

Generalized method for the computational phase correction of arbitrary dual comb signals

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Received 4 April 2019; revised 5 May 2019; accepted 6 May 2019; posted 9 May 2019 (Doc. ID 364262); published 4 June 2019

We demonstrate a computational phase correction algorithm that is able to correct for phase and timing fluctuations of arbitrary dual comb spectra. By augmenting a Kalman filter with a global search and decoupling the interferogram estimation, we show that dual comb signals having a wide range of structures can be predicted and corrected. Furthermore, we derive an upper bound for the accuracy of any self-correction technique and show that the augmented filter is capable of reaching this bound when the phase and frequency noise are bandlimited. Finally, we show how expectation maximization can be used to learn the statistical parameters of a system without any free parameters. This approach is hands-off, robust, and accurate for a wide range of dual comb systems. Demonstration code is provided. © 2019 Optical Society of America

<https://doi.org/10.1364/OL.44.002966>

Dual comb spectroscopy is a powerful technique that allows for the collection of optical spectra using only electrical techniques, in which a radio frequency comb is generated from the multi-heterodyne beating of two optical combs [1,2]. Its performance is often limited by the mutual coherence of the two combs, as incoherence broadens the linewidth of each tooth. This distorts the spectrum when the broadening is small and makes it unusable when the broadening is large. In laboratory environments, mutual coherence can be sustained for seconds, or even hours [3–5], but this is more difficult in chip-scale systems. Adaptive sampling approaches can correct for incoherence by making use of extra reference channels [6,7], but increase system complexity and power consumption. One can also self-correct spectra using only digital techniques [8–11], which is appealing for portable applications, since it requires no additional optics.

Unfortunately, while self-correction techniques have been shown to be effective in a particular use case, they are highly dependent on the structure of the problem. The extended Kalman filter (EKF) [8] and computational coherent averaging [11] approaches track the frequencies of the RF comb's lines continuously in time, making them well-suited for quasi-continuous dual comb systems that lack a center burst (e.g., passive quantum cascade laser [QCL] combs [12,13], electro-optic combs [3], some microresonator combs [14], and

quantum well diode lasers [15]). Though, in principle, they can be applied to the dual comb signal generated by pulsed lasers, and the resulting correction may even *look* reasonable, upon closer inspection one can find that the extracted amplitudes and phases are sometimes inaccurate. By contrast, the ambiguity function and cross-correlation approaches [9,10] are well-suited for pulsed lasers, but are more difficult to apply to quasi-continuous interferograms without clear boundaries. In low signal-to-noise ratio (SNR) conditions they will also become less accurate, as they do not account for the statistics of the underlying phase noise. Here we demonstrate an algorithm that combines the best features of all approaches—the accurate statistical representation of the Kalman filter and the robustness of batch interferogram processing—to correct all manner of comb spectra. We also investigate the fundamental limits of self-correction and show that this method achieves those limits. (The demonstration code is available in [Code 1](#), Ref. [16].)

We assume that the dual comb's RF spectrum is represented by a complex signal $y(t) = \sum_n A_n e^{i\phi_n(t)}$, where A_n is the complex amplitude of the n th comb line, and $\phi_n = \phi_0 + n\phi_r$, the corresponding phase. (ϕ_0 and ϕ_r are the offset and repetition rate phases of the RF comb; f_0 and f_r are the frequencies.) We wish to accomplish two objectives at once:

1. For data sampled at discrete times t_k , we wish to find amplitudes and phases that best fit the data. Collecting all of them into a state variable x_k , we essentially wish to find the x_k 's that minimize $\sum_k |y_k - h(x_k)|^2$, where $h(x_k) = \sum_n A_n e^{i\phi_{nk}}$ is a nonlinear measurement function.
2. The phases at different times should be related. In the absence of phase noise, we expect $\phi_{0,k+1} = \phi_{0,k} + \omega_{0,k}\Delta t$ and $\phi_{r,k+1} = \phi_{r,k} + \omega_{r,k}\Delta t$. Calling this relation $f(x_k)$ the process function, we wish to minimize $\sum_k |f(x_k) - x_{k+1}|^2$.

