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LOCAL REGULARIZATION METHODS FOR INVERSE VOLTERRA EQUATIONS APPLICABLE TO THE STRUCTURE OF SOLID SURFACES

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ABSTRACT. Deconvolution of appearance potential spectra is an old strategy commonly used to investigate electronic properties of solids in the surface region. Recently, this strategy was found to be effective in the study of nanostructures. In this context, the density of unoccupied states in the surface region of a solid is recovered from the measured AP-spectrum data from the governing equation $k * x * x = g$, where k is a Lorentzian type function, g is a measured APS-signal and x is the density function to be recovered. As an important step in solving for x, we need to solve the autoconvolution problem $x * x = f$, which is a nonlinear ill-posed Volterra problem. In this paper, we first improve upon the existing local regularization theory developed in [**9**] for solving the autoconvolution problem, allowing for L_p data, where $1 \leq p \leq \infty$. We prove the solutions of the regularized equation $x_\alpha^{\delta} \in L_\infty(0,1)$ (smoother than $x_\alpha^\delta \in L_2(0,1)$ as in [**9**]) converge to the true solution $\overline{x}$ of the autoconvolution equation in L_∞ norm (stronger than L_2 norm as in [**9**]) when the noise level in the data shrinks to 0. It is worth noting that we obtain the improved convergence theory while imposing less restrictions on the true solution $\overline{x}$; namely $\overline{x} \in C^1(0,1)$ in contrast to $\overline{x} \in W^{2,\infty}(0,1)$. Further, for the stable deconvolution of appearance potential spectra, we apply the local regularization methods to solve a combination of two ill-posed Volterra problems: the linear problem of determining f from $f * k = g$ and then the nonlinear autoconvolution problem of determining x from $x * x = f$. The results include a convergence theory and a fast sequential numerical method which essentially preserves the causal nature of the combined deconvolution problem. Numerical examples are included to show the effectiveness and efficiency of the methods.

1. Introduction. In this paper we first consider the inverse autoconvolution problem of finding $\overline{x} \in L_\infty(0,T)$ solving

$$G(x) = f, \tag{1}$$

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where G is the nonlinear Volterra operator given by

$$G(x)(t) = x * x = \int_0^t x(t-s)\, x(s)\, ds, \quad \text{a.e. } t \in (0,T), \tag{2}$$

and where $f \in \operatorname{Range}(G) \subseteq L_p(0,T)$ for $1 \le p \le \infty$. Without loss of generality, we will henceforth let $T = 1$.

The autoconvolution problem is ill-posed due to the lack of continuous dependence of solutions $\overline{x}$ on data f [**14–16, 18**]. Indeed, for $D(G) \equiv \{x \in L_2(0,1), x(t) \ge 0, \text{ a.e. } t \in (0,1)\}$, the operator $G : D(G) \subset L_2(0,1) \mapsto L_2(0,1)$ is such that the inverse autoconvolution operator G^{-1} is discontinuous at every point f in the range of G; i.e., the autoconvolution equation is locally ill-posed at every point x in $D(G)$. The degree of ill-posedness depends on both the smoothness of the solution $\overline{x}$ and the behavior of $\overline{x}$ at 0 [**16, 18**]. In practice, we only have access to perturbed data f^δ and need to use this noisy data to recover $\overline{x}$. Therefore, regularization methods need to be employed in order to stably solve the autoconvolution problem.

Three main regularization methods for the autoconvolution equation currently exist in the literature: Tikhonov regularization [**13, 18, 40**], Lavrent'ev regularization [**22, 23**] and local regularization [**9**]. It was established in [**9**] that local regularization methods compare favorably to Tikhonov and Lavrent'ev regularization in solving the nonlinear autoconvolution equation, especially in recovering sharp features of the unknown solution. In the following, we will briefly summarize the existing results in comparing these three regularization methods in solving the autoconvolution equation.

The nonlinear autoconvolution equation is Volterra with a causal nature. When solved using the standard discretization without any regularization, we can expect a fast sequential algorithm. As is well known in the case of linear Volterra problems, classical regularization methods, such as Tikhonov, destroys the causal nature of the Volterra problems, generating a full domain problem that is numerically expensive. This disadvantage is only magnified when we have to solve a nonlinear equation at every step. In contrast, both Lavrent'ev and local regularization preserve the casual nature of the autoconvolution problem, leading to fast sequential numerical solutions. As a matter of fact, the cost of the numerical method of local regularization as proposed in

[**9**] is $\mathcal{O}(rN^2 - r^2N)$, which is similar to that of solving the problem without any regularization. The Lavrent'ev is likely to have similar operational counts. Without operation counts available for Tikhonov regularization applied to this nonlinear problem, we will simply point out that the cost of Tikhonov regularization on a general *linear* problem is $\mathcal{O}(N^3)$ flops. As seen from the numerical examples studied in [**9**], the computation time for Tikhonov regularization applied to the autoconvolution problem is at least 150 times that of local regularization in recovering simple $\overline{x}$.

Both found sequentially, local regularization outperforms Lavrent'ev regularization when the signal-to-noise ratio in the data is small over a large part of the domain [**9**]. Local regularization makes use of future data in recovering the value of the solution at current time t, whereas Lavrent'ev approximation does not. The amount of future data used, α, is the regularization parameter for local regularization. Depending on the signal-to-noise ratio in the data, we can adjust α so that meaningful information from data can be used. Without such an ability for adjustment, Lavrent'ev regularization can fail to recover the solution when signal-to-noise ratio in the data is small over a large part of the domain. A modified discrepancy principle has been developed in determining α for the linear convolution problem [**3, 4**]; criteria in selecting α for nonlinear problems, including the nonlinear autoconvolution problem, is still under study.

Another important aspect that makes local regularization methods superior to both Tikhonov and Lavrent'ev regularizations is that it does not require an initial guess $x^\star$ of the unknown true solution $\overline{x}$ as the other two methods. The source conditions needed for convergence rates for Tikhonov regularization as applied to the nonlinear problem (1) require that $\overline{x} - x^\star = G'(\overline{x})^\star w$ for some $w \in L_2(0,1)$ [**12**], where $x^\star$ is an initial guess for $\overline{x}$ and $\overline{x}$ is the true solution of (1). It is not hard to show that the source condition requires that $x^\star(1) = \overline{x}(1)$; since $x^\star$ is part of the Tikhonov algorithm, the method then requires knowledge of the value of the unknown solution $\overline{x}$ at $t = 1$. It is worth noting that more recent study of the method of approximate source conditions for Tikhonov regularization for nonlinear ill-posed problems allows for more flexibility in yielding convergent solutions when the above benchmark source conditions are not satisfied [**21**]. However, the success of the method of approximate source conditions largely relies on the successful balancing of the distance occurring functions which cannot be guaranteed. In the case of Lavrent'ev regularization, it is required that $x^\star(0) = \overline{x}(0)$, which means that $\overline{x}(0)$ must be known in advance (or at least computed using regularized differentiation of noisy data). The performance of both the Lavrent'ev and Tikhonov methods seems fairly dependent on the choice of the initial guess $x^\star$ and of its closeness to $\overline{x}$. The convergence theory for local regularization does require a source condition that includes a particular relationship between $\overline{x}(0)$ and $\|\overline{x}'\|_\infty$, but the numerical methods only make use of the data f^δ without initial guess of the value of $\overline{x}$ at any point.

