Spatial distribution in MSI

Instrument response estimation, image correction, and resolution and clustering

Xavier Loizeau

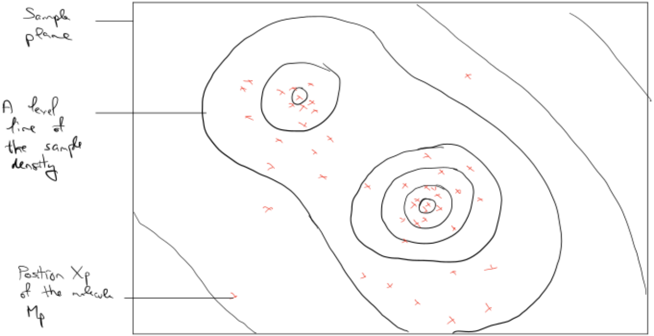
Contents

Contents

General framework

The sample distribution

Figure: Spatial distribution f_X in m^{-2} and a sample $(X_1, \ldots, X_n)$ from it



General framework

The sampling design

- <u>Discrete sampling</u>: the laser stops at q different spots $(y_1, \ldots, y_q)$ for a fixed duration t_0;
- <u>Continuous sampling</u>: the laser is driven along a path Γ and its position at time t is $\Gamma(t)$;

Figure: Sampling design $(y_1, \ldots, y_q)$ in spot mode

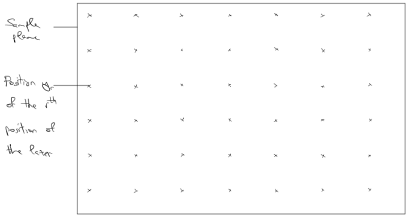


Figure: Sampling design Γ in raster mode

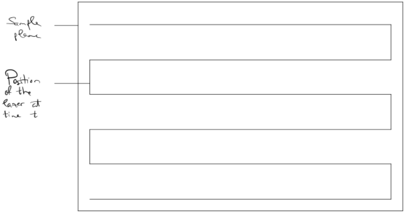


Figure: Laser irradiance $I(x)$ in $W.m^{-2}$

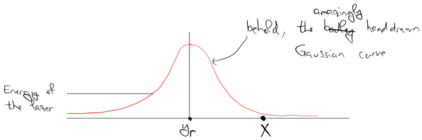


Figure: Ionisation probability function $\mathscr{I}_{\mathbb{P}}(t, y_r - X)$

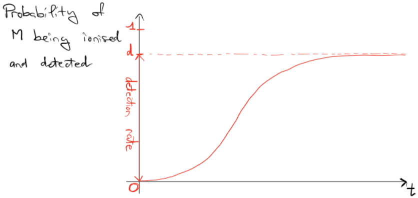
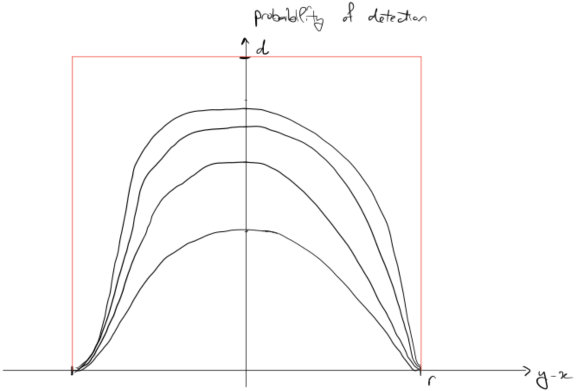


Figure: Ionisation probability function $\mathscr{I}_{\mathbb{P}}(t_0, y-x)$ for different values of t_0



Recorded position: Y is the position of the laser when the molecule is detected;

$$\mathbb{P}(Y = y_r) = (\mathscr{I}_{\mathbb{P}}(t_0, \cdot) \star f_x)(y_r)$$

Figure: The sampling design

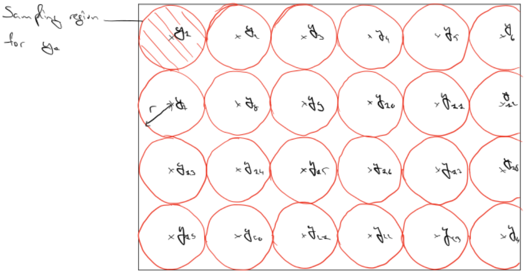


Image:

