MULTI-TARGET DETECTION WITH THE GENERALIZED METHOD OF MOMENTS

Shay Kreymer, Asaf Abas, Ye'Ela Shalit, Ran Weber, Tamir Bendory

School of Electrical Engineering, Tel Aviv University, Tel Aviv, Israel

ABSTRACT

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Index Terms— One, two, three, four, five

1. INTRODUCTION

We study the multi-target detection (MTD) problem of estimating a target signal $x : \{0, \ldots, L-1\} \rightarrow \mathbb{R}$ from a noisy measurement that contains multiple copies of the signal, each randomly translated [1], [2], [3], [4], [5], [6]. Specifically, let $y : \{0, \ldots, N-1\} \rightarrow \mathbb{R}$ be a measurement of the form

$$y[\ell] = \sum_{i=1}^{p} x[\ell - \ell_i] + \varepsilon[\ell], \tag{1}$$

where $\{\ell_i\}_{i=1}^{p} \in \{L+1, \ldots, N-L\}$ are arbitrary translations, and $\varepsilon[\ell]$ is i.i.d. Gaussian noise with zero mean and variance σ^2.

The translations and the number of occurrences of x in y are unknown. Figure 1 presents an example of a measurement y at different signal-to-noise ratios (SNRs). We define SNR $:= \frac{\|x\|_F^2}{L\sigma^2}$, where L is the length of x (in pixels), and σ^2 is the noise variance.

The MTD model arises in several scientific applications, such as passive radar [7], astronomy [8], motion deblurring [9], and system identification [10]. In particular, it serves as mathematical abstraction of the cryo-electron microscopy (cryo-EM) technology for macromolecular structure determination [11], [12], [13]. In a cryo-EM experiment [14], biological macromolecules suspended in a liquid solution are rapidly frozen into a thin ice layer. An electron beam then passes through the sample, and a two-dimensional tomographic projection is recorded. Importantly, the 2-D location

and 3-D orientation of particles within the ice are random and unknown. This measurement, called *micrograph*, is affected by high noise levels and the optical configuration of the microscope. This transformation is typically modeled as a convolution of the model (1) with a point spread function, whose Fourier transform is called contrast transfer function (CTF) [15], [16].

In the current analysis workflow of cryo-EM data [17], [18], [19], the 2-D projections are first detected and extracted from the micrograph, and later rotationally and translationally aligned to reconstruct the 3-D molecular structure. This approach fails for small molecules, which induce low contrast, and thus low SNR. This makes them difficult to detect and align [6], [11], [17], [20], rendering current cryo-EM algorithmic pipeline ineffective. For example, in the limit SNR $\rightarrow 0$, reliable detection of signals' locations within the measurement is impossible [6, Proposition 3.1].

The MTD model was devised in [6] in order to study the recovery of small molecules directly from the micrograph, below the current detection limit of cryo-EM [11], [21]. An autocorrelation analysis technique (see Section 2.1) was implemented to recover low-resolution 3-D structures from noiseless simulated data under a simplified model. Autocorrelation analysis consists of finding an image that best explains the empirical autocorrelations of the measurement. For any noise level, those autocorrelations can be estimated to any desired accuracy for sufficiently large N. Computing the autocorrelations is straightforward and requires only one pass over the data, which is advantageous for massively large datasets, such as cryo-EM datasets [17]. As such, autocorrelation analysis provides an attractive alternative to other computational methods, such as maximum likelihood estimation, which is intractable for the MTD problem [2].
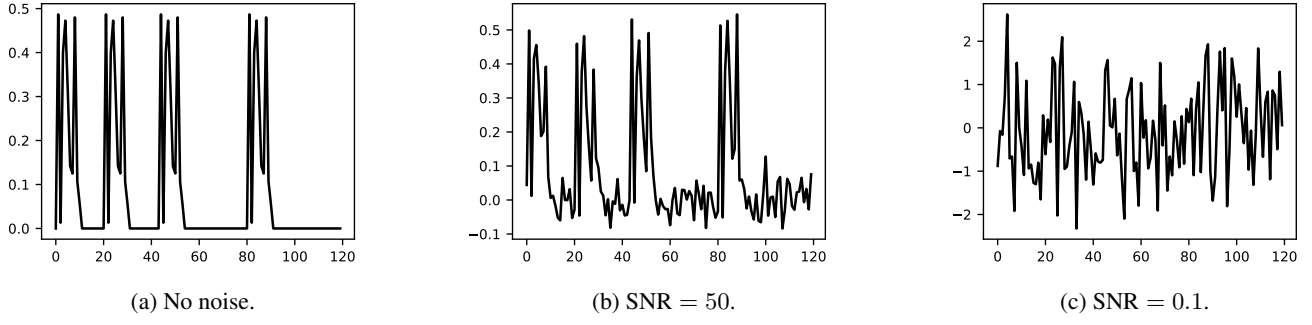
2. MATHEMATICAL FRAMEWORK

