Isotopic pattern analysis based on a new Fourier deconvolution approach

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Aim

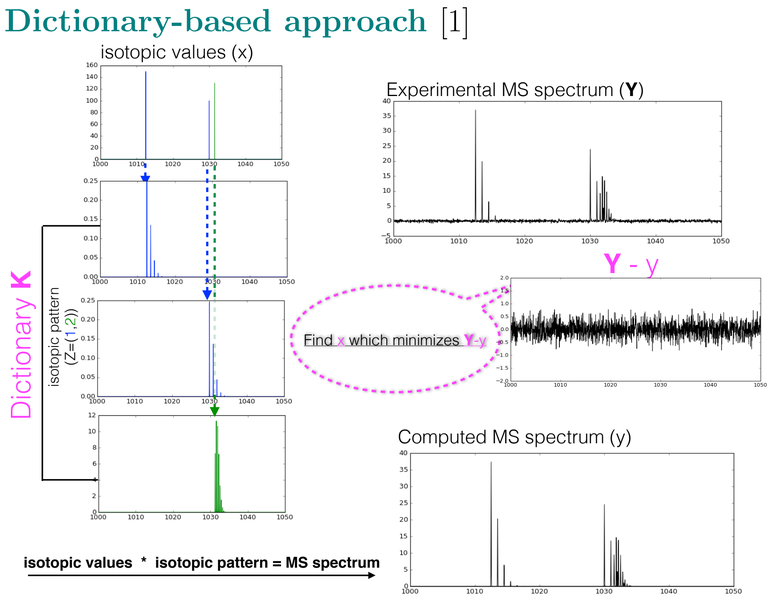
✗ Isotopic pattern deconvolution of peptide spectra.

Method

✗ Use direct spectra
☞ No peak picking!
✗ Use built isotopic pattern using averagine model [2]
☞ Peptide analysis.
✗ Include as well experimental line-shape
☞ Increase in resolution and simplification of spectra.

CONVEX OPTIMIZATION

Dictionary-based approach [1]



Fourier deconvolution approximation

✗ Large size of data with different charge values.
☞ Computational challenge & Large memory resources are needed to store the dictionary.
✓ We suppose that isotopic pattern is locally stable.
✓ Mass axis will be decomposed into windows.
✓ Isotopic pattern will be only calculated for each average mass of each window.
✓ Locally convolution product.
☞ Faster computation & Less memory.

CONCLUSION

✓ 1D deconvolution of isotopic masses of proteins
☞ Generalization of our approach to process any 1D & 2D complex mixture.

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REFERENCES

[1] Afef Cherni, Emilie Chouzenoux, Marc-André Delsuc, "*Fast dictionary-based approach for mass spectrometry data analysis*", in Proc. IEEE ICASSP, pp.x-x, Calgary, 15-20 April 2018.

[2] Michael W Senko, J Paul Speir, and Fred W McLafferty, "*Collisional activation of large multiply charged ions using Fourier transform mass spectrometry*", Analytical Chemistry, vol. 60, no. 18, pp. 2801-2808,1994.

MS SIMULATED SPECTRUM

• **1D Simulated signal**: With 50 ions, charged with z from 1 to 3. On the window m/z values are from 1000 to 1100 Daltons, simulated on 5000 points with 1% noise level. Reconstruction is done with 2000 iterations.

- Memory storage: 572 Mb
- Computation time: 30 s
- Qlty reconstruction: 35.73 dB