In [**9**], we formulated the local regularized equation for the autoconvolution problem and proved the convergence of the solution produced by this regularized equation to $\overline{x}$ as the noise level δ in the data shrinks to zero. The convergence rate of $\mathcal{O}(\delta^{2/5})$ that we obtain for L_2 data is not as good as that $\mathcal{O}(\delta^{1/2})$ obtained by Tikhonov regularization and Lavrent'ev regularization. Only with continuous data are we able to reach the $\mathcal{O}(\delta^{1/2})$ rate of these methods. We improve the convergence theory in [**9**] in several important ways. First of all, instead of restricted only to L_2 and continuous data as in [**9**], we are able to obtain our convergence theory in case data $f^\delta \in L_p(0,1)$, with the rate of convergence $\mathcal{O}(\delta^{p/(2p+1)})$, for $1 \le p \le \infty$. Note that we obtain the optimal rate of convergence $\mathcal{O}(\delta^{1/2})$ in the case of L_∞ data, as obtained by Tikhonov regularization and Lavrent'ev regularization. Secondly, we obtain smoother solutions for the regularized equation of the autoconvolution problem, namely, $x_\alpha^\delta \in L_\infty(0,1)$, rather than $x_\alpha^\delta \in L_2(0,1)$ in [**9**]. It is worth noting that these improvements are made with fewer restrictions on $\overline{x}$ than what was required in [**9**], namely, we can reduce the smoothness requirement on $\overline{x}$ from $\overline{x} \in W^2_\infty(0,1)$ to $\overline{x} \in C^1(0,1)$.

The second part of this paper applies the local regularization methods developed here for the autoconvoluation problem as well as linear Volterra problems [**24–26, 30, 31**] to the devolution of appearance potential spectra. Appearance Potential Spectroscopy (APS) is a generic term which involves several techniques such as Auger Electron Appearance Potential Spectroscopy (AEAPS), Soft X-ray Appearance Potential Spectroscopy (SXAPS) and Disappearance Potential Spectroscopy (DAPS). These techniques involve gradually increasing the energy of the exciting beam and detecting the onset of the excitation of a core level and are used to investigate electronic properties of solids in their surface region. For example, Soft X-ray appearance potential spectra from solids carry information on the local density of unoccupied states in the surface region of the sample. The total soft x-ray yield from a sample bombarded with monoenergetic electrons is measured. As the bombarding energy is varied, sharp increases occur in the radiation yield at energies given by the binding energies of core electrons. The measured signal is called an AP-spectrum of the sample. Approximately, the AP-spectrum can be considered proportional to an autoconvolution of the density function of unoccupied states in the surface region. Our goal is to determine the density of unoccupied state x from equation

$$k * x * x = g, \tag{3}$$

where g is the integrated version of AP-spectrum and the kernel k is assumed to be a Lorentzian function given by

$$k(s) = \frac{1}{1 + (s/\gamma)^2}, \quad s \in \mathbf{R};\ \gamma > 0. \tag{4}$$

This model formed the basis of a number of early models for appearance potential spectra [**1, 10, 11, 20, 37–39, 43**], and appears today in applications related to nano-structures [**17**]. Clearly, the governing equation (3) can be decomposed as a linear Volterra equation of convolution type

$$\int_0^t k(t-s)f(s) = g(t), \quad t \in [0,1], \tag{5}$$

and the nonlinear autoconvolution equation defined by (2). Therefore, determining the density function x from the governing equation (3) can be accomplished in two steps: we first determine f from the linear inverse problem (5) and then use the approximating solution as perturbed data f^δ to solve the nonlinear inverse autoconvolution problem (2). We will apply local regularization to both the outside ill-posed linear Volterra problem and the inside ill-posed nonlinear Volterra problem given that local regularization methods are well-established and well-suited in solving the linear Volterra problem (5) as well as the nonlinear autoconvolution problem (2) as described above [**9, 24–28, 30, 31**]. The result is an effective and efficient method for deconvolution of appearance potential spectra to recover the density of the unoccupied states in the surface region.

2. The regularized autoconvolution equation. Because this paper extends the ideas in [**9**], we will briefly review the ideas of the regularized autoconvolution equation.

We assume that equation (1) holds on an extended interval $[0, 1+\overline{\alpha}]$ for some small $\overline{\alpha} \in (0, 1]$, i.e., $\overline{x}$ solves

$$\int_0^{t+\rho} x(t+\rho-s)\, x(s)\, ds = f(t+\rho), \quad \text{a.e. } t \in (0,1),\ \rho \in (0,\alpha),$$

for any $0 < \alpha < \overline{\alpha}$. After splitting the integral at ρ and t and changing the variable of integration, we obtain

$$2\int_0^{\rho} x(t+\rho-s)\, x(s)\, ds + \int_\rho^{t} x(t+\rho-s)\, x(s)\, ds = f(t+\rho) \tag{6}$$

for a.e. $t \in (0,1)$, $\rho \in (0,\alpha)$. We employ an α-dependent measure $\eta = \eta(\rho) > 0$ in order to consolidate the local future information introduced by the variable ρ; that is, we integrate both sides of (6) with respect to η and obtain

$$\begin{aligned} 2\int_0^{\alpha}\int_0^{\rho} & x(t+\rho-s)\, x(s)\, ds\, d\eta(\rho) \\ &+ \int_0^{\alpha}\int_\rho^{t} x(t+\rho-s)\, x(s)\, ds\, d\eta(\rho) \\ &= \int_0^{\alpha} f(t+\rho)\, d\eta(\rho) \quad \text{a.e. } t \in (0,1). \end{aligned} \tag{7}$$

Note that $\overline{x}$ still satisfies (7) exactly.

Here, the Borel measure $\eta = \eta(\rho)$ is similarly defined as in [**9**], namely,

$$\int_0^{\alpha} g(\rho)\, d\eta(\rho) \equiv \int_0^{\alpha} g(\rho)\, \omega(\rho,\alpha)\, d\rho, \quad g \in L_2(0,\alpha), \tag{8}$$

where the family $\{\omega(\cdot,\alpha) \in L_\infty(0,\alpha)\}_{\alpha\in(0,\overline{\alpha}]}$ is such that there exist $\underline{\omega}$, $\overline{\omega} > 0$ independent of α so that

$$0 < \underline{\omega} \le \omega(\rho,\alpha) \le \overline{\omega}, \quad \text{a.e. } \rho \in (0,\alpha], \tag{9}$$

for all α sufficiently small. Note that a property for such an η is that, for any real $m \geq 0$, there exist constants $K(m) > 0$ independent of α so that

$$\frac{\int_0^\alpha \rho^m \, d\eta(\rho)}{\int_0^\alpha \rho \, d\eta(\rho)} \leq K(m)\alpha^{m-1} \tag{10}$$

for all $\alpha > 0$ sufficiently small. This class of Borel measures is frequently used in local regularization of linear and nonlinear Volterra problems ([**5–7, 24–27, 29, 30, 32, 34, 35, 41**]).