- 1 pixel $=1$ laser position
- pixel r contains $Z_r = \frac{1}{n}\sum_{p=1}^{n} \mathbb{1}_{\{Y_p = y_r\}}$

$$\mathbb{P}(Z_r = p) = \binom{n}{n \cdot p} \cdot ((\mathscr{I}_{\mathbb{P}}(t_0,\cdot) \star f_X)(y_r))^{n \cdot p} \cdot (1 - (\mathscr{I}_{\mathbb{P}}(t_0,\cdot) \star f_X)(y_r))^{n \cdot (1-p)}$$

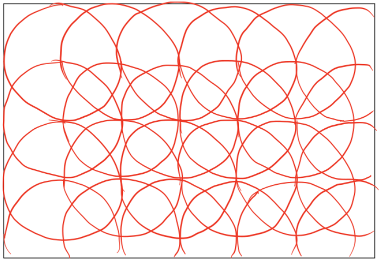
$$\mathbb{E}\left[Z_r\right] = (\mathscr{I}_{\mathbb{P}}(t_0,\cdot) \star f_X)(y_r)$$

$$\mathbb{V}\left[Z_r\right] \leq \frac{1}{4 \cdot n}$$

Recorded position: Y is the position of the laser when the molecule is detected;

$$\mathbb{P}(Y = y_r) = (\mathscr{I}_{\mathbb{P}}(t_0, \cdot) \star f_x)(y_r) \cdot \prod_{s=1}^{r-1} (1 - (\mathscr{I}_{\mathbb{P}}(t_0, \cdot) \star f_X)(y_s))$$

Figure: The sampling design



Oversampling: Distribution of the observation

$$\mathbb{P}(Z_r = p) = \binom{n}{n \cdot p} \cdot (\mathbb{P}(Y = y_r))^{n \cdot p} \cdot (1 - \mathbb{P}(Y = y_r))^{n \cdot (1-p)}$$

$$\mathbb{E}[Z_r] = (\mathbb{P} \star f_x)(y_r) \cdot \prod_{s=1}^{r-1} (1 - (\mathbb{P} \star f_X)(y_s))$$

$$\mathbb{V}[Z_r] \leq \frac{1}{4 \cdot n}$$

Contents

MSI spatial distribution: a proposal for modelling

What is the point?

