

Figure 1

After the stop of running the script from the demo, Figure 1 will be obtained. The "Best point" in the Figure shows the optimal values of two parameters of multivariate Gaussian fitting function. The "Best Function value" in the Figure is the optimum RMSECV (minimum RMSECV).

It is worth noting that the results obtained by demo are slightly different from those of the paper, the reasons are the different calibration set and prediction, RMSECV was used in the demo, RMSEV was used in the paper.

## References

X.J. Chen, Y. J. Lai, X. Chen, Y. J. Shi, D. H. Zhu, A novel spectral multivariate calibration approach based on Multiple Fitting method, *Analyst*, 2016, DOI: 10.1039/C6AN01201A.

Write us for comments, questions or if you find bugs we didn't see, <a href="mailto:chenxj@wzu.edu.cn">chenxj@wzu.edu.cn</a> (Xiaojing Chen)