If the measurement is perturbed by additive white Gaussian noise with covariance $2\sigma^2$ and process noise covariance Q_k , we can combine these by minimizing the cost: $J = \|x_0 - x_p\|_{P^{-1}}^2 + \sum_k \frac{1}{\sigma^2} |y_k - h(x_k)|^2 + \|f(x_k) - x_{k+1}\|_{Q_k^{-1}}^2$, where $\|x\|_C^2 \equiv x^T C x$ weights the covariances, and where x_p and P represent the prior mean and covariance. This cost is extremely general and is implicitly what was minimized by all previously demonstrated methods.

Though nonlinear Kalman filters can converge to a local minimum of the cost, they cannot guarantee convergence at

all or to a global minimum. Solving this problem, in general, is difficult, because the measurement component contains many sinusoidal terms that make it highly non-convex. We make two assumptions that greatly simplify the problem. First, we assume that the amplitudes and phases of the N comb lines (i.e., the interferogram) are slowly varying; they can then be determined by demodulation. This means that we only have four state variables, rather than the $2N + 4$ that are needed to keep track of all of the amplitudes and phases. Secondly, we collect all of the process noise of a finite length of data into a single time—making it 0 for all times in between—and divide the data into batches of length M , where $M\Delta t \sim 1/f_r$. We then minimize a simpler expression for each batch:

$$J_b(x) = \|x - x_p\|_{P^{-1}}^2 + \sum_{k=0}^{M-1} \frac{1}{\sigma^2} |y_k - h_k(x)|^2, \quad (1)$$

where $x = [\phi_0, \phi_r, \omega_0, \omega_r]^T$ is the state of the system at the first time in the batch, P is the prior covariance at the start of the batch, and the measurement h_k now includes phase evolution, i.e., $h_k(x) = \sum_n A_n e^{i(\phi_0 + \omega_0 t_k + n(\phi_r + \omega_r t_k))}$. In other words, Eq. (1) assumes that the phase is piecewise linear; this requires that the phase and frequency noise be bandlimited to $f_r/2$.

Minimizing J_b solves a maximum a posteriori problem, selecting the measurement component at low noise levels and the prior at high noise levels. It is well-known that Eq. (1) can be locally minimized using iterated EKF [17], as the approach essentially mimics Gauss–Newton minimization. Unfortunately, this local minimum is frequently suboptimal, so a global search strategy must be employed. ϕ_0 represents a global phase and can quickly be found, given the other three parameters. The remaining parameters can be found by constructing a discrete grid that ranges over their possible values, using fast Fourier transform (FFT) methods to rapidly evaluate (1) over the grid. In addition, all sums of the form $p(t) = \sum_n A_n e^{i2\pi n t}$ can be avoided by placing the A_n 's onto a grid, using an FFT to compute $p(t)$, and interpolating, a process that is significantly faster than a direct summation when N is large. After J_b is minimized for a given batch, the state and covariance are updated using the usual iterated EKF update relations, and the complex amplitude of the n th line is estimated by demodulation ($A_n = \langle y_k e^{-i\phi_{n,k}} \rangle$). Once this has been done for all batches, the phases are resampled onto the original time grid and filtered to remove any residual components above $f_r/2$.

This approach combines many of the advantages of previous approaches. The approach in Ref. [8] can correctly reproduce spectra, even in the case of large phase noise and low signal-to-noise levels, but can converge to false minima (particularly at rational number multiples of the repetition rate). Here this problem is eliminated by the global search. The method in Ref. [9], by contrast, works well for pulsed lasers with thousands of lines, but ignores the statistics of the underlying noise. [One can show that maximizing the ambiguity function maximizes the measurement term of Eq. (1) alone.] Thus, its performance will suffer in high-noise conditions.