2.1. Autocorrelation analysis

The autocorrelation of order q of a random signal $z \in \mathbb{R}^N$ is defined as

$$A_z^q[\ell_1, \ldots, \ell_{q-1}] := \mathbb{E}_z \Big[\frac{1}{N^2} \sum_{i \in \mathbb{R}^2} z[i] z[i+\ell_1] \cdots z[i+\ell_{q-1}] \Big], \tag{2}$$

(a) No noise.   (b) SNR = 50.   (c) SNR = 0.1.

Fig. 1: Three measurements y from (1) at different noise levels: no noise (left); SNR = 50 (middle); SNR = 0.1 (right). Each measurement contains multiple copies of the target signal in arbitrary locations. In this work, our goal is to estimate the target signal directly from y. We focus on the low SNR regime (e.g., panel (c)) in which the signal occurrences are swamped by the noise, and the locations of the signal occurrences cannot be detected reliably.

where $\ell_1, \ldots, \ell_{q-1}$ are integer shifts. Indexing out of bounds is zero-padded, that is, $z[i] = 0$ out of the range $\{0, \ldots, N-1\}$. In this work, we use the first three autocorrelations which are explicitly given by

$$A_z^1 = \mathbb{E}_z \left[\frac{1}{N} \sum_{i \in \mathbb{Z}} z[i] \right], \tag{3}$$

$$A_z^2[\ell] = \mathbb{E}_z \left[\frac{1}{N} \sum_{i \in \mathbb{Z}} z[i]\, z[i+\ell] \right], \tag{4}$$

$$A_z^3[\ell_1, \ell_2] = \mathbb{E}_z \left[\frac{1}{N} \sum_{i \in \mathbb{Z}} z[i]\, z[i+\ell_1]\, z[i+\ell_2] \right]. \tag{5}$$

As N grows indefinitely, the empirical autocorrelations of z almost surely (a.s.) converge to the population autocorrelations of z:

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i \in \mathbb{Z}^2} z[i]z[i+\ell_1] \cdots z[i+\ell_{q-1}] \stackrel{\text{a.s.}}{=} A_z^q[\ell_1, \ldots, \ell_{q-1}]. \tag{6}$$

Our goal is to relate the autocorrelations of the measurement with the target signal x. In particular, the first-order autocorrelation is defined as

$$A_y^1 := \frac{1}{N} \sum_{i \in \mathbb{Z}} y[i]. \tag{7}$$

This is the mean of the measurement. The second-order autocorrelation of y, $A_y^2 : \mathbb{Z} \to \mathbb{R}$, is defined by

$$A_y^2[\ell_1] := \frac{1}{N} \sum_{i \in \mathbb{Z}} y[i]y[i+\ell_1], \tag{8}$$

and the third-order autocorrelation $A_y^3 : \mathbb{Z}y \times \mathbb{Z} \to \mathbb{R}$ by

$$A_M^3[\ell_1, \ell_2] := \frac{1}{N} \sum_{i \in \mathbb{Z}} y[i]y[i+\ell_1]y[i+\ell_2]. \tag{9}$$

2.2. Generalized method of moments

3. NUMERICAL EXPERIMENTS

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4. CONCLUSION

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