In practice, we almost always have to replace the "ideal" data f by the perturbed f^δ, in which case we need to regularize the original equation (1), or its equivalent (7) to find a suitable approximation of $\overline{x}$. Local regularization suggests that we momentarily hold x constant on a small local interval $[t, t+\alpha]$, i.e., we replace $x(t+\rho-s)$ by $x(t)$ in the first term of (7) for values of ρ, s such that $\rho - s \in [0, \alpha]$. The length of the local interval we use, α, serves as the regularization parameter. We then obtain the regularization equation

$$a_\alpha(x)x + F_\alpha(x) = f_\alpha^\delta, \tag{11}$$

where, for almost every $t \in (0,1)$,

$$a_\alpha(x) \equiv 2\int_0^\alpha \int_0^\rho x(s)\, ds\, d\eta(\rho), \tag{12}$$

$$F_\alpha(x)(t) \equiv \int_0^\alpha \int_\rho^t x(t+\rho-s)\, x(s)\, ds\, d\eta(\rho), \tag{13}$$

$$f_\alpha^\delta(t) \equiv \int_0^\alpha f^\delta(t+\rho)\, d\eta(\rho). \tag{14}$$

The nonlinear operator G which defines the original problem (1) appears in the regularized equation in the form of two terms on the left hand side of (11). The coefficient of x in first term $a_\alpha(x)$ depends only on the restriction of x on the interval $[0, \alpha]$, and as such is not as difficult to handle as is the second term $F_\alpha(x)$ on the left of (11), which we linearize about the true solution $\overline{x}$. That is, using arguments quite similar to those in the proof of Lemma 2.3 in [**9**], we can conclude that the operator $F_\alpha : L_\infty(0,1) \to L_\infty(0,1)$ as defined in (13) is Fréchet differentiable with

$$F'_\alpha(x)(h)(t) = 2\int_0^\alpha \int_\rho^t x(t+\rho-s)\,h(s)\,ds\,d\eta(\rho), \quad \text{a.e. } t \in (0,1), \tag{15}$$

for $h \in L_\infty(0,1)$. Further, F'_α is uniformly Lipschitz in $L_\infty(0,1)$ for all $\alpha > 0$ sufficiently small, i.e.,

$$\|F'_\alpha(x_1) - F'_\alpha(x_2)\| \le 2\int_0^\alpha d\eta(\rho)\|x_1 - x_2\|_\infty \tag{16}$$

for $x_1, x_2 \in L_\infty(0,1)$, where $\|\cdot\|$ denotes the usual $\mathcal{L}(L_\infty(0,1))$ operator norm.

We define the closed ball in $L_\infty(0,1)$ centered at x_0 with radius r as

$$\mathcal{B}(x_0, r) = \{z \in L_\infty(0,\infty),\ \|z - x_0\|_\infty \le r\}. \tag{17}$$

Following the same arguments as in the proof of Lemma 2.4 in [**9**], we know that the remainder terms of the linearization defined as

$$\mathcal{R}_\alpha(x,v) \equiv F_\alpha(x+v) - F_\alpha(x) - F'_\alpha(x)v \tag{18}$$

for $v, v_1, v_2 \in \mathcal{B}(0,r) \subseteq L_\infty(0,1)$ and $x \in L_\infty(0,1)$, satisfies

$$\|\mathcal{R}_\alpha(x,v)\|_\infty \le \frac{1}{2}\int_0^\alpha d\eta(\rho)\,\|v\|_\infty^2 \tag{19}$$

and

$$\|\mathcal{R}_\alpha(x,v_1) - \mathcal{R}_\alpha(x,v_2)\|_\infty \le \int_0^\alpha d\eta(\rho)\ \max\{\|v_1\|_\infty,\ \|v_2\|_\infty\}\,\|v_1 - v_2\|_\infty$$

for all $\alpha > 0$ sufficiently small [**8, 9, 23**].

3. Convergence results. As in [**9**], in order to begin the arguments needed to prove the main convergence results, we first rewrite the original autoconvolution equation (7) using similar notation to that used in the regularization equation (11). That is, the solution $\overline{x}$ of the original autoconvolution equation satisfies

$$a_\alpha(\overline{x})\overline{x} + F_\alpha(\overline{x}) = f_\alpha + \varepsilon_\alpha, \tag{20}$$

where

$$\varepsilon_\alpha(t) \equiv 2\int_0^\alpha \int_0^\rho (\overline{x}(t) - \overline{x}(t+\rho-s))\,\overline{x}(s)\,ds\,d\eta(\rho), \quad \text{a.e. } t \in (0,1), \tag{21}$$

$a_\alpha(\overline{x})$ and $F_\alpha(\overline{x})$ are defined as in (12)–(13), using $\overline{x}$ instead of x, and f_α is defined as in (14) using f instead of f^δ.

We rewrite the regularized equation (11) using the expansion of $F_\alpha(x)$ as

$$a_\alpha(x)x + F_\alpha(\overline{x}) + F'_\alpha(\overline{x})(x-\overline{x}) + \mathcal{R}_\alpha(\overline{x}, x-\overline{x}) = f_\alpha^\delta. \tag{22}$$

Combining (20) and (22), we obtain

$$\begin{aligned}(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))(x-\overline{x}) = {} & f_\alpha^\delta - f_\alpha - \varepsilon_\alpha - \mathcal{R}_\alpha(\overline{x}, x-\overline{x}) \\ & + D_\alpha(\overline{x})(x-\overline{x}) + (a_\alpha(\overline{x}) - a_\alpha(x))x,\end{aligned} \tag{23}$$

where I is the identity operator on $L_\infty(0,1)$, and

$$\begin{aligned} B_\alpha(\overline{x})(h)(t) &\equiv 2\int_0^\alpha \int_0^t \overline{x}(t+\rho-s)\,h(s)\,ds\,d\eta(\rho), \\ D_\alpha(\overline{x})(h)(t) &\equiv 2\int_0^\alpha \int_0^\rho \overline{x}(t+\rho-s)\,h(s)\,ds\,d\eta(\rho)\end{aligned}$$

for almost every $t \in (0,1)$. We further denote for $v \in L_\infty(0,1)$ that

$$E_\alpha(\overline{x}, v) = D_\alpha(\overline{x})(v) - a_\alpha(v)\,\overline{x}. \tag{24}$$