In order to assess the efficacy of this approach, we first focus on two types of synthesized data. First, we consider a quasi-continuous comb with relatively few lines ($N_l = 100$) and a repetition rate of 5 MHz, similar to multiheterodyne signals generated by (QCLs) [12,13,18] and some microresonators [14]. Next, we consider a comb with many lines

($N_l = 4000$) and a repetition rate of 10 kHz, similar to the signal generated by the mode-locked lasers in Ref. [9]. Since spectral leakage between nearby lines frequently occurs with suboptimal techniques, we impose deep absorption features onto the dual comb spectra to see whether leakage occurs. The offset noise in the two cases has peak-to-peak fluctuations of $8f_r$ and $15f_r$ for the continuous and pulsed signals, respectively, ensuring that both spectra are fully mutually incoherent.

Figure 1(a) shows the result of this correction for the case of a quasi-continuous comb. The raw data are shown in red, the corrected data are shown in blue, and the actual amplitudes are shown in orange. Note that the correction is essentially perfect and practically the comb's entire spectrum is captured by the correction. As a result, the agreement between the true amplitudes and the corrected amplitudes is excellent. This is also evident in the time domain, which is shown in Fig. 1(b). The extracted frequency noise and the actual frequency noise agree extremely well, a consequence of the fact that Kalman filters can nearly perfectly estimate signals when the linearization is adequate. Figure 2 shows the same results for the case of the mode-locked laser. The RF comb is significantly denser and contains many more lines, but the correction nonetheless remains accurate. In terms of the computation time, on a typical computer, Fig. 1 requires 10 s to process 100 μ s of data, while Fig. 2 requires 30 s to process 70 ms of data.

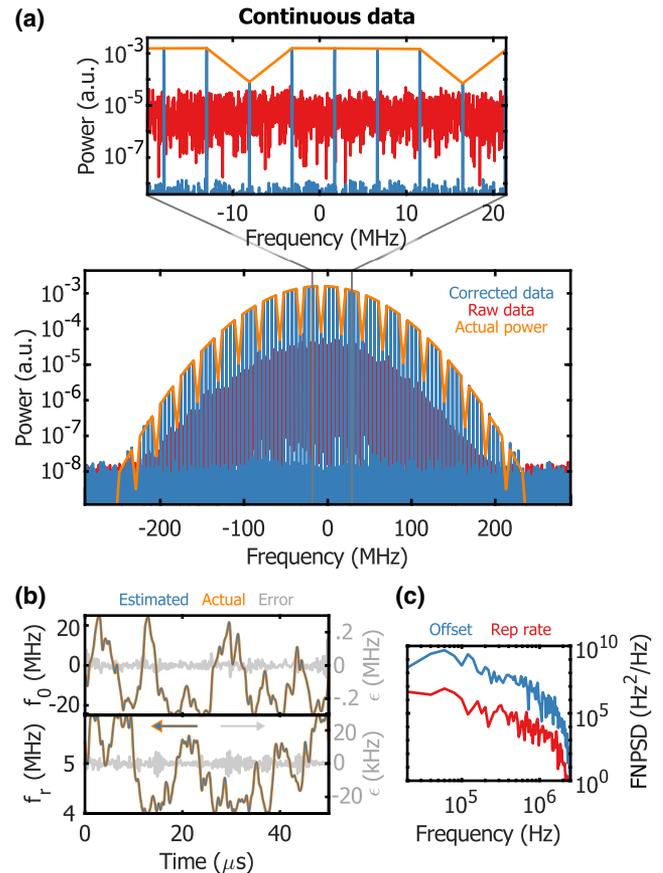


Fig. 1. (a) Frequency-domain correction of a quasi-continuous signal using an augmented Kalman filter. The accuracy is limited only by measurement noise [residuals plotted in Fig. 3(a)]. (b) Extracted frequencies in the time domain. (c) Power spectral densities of f_0 and f_r .