- Instrument response estimation
- Image correction

Figure: Data in 2D

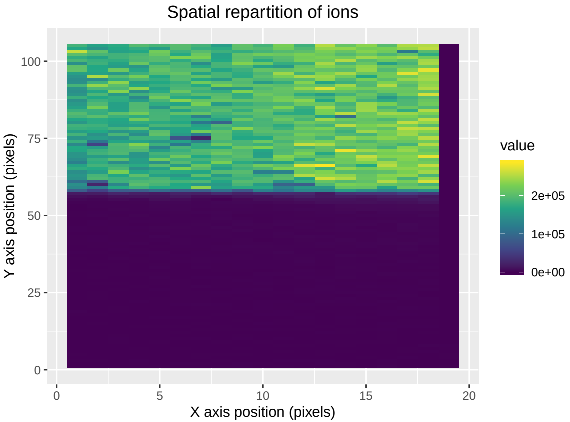


Figure: Data in 1D

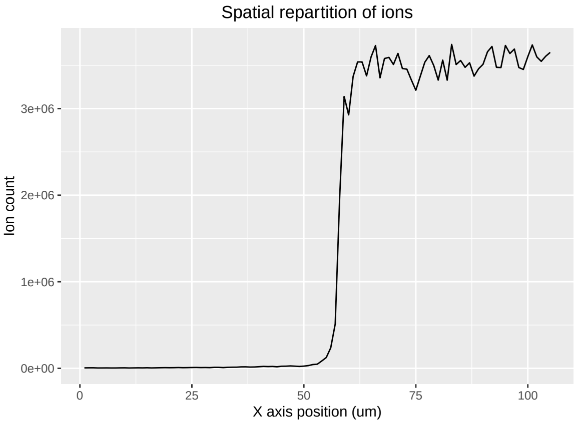


Figure: Spectra of the data in 2D

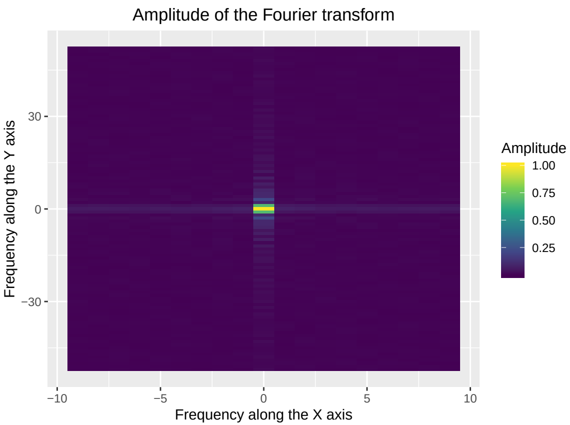


Figure: Spectra of the data in 1D

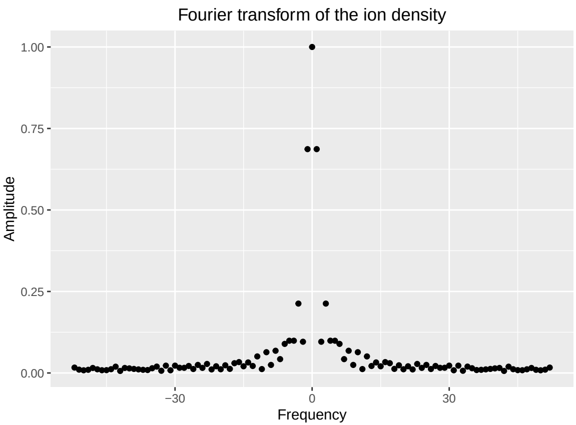


Figure: Adaptive shrinkage estimator in 1D

Figure: Edge in 2D

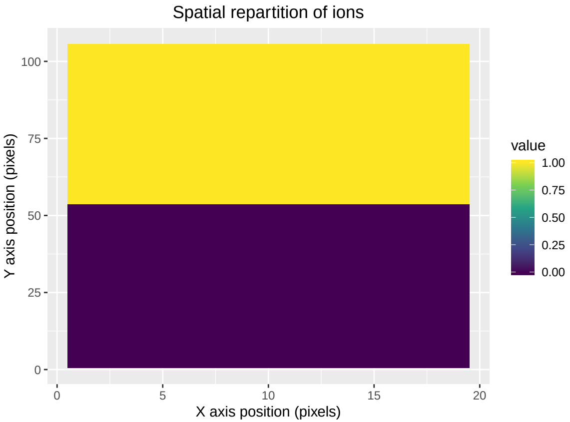


Figure: Edge in 1D

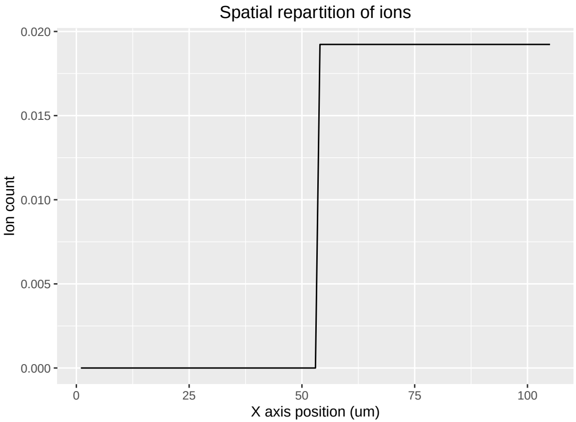


Figure: Spectra of the edge in 2D

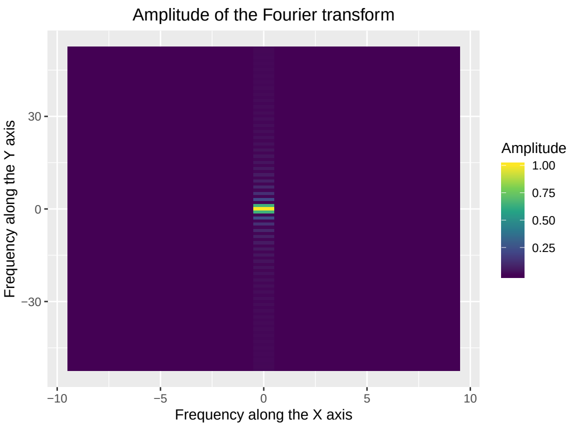


Figure: Spectra of the edge in 1D

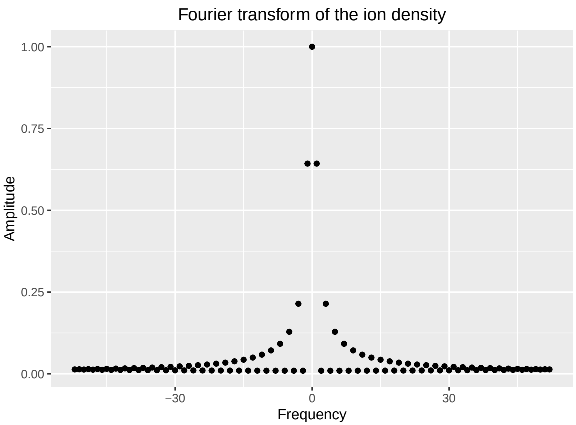


Figure: Adaptive shrinkage estimator of $\mathscr{I}_{\mathbb{P}}(t_0, \cdot)$ in 1D

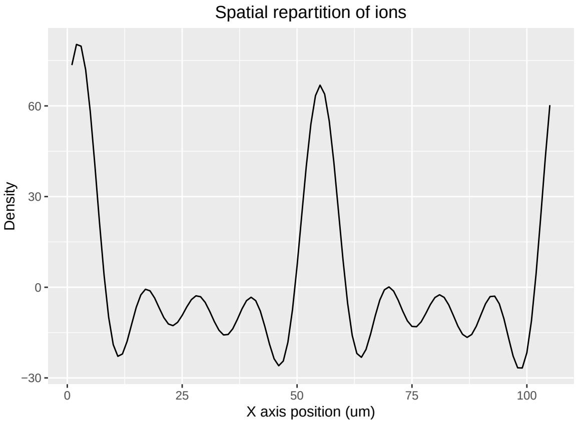