Then (23) becomes

$$\begin{aligned}(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))(x-\overline{x}) = {} & f_\alpha^\delta - f_\alpha - \varepsilon_\alpha - \mathcal{R}_\alpha(\overline{x}, x-\overline{x}) \\ & + E_\alpha(\overline{x}, x-\overline{x}) + (a_\alpha(x) - a_\alpha(\overline{x}))(\overline{x} - x)\end{aligned} \tag{25}$$

Without loss of generality, we will henceforth assume that $\overline{x}(0) > 0$. Notice that the solutions of the autoconvolution problem always show up in pairs: if $\overline{x}$ is a solution to the autoconvolution problem, then so is $-\overline{x}$. Therefore, it is reasonable to make the assumption that $\overline{x}(0) > 0$. According to Lemma (3.5) of [**9**], if $\overline{x} \in C^1[0, 1+\beta\overline{\alpha}]$ satisfies $\overline{x}(0) > 0$, then for the measure η satisfying (8)–(9), we have $a_\alpha(\overline{x}) > 0$ and

$$\frac{1}{a_\alpha(\overline{x})} \leq \frac{1}{\overline{x}(0)\int_0^\alpha \rho\, d\eta(\rho)}, \tag{26}$$

as long as $\alpha > 0$ is sufficiently small.

In [**9**], it is the accretivity of the operator $B_\alpha(\overline{x})$ that guaranteed the invertibility of the operator $(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))$. To obtain the accretivity of the operator $B_\alpha(\overline{x})$ in [**9**], we imposed two conditions on the true solution $\overline{x}$ of the autoconvolution problem that are crucial. First, $\overline{x}$ was required to be sufficiently smooth, namely, $\overline{x} \in W^{2,\infty}[0, 1+\overline{\alpha}]$; secondly, it was required that the true solution $\overline{x}$ does not cross the horizontal axis, i.e., $\overline{x}$ is either strictly positive or strictly negative. It is worth noting that, even though these two constraints on $\overline{x}$ are both also required with the Lavent'ev regularization [**22, 23**], the Tikhonov regularization does not require $\overline{x}$ to be strictly positive (or strictly negative) [**14**]. However, it is quite reasonable to assume that $\overline{x} > 0$ given that $\overline{x}$ almost always represents some type of density function in practice. In this paper, we are able to establish the invertibility of the operator $(a_\alpha(\overline{x})I + B_\alpha(\overline{x})) \in \mathcal{L}(L_\infty(0,1))$ without requiring $B_\alpha(\overline{x})$ to be accretive. In doing so, we can get away with requiring excessive smoothness on $\overline{x}$ which is needed in [**9**]. Even though we do not have to explicitly require that $\overline{x}$ does not cross the horizontal axis, the condition is implied by convergence theory. In order to establish the invertibility of the operator $(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))$, we introduce the following lemma.

Lemma 1. *Let h satisfy*

$$a_\alpha(\overline{x})h(t) + B_\alpha(\overline{x})(h)(t) = g(t), \tag{27}$$

almost everywhere $t \in (0,1)$ for $g \in L_\infty(0,1)$. If $\overline{x} \in W^{1,\infty}[0, 1+\overline{\alpha}]$ and, for some $k > 1$,

$$\frac{k}{k-1}\frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} < 1. \tag{28}$$

Then equation (27) *has a unique solution* $h \in L_\infty(0,1)$ *and*

$$\|h\|_\infty \le \frac{C}{a_\alpha(\overline{x})}\|g\|_\infty, \tag{29}$$

where

$$C = \frac{2(k-1)\overline{x}(0)}{(k-1)\overline{x}(0) - k\|\overline{x}'\|_\infty}. \tag{30}$$

Proof. To simplify notation, we define, for $t \in [0,1]$, $b_\alpha(t) \equiv 2\int_0^\alpha \overline{x}(t+\rho)\,d\eta(\rho)$; then we can write, for $h \in L_\infty(0,1)$, $B_\alpha(\overline{x})(h)(t) = \int_0^t b_\alpha(t-s)h(s)\,ds$.

We further define $K_\alpha(t) = (b_\alpha(t))/(b_\alpha(0))$ and $\varepsilon(\alpha) = (a_\alpha(\overline{x}))/(a_\alpha(0))$, so that equation (27) can be written as

$$h(t) + \frac{1}{\epsilon(\alpha)}\int_0^t K_\alpha(t-s)h(s)ds = \frac{g(t)}{a_\alpha(\bar{x})} \tag{31}$$

almost everywhere $t \in (0,1)$.

Note that, under the assumption that $\overline{x}(0) > 0$, for α sufficiently small, we have $b_\alpha(0) = 2\int_0^\alpha \overline{x}(\rho)\,d\eta(\rho) > 0$ and $\varepsilon(\alpha) > 0$ (independent of t). From the proof of Lemma 4.1 in [**35**], we have

$$h(t) = \int_0^t G(t,s)h(s)\,ds + \left[\frac{g(t)}{a_\alpha(\overline{x})} - \psi(t,\varepsilon) * \frac{g(t)}{a_\alpha(\overline{x})}\right] \tag{32}$$

almost everywhere $t \in [0,1]$, where $\psi(t,\varepsilon)$ is defined as

$$\psi(t,\varepsilon) \equiv \begin{cases} 0 & t < 0 \\ (1/\varepsilon)e^{-t/\varepsilon} & t \ge 0 \end{cases} \tag{33}$$

for a given $\varepsilon > 0$, and

$$G(t,s) \equiv \int_s^t \psi(t-\tau,\varepsilon)(-K_\alpha'(\tau - s))\,d\tau$$

for $0 \le s \le t \le 1$. However, there exists a $\xi \in [0, \alpha]$ and some $k > 1$ (to be determined later), such that

$$\begin{aligned}
|G(t,s)| &\le \|K_\alpha'\|_\infty \left| \int_s^t \frac{1}{\varepsilon} e^{-(t-\tau)/\varepsilon} d\tau \right| \\
&= \|K_\alpha'\|_\infty (1 - e^{-(t-s)/\varepsilon}) \le \|K_\alpha'\|_\infty = \left\| \frac{b_\alpha'(t)}{b_\alpha(0)} \right\|_\infty \\
&= \left\| \frac{\int_0^\alpha \overline{x}'(t+\rho)\, d\eta(\rho)}{\int_0^\alpha \overline{x}(\rho)\, d\eta(\rho)} \right\|_\infty \le \left\| \frac{\|\overline{x}'\|_\infty \int_0^\alpha d\eta(\rho)}{\int_0^\alpha [\overline{x}(0) + \overline{x}'(\xi)\rho]\, d\eta(\rho)} \right\|_\infty \\
&= \left\| \frac{\|\overline{x}'\|_\infty \int_0^\alpha d\eta(\rho)}{\int_0^\alpha \overline{x}(0)[1 + (\overline{x}'(\xi))/(\overline{x}(0))\rho]\, d\eta(\rho)} \right\|_\infty \\
&\le \frac{\|\overline{x}'\|_\infty \int_0^\alpha d\eta(\rho)}{\overline{x}(0) \int_0^\alpha (1 - (1/k))\, d\eta(\rho)} \\
&= \frac{k}{k-1} \frac{\|\overline{x}'\|_\infty}{\overline{x}(0)},
\end{aligned}$$