(The calculation time is dominated by the grid search; in principle this can be parallelized by GPU processing.)

Of course, for spectroscopy, the ultimate test is not whether or not these methods can reproduce the underlying frequency noise, but whether or not they can correctly reproduce the underlying spectra. In fact, there is a fundamental limit to how accurately any data can be used to phase-correct itself. Consider the case of a single line with phase noise. If the phase noise is known, its power can be estimated by using simple demodulation and taking the magnitude squared of the result (i.e., homodyne detection). This is the *coherent* power estimate. When the phase noise is not known, one must estimate the power by integrating the power spectrum over its bandwidth. This is the *incoherent* estimate, and is equivalent to taking the phase of the signal and using that to perform self-correction. One can show that in the presence of additive white Gaussian measurement noise with covariance $2\sigma^2$, the variance of the power estimate of a line with power P using N samples will be given by

$$\sigma_{\text{coherent}}^2 = \frac{4\sigma^2}{N} \left(P + \frac{\sigma^2}{N} \right), \quad \sigma_{\text{incoherent}}^2 = \frac{4\sigma^2}{N} (P + \sigma^2). \quad (2)$$

When N is large, the coherent power estimate has a SNR that is a factor of $1 + \frac{\sigma^2}{P}$ larger. This increase of $\frac{\sigma^2}{P}$ is exactly the variance associated with the estimate of the phase of a signal given noisy measurements, because the increase in the SNR in the coherent case can be interpreted as coming from the fact that we are supplied with the phase and do not need to estimate it. For weak signals ($P \ll \sigma^2$), the increase is dramatic, explaining

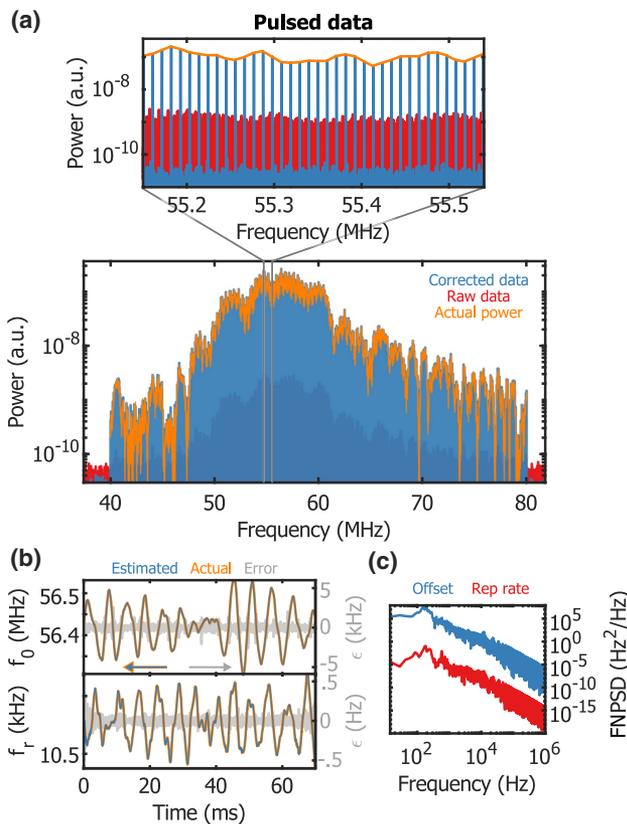


Fig. 2. (a) Frequency-domain correction of a pulsed signal using an interferogram-augmented Kalman filter [residuals plotted in Fig. 3(b)]. (b) Extracted frequency fluctuations in the time domain. (c) Power spectral densities of f_0 and f_r .

why homodyne detection is generally needed to recover them. For strong signals, this gain is small, and coherent integration is not much better than incoherent integration.

