the basis vectors is mathematically sufficient, it is hard to visualize the overall effect of the transformation.
- We prefer to use coloured spheres.

Displaying the SVD

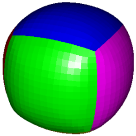
$$A = \begin{pmatrix} 1 & 0.1 & 0.1 \\ 2 & 1 & 0.1 \\ 0.1 & 0.1 & 0.5 \end{pmatrix}$$



Identity

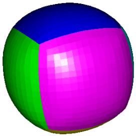


A



U

D



V

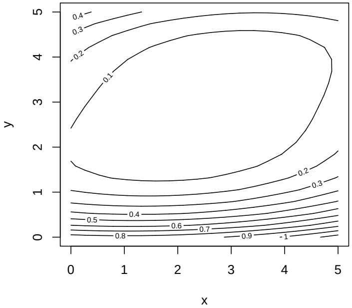
The Nelder-Mead Simplex Method

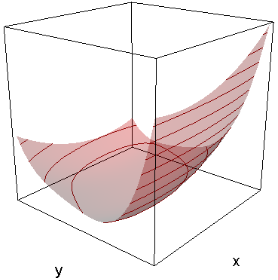
- A robust derivative-free multi-dimensional minimizer.
- Easy to describe and to visualize
- Implementations of it are within the reach of our introductory students.
- Not very fast, and the visualizations help to illustrate why.
- Our demonstration is based on the implementation in R, which is adapted from Nash (1990).

How Nelder-Mead Works

- Start with a non-degenerate simplex in the space of the arguments to the target function.
- Iterate through updates of the simplex until the simplex is determined to be close enough to a local minimum.
- Updates replace the vertex with the highest function value with a new one, either by shrinking, expanding, or reflecting the simplex through the centroid of the other vertices, or shrink the entire simplex.

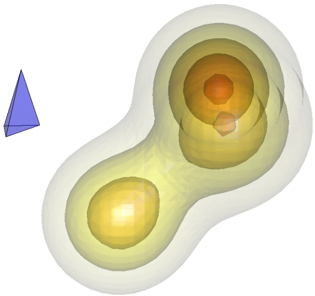
Two Dimensional Example





$$f(x,y) = [(x-y)^2 + (x-2)^2 + (y-3)^4]/100$$

Three Dimensional Example



Density of mixture of three normals (from `misc3d` package), together with initial simplex.

Conclusions

- We show students that it is possible to generate relatively sophisticated graphics in a fairly easy way.
- Students are already computer users (as game players, etc.); in our class they learn that they can be in control.
- They also learn something about linear algebra, optimization, Monte Carlo methods.