for almost every $0 \le s \le t \le 1$. Further, for almost every $t \in [0,1]$,

$$\begin{aligned}
\frac{g(t)}{a_\alpha(\overline{x})} - \psi(t,\varepsilon) * \frac{g(t)}{a_\alpha(\overline{x})} &\le \left\| \frac{g(\cdot)}{a_\alpha(\overline{x})} \right\|_\infty \left[1 + \int_0^t \psi(t-\tau,\varepsilon)\, d\tau \right] \\
&\le 2 \left\| \frac{g(\cdot)}{a_\alpha(\overline{x})} \right\|_\infty .
\end{aligned}$$

Combining the above estimates with equation (32), we have

$$\|h\|_\infty \le \frac{k}{k-1} \frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} \|h\|_\infty + 2 \left\| \frac{g(\cdot)}{a_\alpha(\overline{x})} \right\|_\infty .$$

Provided that $k/(k-1)\|\overline{x}'\|_\infty/(\overline{x}(0)) < 1$, we obtain inequality (29). $\square$

From Lemma (1), we conclude that, for $\overline{x} \in W^{1,\infty}[0, 1 + \overline{\alpha}]$ satisfying

$$\frac{k}{k-1} \frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} < 1,$$

for some $k > 1$, we have $(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))^{-1} \in \mathcal{L}(L_\infty(0,1))$, and the linear operator norm is bounded,

$$\|(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))^{-1}\| \le \frac{C}{a_\alpha(\overline{x})}, \tag{34}$$

with C given by equation (30). Note that this is similar to the upper bound for the operator norm of $(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))^{-1}$ we obtained in [**9**], with constant 1 replaced by C. To be able to obtain this bound for the general solution $\overline{x}$, we have to impose an *a priori* condition of $\overline{x}$ given by (28). We will see later the implication of this *a priori* condition.

We can now rewrite our regularized equation (11) as

$$x = H_\alpha x, \tag{35}$$

where, from (25), $H_\alpha : L_\infty(0,1) \mapsto L_\infty(0,1)$ is given by

$$\begin{aligned} H_\alpha x = (a_\alpha(\overline{x})I + B_\alpha(\overline{x}))^{-1}[f_\alpha^\delta - f_\alpha - \varepsilon_\alpha - \mathcal{R}_\alpha(\overline{x}, x - \overline{x}) \\ + E_\alpha(\overline{x}, x - \overline{x}) + (a_\alpha(x) - a_\alpha(\overline{x}))(\overline{x} - x)] + \overline{x}. \end{aligned} \tag{36}$$

The following two lemmas will bound relevant quantities on the right-hand side of (36).

Lemma 2. *Let* $f \in L_p(0, 1+\overline{\alpha})$, $1 \le p \le \infty$, *and let the measure* η *be given satisfying* (8)–(9). *Then* $f_\alpha \in L_\infty(0,1)$ *for* $\alpha \in (0, \overline{\alpha}]$. *Further, if* $f, f^\delta \in L_p(0, 1+\overline{\alpha})$ *with* $\|f - f^\delta\|_{L_p} \le \delta$, *then*

$$\|f_\alpha - f_\alpha^\delta\|_\infty \le \delta \overline{\omega} \alpha^{1/q} \tag{37}$$

for $\overline{\omega}$ *given in* (9) *and* q *satisfying* $(1/p) + (1/q) = 1$.

Proof. For almost every $t \in (0,1)$ and q such that $(1/p) + (1/q) = 1$,

$$\begin{aligned} |f_\alpha(t)| &= \left| \int_0^\alpha f(t+\rho)\, d\eta(\rho) \right| = \left| \int_0^\alpha f(t+\rho)\omega(\rho)\, d\rho \right| \\ &\le \|f(t+\cdot)\|_{L_p(0,\alpha)} \|\omega\|_{L^q(0,\alpha)} \le \|f\|_{L_p(0,1+\overline{\alpha})} \cdot \overline{\omega} \cdot \left(\int_0^\alpha 1\, d\rho \right)^{1/q}. \end{aligned}$$

Therefore, for any $\alpha \in (0, \overline{\alpha}]$, we have $f_\alpha \in L_\infty(0,1)$ and

$$\|f_\alpha\|_{L_\infty(0,1)} \le \|f\|_{L_p(0,1+\overline{\alpha})} \cdot \overline{\omega} \cdot R^{1/q}.$$

Similarly, for almost every $t \in [0,1]$,

$$|f_\alpha^\delta(t) - f_\alpha(t)| \le \|f^\delta - f\|_{L_p(0,1+\overline{\alpha})} \cdot \overline{\omega} \cdot R^{1/q}.$$

Equation (37) immediately follows given that $\|f^\delta - f\|_{L_p(0,1+\overline{\alpha})} \le \delta$. $\square$

Lemma 3. *Let $\overline{x} \in C^1[0,1+\overline{\alpha}]$ satisfy $\overline{x}(0) > 0$. Assume the measure η satisfies* (8)–(9)*. Let $x_1, x_2 \in L_\infty(0,1)$. Then*

$$\|E_\alpha(\overline{x}, x_1 - x_2)\|_\infty \le \|\overline{x}'\|_\infty \|x_1 - x_2\|_\infty \int_0^\alpha \rho^2 \, d\eta(\rho), \tag{38}$$

$$\|\varepsilon_\alpha\|_\infty \le \|\overline{x}'\|_\infty \left(3\overline{x}(0) \int_0^\alpha \rho^2 \, d\eta(\rho) + \frac{5}{3} \int_0^\alpha \rho^3 \, d\eta(\rho) \|\overline{x}'\|_\infty\right) \tag{39}$$

and

$$|a_\alpha(x_1) - a_\alpha(x_2)| \le \|x_1 - x_2\|_\infty \int_0^\alpha \rho \, d\eta(\rho). \tag{40}$$

Proof. Similar arguments to Lemma 3.6 of [**9**]. $\square$

We are now ready to state the main convergence theorem.