What limit should apply in the multiheterodyne case? Despite the fact that we do not have a clean phase reference, we are using all of the comb's lines to estimate the phase and timing signal. In other words, the power that goes into the phase and timing estimation is effectively the power of the whole comb, not just the power of a single line (i.e., P is large). Therefore, we can expect to obtain results that are close to the *coherent* estimate. This is confirmed in Figs. 3(a) and 3(b), which plots the residual of our corrected power estimates for the spectra shown above. Note that in both cases we are able to reach the coherent limit, even though there is no coherent reference; the phase reference is derived from the other lines. Even weak lines originally below the noise floor will reappear once corrected, similar to what happens in the homodyne measurements of weak signals. The correction is optimal, provided that we satisfy the constraint that the underlying phase and frequency noise are bandlimited. Only noise outside $f_r/2$ deg rades the correction [Figs. 3(c) and 3(d)].

Lastly, we examine the issue of hyperparameters. Until now, we have made a critical assumption about the system being corrected: that its noise statistics Q and σ^2 are known and correctly modeled. However, for most real data, we do not have these parameters. The measurement noise can be quickly ascertained by examining the white noise level of the signal, but the process noise Q can be much more elusive, since it reflects the phase noise statistics of the signal we are trying to estimate. Not only can phase noise have components of different color (for example, due to a mixture of white and Brownian frequency noise), but it can also be strongly correlated. For example, in semiconductor lasers, both offset and repetition rate fluctuations can be

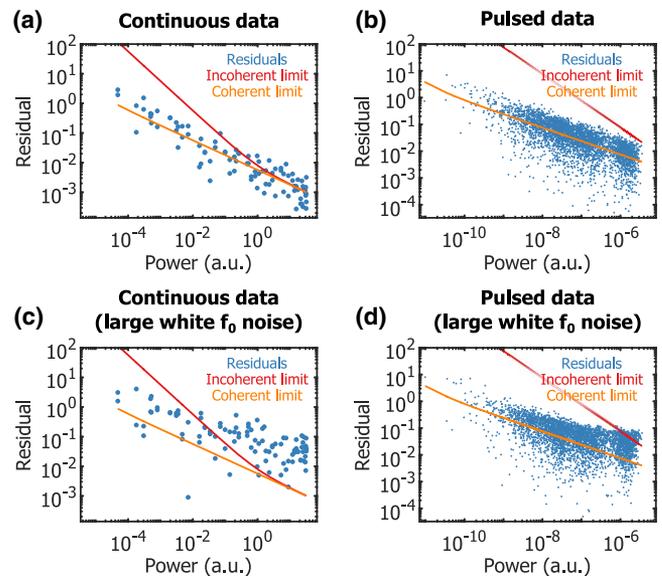


Fig. 3. (a), (b) Fractional error corresponding to the spectra in Figs. 1 and 2, respectively, along with σ_{coherent} and $\sigma_{\text{incoherent}}$. In both cases, the residuals closely match the coherent estimate's standard deviation, so the augmented filter achieves the best possible SNR. (c), (d) Residuals of the previous cases with extra white frequency noise (20 MHz and 400 kHz, respectively, causing phase walk of variance $(\pi/2)^2$ per $1/f_r$). The correction suffers, but remains informative.

generated by current fluctuations, changing both the refractive index and the intracavity power [19]. Ideally, we would like to estimate Q from our data, but this amounts to an intractable maximum likelihood estimation problem. Instead, we solve it iteratively by employing the well-known *expectation maximization* (EM) algorithm [20]. In essence, we alternate between two steps: expectation—running the augmented Kalman filter using a given $Q^{(i)}$ —and maximization—choosing $Q^{(i+1)}$ by maximizing the log-likelihood of the filter output, finding

$$\begin{aligned} \arg \min_Q \sum_b \text{Tr} Q^{-1} \langle (x_{b+1} - f(x_b))(x_{b+1} - f(x_b))^T \rangle - \ln |Q^{-1}| \\ = \frac{1}{N_b - 1} \sum_b \langle (x_{b+1} - f(x_b))(x_{b+1} - f(x_b))^T \rangle. \end{aligned}$$