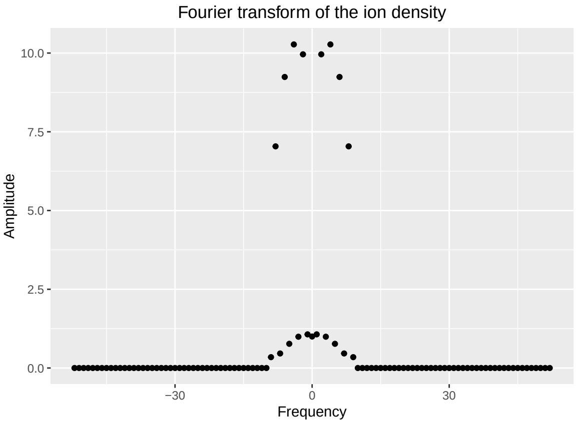


Figure: Adaptive shrinkage estimator of $\mathscr{I}_{\mathbb{P}}(t_0, \cdot)$ in 1D



- complete implementation in 2D;
- estimate quantiles of $\mathscr{I}_{\mathbb{P}}$;
- confidence bands for $\mathscr{I}_{\mathbb{P}}$;
- far future (spatial statistic): from estimations of $\mathscr{I}_{\mathbb{P}}$ for a set of parameters (time, laser profile, end-member nature,...) estimate it for new values of parameters.

Image correction

- Given: an estimate $\widehat{\mathscr{I}_{\mathbb{P}}}$ of $\mathscr{I}_{\mathbb{P}}$ and an image $(Z_r)_{r\in[\![1,q]\!]}$ of a sample with unknown end-member spatial distribution f_X;
- Goal: estimate f_X by deconvolving $\widehat{\mathscr{I}_{\mathbb{P}}}$ from $(Z_r)_{r\in[\![1,q]\!]}$.