Theorem 4. *Assume that $f^\delta \in L_p(0, 1+\overline{\alpha})$, $1 \le p \le \infty$ satisfies*

$$\|f^\delta - f\|_{L_p} \le \delta.$$

Assume that the measure $\eta(\rho) > 0$ satisfies (8)–(9) *and that the autoconvolution problem* (1) *has a solution $\overline{x} \in C^1[0, 1+\overline{\alpha}]$ satisfying*

$$\overline{x}(0) > \left(4\sqrt{2}b + 1\right)^2 \|\overline{x}'\|_\infty \tag{41}$$

for $b \ge 2\overline{\omega}/\underline{\omega}$, where $\overline{\omega}, \underline{\omega}$ are given in (8)*. Then there exist constants $k_1 > 0$ and $\widehat{C} > 0$ independent of α such that, if $\delta = \delta(\alpha) > 0$ satisfies*

$$\delta \le k_1 \alpha^{2+(1/p)}, \tag{42}$$

then for all $\alpha > 0$ sufficiently small, the regularized equation (35) *has a unique solution $x_\alpha^\delta \in L_\infty(0,1)$ satisfying*

$$\|x_\alpha^\delta - \overline{x}\|_\infty \le \widehat{C}\alpha. \tag{43}$$

Further, $x_\alpha^\delta \in L_\infty(0,1)$ depends continuously on $f^\delta \in L_p$ for all $\alpha > 0$ sufficiently small.

Proof. We will apply the contraction mapping principle to the regularized equation (35) in the ball $\mathcal{B}(\overline{x}, \widehat{C}\alpha)$. From Lemmas 1, 2 and 3 and inequalities (16), (19), (26) and (34), if $\overline{x}$ satisfies

$$0 < \frac{k}{k-1}\frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} < 1, \tag{44}$$

for some $k > 1$, we then have

$$\begin{aligned}
\|H_\alpha x - \overline{x}\|_\infty \le \frac{C}{\alpha(\overline{x})}\|f_\alpha^\delta - f_\alpha\|_\infty \\
&+ \frac{C}{\alpha(\overline{x})}\|\mathcal{R}_\alpha(\overline{x}, x-\overline{x})\|_\infty + \frac{C}{\alpha(\overline{x})}\|\varepsilon_\alpha\|_\infty \\
&+ \frac{C}{\alpha(\overline{x})}\|E_\alpha(\overline{x}, x-\overline{x})\|_\infty + \frac{|a_\alpha(x) - a_\alpha(\overline{x})|}{a_\alpha(\overline{x})}\|x-\overline{x}\|_\infty \\
\le{}& \frac{2C}{\overline{x}(0)}\frac{\overline{\omega}}{\underline{\omega}}\alpha^{(1/q)-2}\delta + \frac{C}{\overline{x}(0)}\,\frac{\overline{\omega}}{\underline{\omega}}\,\alpha^{-1}\|x-\overline{x}\|_\infty^2 \\
&+ C\|\overline{x}'\|_\infty\left(\frac{2\overline{\omega}}{\underline{\omega}}\,\alpha + \frac{5\|\overline{x}'\|_\infty}{3\,\overline{x}(0)}\,K(3)\,\alpha^2\right) \\
&+ \frac{C\,\|\overline{x}'\|_\infty}{\overline{x}(0)}\,K(2)\,\alpha\|x-\overline{x}\|_\infty + \frac{2C}{\overline{x}(0)}\|x-\overline{x}\|_\infty^2,
\end{aligned}$$

for $C = [2(k-1)\overline{x}(0)]/[(k-1)\overline{x}(0) - k\|\overline{x}'\|_\infty]$ and q satisfying $1/p + 1/q = 1$. Using assumption (42) and the fact that $\|x - \overline{x}\|_\alpha \le \widehat{C}\alpha$, we have

$$\begin{aligned}
\|H_\alpha x - \overline{x}\|_\infty \le{}& \frac{2C}{\overline{x}(0)}\frac{\overline{\omega}}{\underline{\omega}}k_1\alpha + \frac{C}{\overline{x}(0)}\,\frac{\overline{\omega}}{\underline{\omega}}\,\widehat{C}^2\alpha \\
&+ C\|\overline{x}'\|_\infty\frac{2\overline{\omega}}{\underline{\omega}}\alpha + \frac{5C\|\overline{x}'\|_\infty^2}{3\,\overline{x}(0)}\,K(3)\,\alpha^2 \\
&+ \frac{C\,\|\overline{x}'\|_\infty}{\overline{x}(0)}\,K(2)\,\widehat{C}\alpha^2 + \frac{2C}{\overline{x}(0)}\widehat{C}^2\alpha^2.
\end{aligned}$$

Therefore, to have $\|H_\alpha x - \overline{x}\|_\infty \le \widehat{C}\alpha$ for some $\widehat{C} > 0$ and all $\alpha > 0$ sufficiently small, a sufficient condition is that

$$\frac{C}{\overline{x}(0)}\,b\,k_1 + \frac{C}{\overline{x}(0)}\,b\,\widehat{C}^2 + C\|\overline{x}'\|_\infty\,b < \widehat{C}. \tag{45}$$

If we let

$$k_1 = \|\overline{x}'\|_\infty \, \overline{x}(0), \tag{46}$$

then (45) becomes

$$L(\widehat{C}) \equiv \frac{Cb}{\overline{x}(0)} \widehat{C}^2 - \widehat{C} + 2\, b\, C \, \|\overline{x}'\|_\infty < 0. \tag{47}$$

In order for $L(\widehat{C}) = 0$ to have two distinct positive solutions $0 < \widehat{C}_1 < \widehat{C}_2$, we will require the discriminant of $L(\widehat{C})$ to be positive, i.e.,

$$\Delta = 1 - \frac{8b^2C^2}{\overline{x}(0)} \|\overline{x}'\|_\infty > 0. \tag{48}$$

After plugging in the value for C and some algebraic manipulation, inequality (48) becomes, for $k > 1$,

$$1 > 4\sqrt{2}\, b \left(\frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} \right)^{1/2} + \frac{k}{k-1} \frac{\|\overline{x}'\|_\infty}{\overline{x}(0)}. \tag{49}$$

Under the prior assumption given by (44), a sufficient condition for $\Delta > 0$ is that

$$1 > \left(4\sqrt{2}\, b + \sqrt{\frac{k}{k-1}} \right) \left(\frac{\|\overline{x}'\|_\infty}{\overline{x}(0)} \right)^{1/2}. \tag{50}$$

This poses a more stringent condition on $\overline{x}$ than (44). We pick k sufficiently large; then it is not hard to see that $L(\widehat{C}) = 0$ to have two distinct positive solutions $0 < \widehat{C}_1 < \widehat{C}_2$ by assumption (41). Then, for $\widehat{C}$ satisfying $\widehat{C}_1 < \widehat{C} < \widehat{C}_2$, we have $L(\widehat{C}) < 0$, and thus $\|H_\alpha x - \overline{x}\|_\infty \le \widehat{C}\alpha$ for all $\alpha > 0$ sufficiently small.