An initial guess of $Q^{(1)}$ must be provided, but for all systems tested it is extremely well-behaved and practically always converges, even when initialized many orders of magnitude away from the underlying statistics. A similar expression can be derived for the measurement noise, allowing the EM algorithm to efficiently learn all of the relevant statistics— σ^2 and the 10 components of Q . Figure 4(a) shows the result of this process for the quasi-continuous data with wildly different initial conditions (Q and σ^2 ranging across six orders of magnitude). In each case, the EM algorithm converges to the same optimal value in just a few iterations. Because EM is iterative, it requires that the filter be run several times, a process which can be time-consuming. Fortunately, provided the noise is stationary, it does not need to be performed frequently, or even for an entire set of data. It need only be performed on a small subset of the data collected and can be subsequently reused.

Figure 4(b) shows the result of correction during the EM process. When $Q^{(1)}$ is poorly chosen, the resulting correction is inaccurate, and the residual is far from the white noise level.

However, by running EM, all the correct parameters are found, and the spectrum is well-corrected. Figure 4(c) shows the result of running EM on terahertz QCL dual comb data [8]. With a poor choice of $Q^{(1)}$ one still obtains a correction that looks reasonable but, upon closer inspection, it is actually smeared out: different lines leak into their neighbors. The lines indicated by arrows are initially thought to differ by only 11 dB, but subsequent iterations show them to be 28 dB apart. Convergence occurs rapidly, and iterations 2 and 3 are practically identical. Interestingly, the final value of Q has a Pearson correlation coefficient of $\rho_{f_0, f_r} = 0.6$, indicating a strong correlation between f_0 and f_r noise.

In conclusion, we have demonstrated a method by which the phase and timing noise of an arbitrary mutually incoherent comb can be computationally corrected. By augmenting a Kalman filter with a global search, we have shown that both quasi-continuous and pulsed dual comb signals can be accurately corrected. We showed that power estimates derived from this method can approach the estimates of a mutually coherent comb—limited only by the SNR of the underlying signal—and demonstrated how EM could be used to learn the statistics of a system without any free parameters [16].

Acknowledgment. The authors thank Yang Yang and Qing Hu for use of the QCL data and Bradley Smith, Matthew Day, and Steve Cundiff for valuable discussions.

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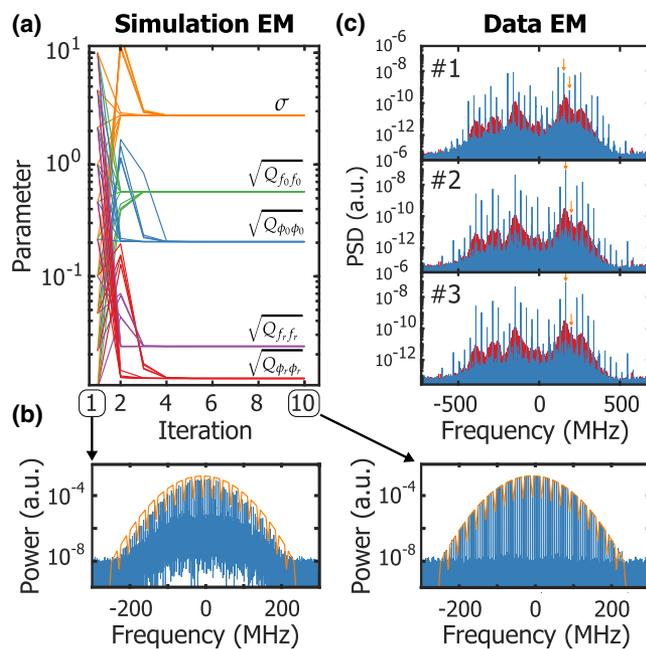


Fig. 4. (a) Expectation maximization convergence on continuous data with widely varying initial conditions. (b) Correction results after the first and last iteration. (c) First three iterations of EM running on real dual comb data, with poor initialization of Q .