

# Points, Curves and Haystacks: Datavis and Metabolomics

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A challenge to researchers using *R* for analysis of large datasets is the lengthy computation time associated with visualization and the static nature of such images generated using base graphics. This limits opportunities to rapidly gain insights into data structures. One solution is to use a new *R* package, **qtpaint**; rendering graphics much more quickly, especially for large datasets. However, **qtpaint** offers only methods for drawing low-level graphical elements and requires an investment of time and effort on the part of the researcher, both in skill acquisition and programming, to implement. `qtpaintgui()` is a tool created to support portable graphics development, accessible via command-line interaction and a point-and-click GUI. We examine how graphics generated using `qtpaintgui()` allow data visualization approaches to support efforts of the Metabolomics community to encourage transparency and automation in data processing.

## References

- A. Buja, D. Cook, and D.F. Swayne, (1996) *Interactive High-Dimensional Data Visualization*, *Journal of Computational and Graphical Statistics*, vol. 5, pp. 78-99.
- M. Guzdial (2004). Programming environments for novices. *Computer Science Education Research*, S. Fincher and M. Petre, Eds. Taylor & Francis, Abingdon, U.K., 2004: 127–154.
- E. Lahtinen, K. Ala-Mutka, H. Järvinen, (2005) *A Study of the Difficulties of Novice Programmers*, Proceedings of the 10th annual SIGCSE conference on Innovation and technology in computer science education, 2005: pp. 14-18
- M. Lawrence (2010). *Interfaces to the Qt framework from R*.  
<http://r-forge.r-project.org/projects/qtinterfaces/>
- J. Yi, Y. Kang, J. Stasko, J. Jacko, (2007). *Toward a Deeper Understanding of the Role of Interaction in Information Visualization*, *IEEE transactions on visualization and computer graphics*, 2007: 13(6), pp. 1224-1231