To further demonstrate that H_α is a contraction on $\mathcal{B}(\overline{x}, \widehat{C}\alpha)$, we let $x_1, x_2 \in \mathcal{B}(\overline{x}, \widehat{C}\alpha)$, and note that

$$\begin{aligned}
&\|H_\alpha x_1 - H_\alpha x_2\|_\infty \\
&= \|(a_\alpha(\overline{x})I + B_\alpha(\overline{x}))^{-1}\{\mathcal{R}_\alpha(\overline{x}, x_2 - \overline{x}) - \mathcal{R}_\alpha(\overline{x}, x_1 - \overline{x}) + E_\alpha(\overline{x}, x_1 - x_2) \\
&\quad - [(a_\alpha(x_1) - a_\alpha(\overline{x}))(x_1 - \overline{x}) - (a_\alpha(x_2) - a_\alpha(\overline{x}))(x_2 - \overline{x})]\}\|_\infty \\
&\le T_\alpha(x_1, x_2),
\end{aligned}$$

where

$$\begin{aligned} T_\alpha(x_1,x_2) \equiv \frac{C}{a_\alpha(\overline{x})}\|\mathcal{R}_\alpha(\overline{x},x_2-\overline{x})-\mathcal{R}_\alpha(\overline{x},x_1-\overline{x})\|_\infty \\ + \frac{C}{a_\alpha(\overline{x})}\|E_\alpha(\overline{x},x_1-x_2)\|_\infty \\ + \frac{C}{a_\alpha(\overline{x})}\|(a_\alpha(x_1)-a_\alpha(\overline{x}))(x_1-\overline{x}) \\ -(a_\alpha(x_2)-a_\alpha(\overline{x}))(x_2-\overline{x})\|_\infty. \end{aligned}$$

Since

$$\begin{aligned} &\frac{1}{a_\alpha(\overline{x})}\|(a_\alpha(x_1)-a_\alpha(\overline{x}))(x_1-\overline{x})-(a_\alpha(x_2)-a_\alpha(\overline{x}))(x_2-\overline{x})\|_\infty \\ &= \frac{1}{a_\alpha(\overline{x})}\|(a_\alpha(x_1)-a_\alpha(x_2))(x_1-\overline{x})+(a_\alpha(x_2)-a_\alpha(\overline{x}))(x_1-x_2)\|_\infty \\ &\le \frac{|a_\alpha(x_1)-a_\alpha(x_2)|}{a_\alpha(\overline{x})}\|x_1-\overline{x}\|_\infty + \frac{|a_\alpha(x_2)-a_\alpha(\overline{x})|}{a_\alpha(\overline{x})}\|x_1-x_2\|_\infty \\ &\le \frac{2\|x_1-x_2\|_\infty \int_0^\alpha \rho\, d\eta(\rho)}{\overline{x}(0)\int_0^\alpha \rho\, d\eta(\rho)}\|x_1-\overline{x}\|_\infty \\ &\quad + \frac{2\|x_2-\overline{x}\|_\infty \int_0^\alpha \rho\, d\eta(\rho)}{\overline{x}(0)\int_0^\alpha \rho\, d\eta(\rho)}\|x_1-x_2\|_\infty \\ &\le \frac{4\widehat{C}\alpha}{\overline{x}(0)}\|x_1-x_2\|_\infty, \end{aligned}$$

we have

$$\begin{aligned} T_\alpha(x_1,x_2) \le \left[\frac{C}{\overline{x}(0)}\,\frac{2\overline{\omega}}{\underline{\omega}}\,\widehat{C}\right]\|x_1-x_2\|_\infty \\ + \left[\frac{C\,\|\overline{x}'\|_\infty}{\overline{x}(0)}\,K\,(3)\,\alpha + \frac{4C\widehat{C}\alpha}{\overline{x}(0)}\right]\|x_1-x_2\|_\infty. \end{aligned}$$

Thus, if we require that

$$\widehat{C} < \frac{\overline{x}(0)}{b\,C}, \tag{51}$$

it follows that

$$\widehat{C} < \frac{\overline{x}(0)}{C}\,\frac{\underline{\omega}}{2\overline{\omega}} \tag{52}$$

and, for $\alpha > 0$ sufficiently small,

$$\|H_\alpha x_1 - H_\alpha x_2\|_\infty \le T_\alpha(x_1, x_2) \le q\,\|x_1 - x_2\|_\infty \tag{53}$$

for any $x_1, x_2 \in \mathcal{B}(\overline{x}, \widehat{C}\alpha)$ with some $q < 1$. Further, we note that $\overline{(\widehat{C}_1 + \widehat{C}_2)/2} = (\overline{x}(0))/(b\,C)$, and therefore our regularized equation (35) has a unique solution x_α^δ in $\mathcal{B}(\overline{x}, \widehat{C}\alpha)$ for $\widehat{C}$ satisfying $\widehat{C}_1 < \widehat{C} < (\overline{x}(0))/(b\,C)$.

Similar arguments to those of Theorem 3.7 in [**9**] give the continuous dependence of solutions on data for the regularized equation (35). $\square$

The following theorem gives the convergence rate of the solution for the regularized equation (35). It immediately follows from Theorem 4.

Theorem 5. *Assume $f^\delta \in L_p(0, 1 + \overline{\alpha})$, $1 < p < \infty$, satisfies the*

$$\|f^\delta - f\|_{L_p} \le \delta.$$

Let the measure η be given satisfying (8)–(9).

Then there exist $\overline{C} > 0$ and $\kappa_1 > 0$, $\kappa_2 > 0$ independent of α such that, if the true solution $\overline{x} \in C^1[0, 1+\overline{\alpha}]$ of the autoconvolution equation satisfies

$$\overline{x}(0) > \overline{C}\,\|\overline{x}'\|_\infty, \tag{54}$$

then, for $\alpha = \alpha(\delta) > 0$ selected satisfying

$$\kappa_1 \delta^{p/(2p+1)} \le \alpha(\delta) \le \kappa_2\, \delta^{p/(2p+1)} \tag{55}$$

as $\delta \to 0$, it follows that there is a unique solution $x^\delta_{\alpha(\delta)}$ of the regularization equation (11) *associated with data f^δ which depends continuously on $f^\delta \in L_p(0, 1)$ and which satisfies*

$$\|x^\delta_{\alpha(\delta)} - \overline{x}\|_{L_\infty(0,1)} = \mathcal{O}(\delta^{p/(2p+1)}) \tag{56}$$

as $\delta \to 0$. Thus, the best rate occurs as $p \to \infty$, i.e., in the case of L_∞ data, with rate approaching $\mathcal{O}(\delta^{1/2})$.