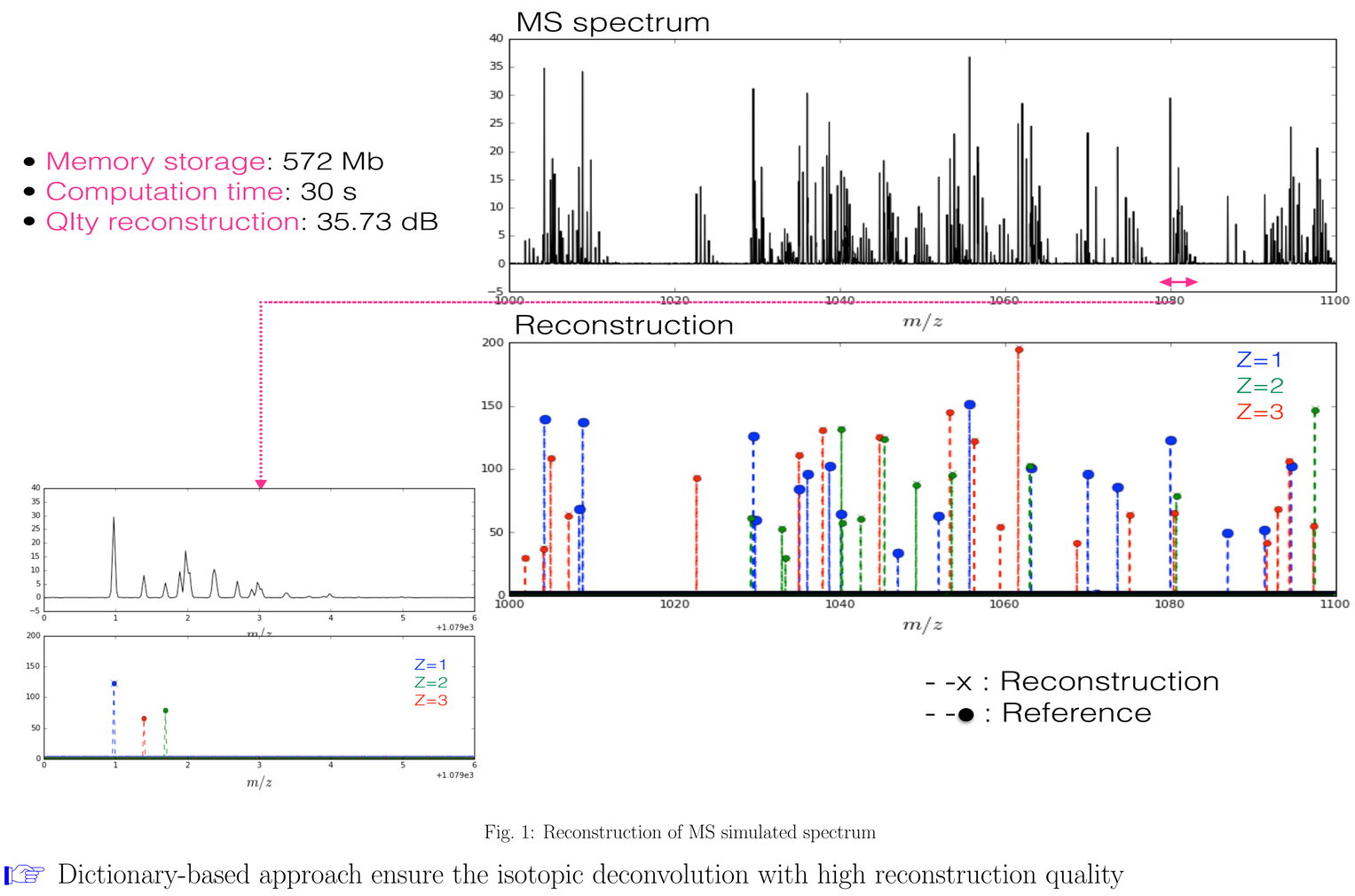
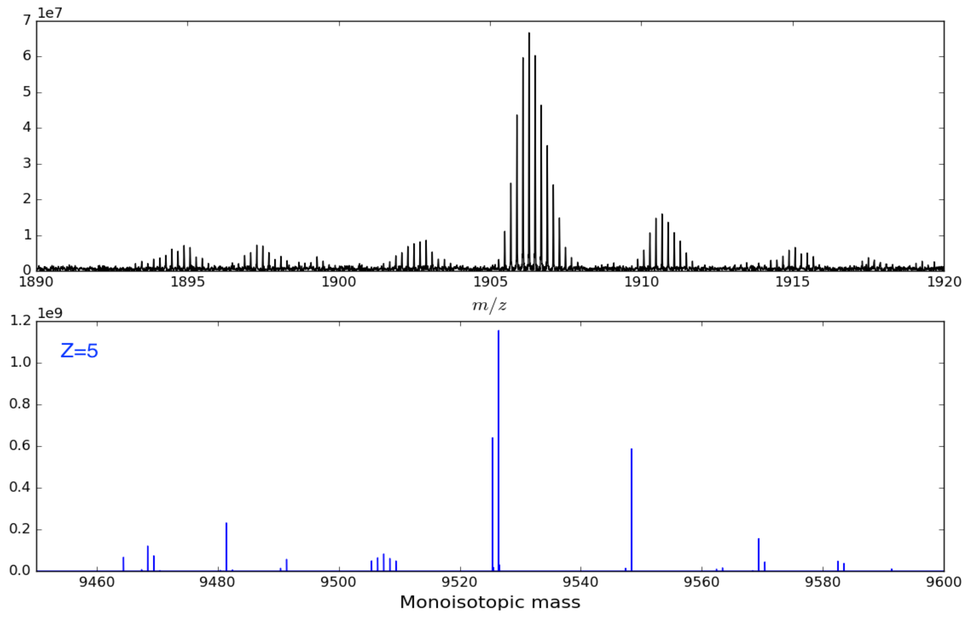


Fig. 1: Reconstruction of MS simulated spectrum

☞ Dictionary-based approach ensure the isotopic deconvolution with high reconstruction quality

EXPERIMENTAL MS SPECTRUM

• Measure 1:
3 μM fo the **peptide** "EVEALEKKVAALESKVQALEKKVEALEHG-NH2" ($C_{140}H_{240}N_{38}O_{45}$) in its **trimer** form in 50 mM of NH_4OAc, acquired in native conditions.
FT-ICR spectrum with size **M=8130981**, $m \in$ [153.57, 4999.96 Daltons], $z \in$ [1, 5].
• Isotopic deconvolution:



	SNR (dB)	Computation Time (s)
Dictionary-based	101	84.46
Optimization strategy (window = 2)	101	80.90
Optimization strategy (window = 5)	99.5	26.84
Optimization strategy (window = 10)	99.5	13.69

Fig. 2: Analysis of the real FT-ICR-MS spectrum of a peptide in trimer form: (top) zoom on the acquired data; (bottom) recovered spectrum at z = 5 using dictionary-based approach.

✓ Major peak at $m = 9526.439$ Daltons fits well with the theoretical monoisotopic mass of the studied peptide equals to $m = 9526.337$ Daltons.
✓ A second peak shifted by -1 Dalton due to unavoidable grid ambiguity.
✓ A third peak distant with +21.959 Daltons of the main peak, identifies the Sodium adduct (theoretical relative position of +21.982 Daltons).
☞ Faithfull approach.

✓ High quality of isotopic deconvolution.
✓ Fast approach devoted to big data.
✓ Limited memory resources needed.

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