Remark. A collocation based discretization of the regularization equation (11) leads to a stable numerical method to solve for x on the interval $[0,1]$. The resulting method is linear and sequential in recovering x on the interval $[\alpha,1]$ but nonlinear and nonsequential on the interval $[0,\alpha]$ due to the coefficient term $a_\alpha(x)$. Even though the interval where the nonlinearity remains is small, it motivated us to look for alternative methods in recovering $x(t)$ on the interval $0 \le t \le \alpha$. As justified in [**9**], any $\mathcal{O}(\alpha^p)$ approximation of $\overline{x}$ on $[0,\alpha]$ for some $p > 1$ is good enough to use in the approximating equation to recover $x(t)$ on the interval $[\alpha, 1]$. This gives us various options in practice for alternative methods on $[0,\alpha]$. For example, if we know $\overline{x}(0)$, we can simply form an $\mathcal{O}(\alpha)$ approximation of $\overline{x}$ via $x_\alpha(t) = \overline{x}(0)$; or if we know both $\overline{x}(0)$ and $\overline{x}'(0)$, we can form an $\mathcal{O}(\alpha^2)$ approximation of $\overline{x}$ via $x_\alpha(t) = \overline{x}(0) + \overline{x}'(0)t$. However, as shown in [**8**], such approximations on $[0,\alpha]$ do not perform as well as approximations based on solving the unregularized equation (1) using a simple collocation-based discretization, which is an $\mathcal{O}(\alpha)$ approximation of $\overline{x}$ on $[0,\alpha]$. This is likely due to the fact that collocation-based discretization, even though unregularized, makes good use of the data f^δ, where the approximations based on Taylor expansion completely ignores the data f^δ. The exact statements of the theoretical results justifying these other choices of recovering x on $[0,\alpha]$ can be found in [**9**], with proofs similar to those in [**9**] but making use of Theorem 4 in this paper with loosened restrictions on $\overline{x}$.

4. Application to devolution of the appearance potential spectra. We now turn to devolution of the appearance potential spectra, where we recover the density function $\overline{x} > 0$ from solving equation (3) in two steps. We first solve the outside linear Volterra equation and then use what we recover as data to solve the inside autoconvolution equation, using local regularization at both steps. Local regularization methods have the advantage of preserving the causal nature of Volterra problems, allowing for fast sequential solution methods. These methods have proved to be effective and efficient regularization procedures for both linear and nonlinear Volterra problems [**9, 24–28, 30, 31**].

Let $\overline{x}$ be the true solution satisfying equation (3); then $\overline{f} = \overline{x} * \overline{x}$ satisfies the linear Volterra equation (5) with the Lorentzian kernel defined in (4). It is not hard to see that the kernel k is 1-smoothing, i.e., $k \in C^1[0,1]$ and $k(0) = 1 \neq 0$. We will first solve this mildly ill-posed linear Volterra problem using local regularization.

We use the same underlying rationale for local regularization methods to derive the regularized equation, namely, we utilize future data on a small future interval beyond t in recovering solution at time t. We first extend equation (5) slightly into the future by assuming it holds on an extended interval $[0, 1+\overline{\beta}]$ for some small $\overline{\beta} \in (0, 1]$ and then consolidate the future information by integrating both sides of the equation with respect to a suitable Borel measure $\eta = \eta_\beta(\rho)$ where $\beta \in [0, \overline{\beta}]$. The resulting equation is:

$$\int_0^t \int_0^\beta k(t+\rho-s)\, d\eta_\beta(\rho) f(s)\, ds + \int_0^\beta \int_0^\rho k(\rho-s) f(t+s)\, ds\, d\eta_\beta(\rho) = \int_0^\beta g(t+\rho) d\eta_\beta(\rho), \quad t \in [0,1].$$

We still have an equation that $\overline{f}$ satisfies exactly. In reality, we only have access to the perturbed data $g^\delta \in C[0, 1+\overline{\beta}]$ satisfying $||g^\delta - g||_\infty \leq \delta$; therefore, we regularize the equation by holding f constant on a small local interval of length $[t, t+\beta]$, where the length β of this local interval serves as the regularization parameter. We obtain the regularized equation as follows:

$$\int_0^t \widetilde{k}_\beta(t-s) f(s)\, ds + a_\beta f(t) = \widetilde{g}^\delta_\beta(t), \quad t \in [0,1], \tag{57}$$

where

$$\widetilde{k}_\beta(t) = \int_0^\beta k(t+\rho)\, d\eta_\beta(\rho), \tag{58}$$

$$\widetilde{g}^\delta_\beta(t) = \int_0^\beta g^\delta(t+\rho) d\eta_\beta(\rho), \tag{59}$$

$$a_\beta = \int_0^\beta \int_0^\rho k(\rho - s)\, ds\, d\eta_\beta(\rho). \tag{60}$$

Signed Borel measures are needed to establish stability and convergence for the local regularization of linear μ-smoothing Volterra problems for all $\mu = 1, 2, \ldots$ [**30**]. However, since our problem is only 1-smoothing, we can use simpler measures $\eta_\beta(\rho) > 0$ defined similarly to $\eta(\rho)$ by equations (8) and (9), with α replaced by β in those equations. With the positive measure $\eta_\beta(\rho)$ defined this way, we can see that $a_\beta \neq 0$ for all $\beta > 0$ sufficiently small. Therefore, there is a unique solution $f^\delta_{\beta(\delta)} \in L_2(0,1)$ of equation (57) which depends continuously on data g^δ in $C[0,1]$ or $L_2(0,1)$ topologies. If we assume smooth or piecewise smooth data g^δ, it is clear that $f^\delta_{\beta(\delta)} \in C[0,1]$. It is shown in [**24**] that the regularized solution $f^\delta_{\beta(\delta)}$ converges to $\overline{f}$ in the case of one-smoothing kernels as δ, the level of noise in the data, goes to zero, with a resulting convergence rate of order $\mathcal{O}(\delta^{1/2})$. The following theorems give the convergence of regularized equation (57) for the outside linear Volterra problem in the deconvolution of appearance potential spectra.

Theorem 6. *Assume $\overline{f}$ is the true solution to equation* (5) *with the kernel given by* (4)*. Assume $g^\delta \in C[0,1+\overline{\beta}]$ such that $||g^\delta - g||_\infty \leq \delta$. Let the measure $\eta_\beta(\rho)$ be defined by equations* (8) *and* (9)*, with α replaced by β in those equations. Then, for $\beta = \beta(\delta) > 0$ sufficiently small, the regularized equation* (57) *has a unique solution $f^\delta_{\beta(\delta)} \in L_2(0,1)$. Further, as $\delta \to 0$,*

$$\beta(\delta) \longrightarrow 0,$$

and

$$||f^\delta_{\beta(\delta)} - \overline{f}|| \longrightarrow 0.$$

Once $f^\delta_{\beta(\delta)}$ is solved, we can then use it as the noisy data f^δ for the autoconvolution problem. The convergence theorem that ultimately recovers $\overline{x}$ immediately follows from Theorem 5.

Theorem 7. *Assume $\overline{x} \in C^1[0,1+\overline{\alpha}]$ is the true solution to equation* (3) *satisfying*

$$\overline{x}(0) > \overline{C}\, \|\overline{x}'\|_\infty, \tag{61}$$

for some $\overline{C} > 0$. Let the measure $\eta(\rho)$ be defined by equations (8) *and* (9)*. Then $\alpha = \alpha(||f^\delta_{\beta(\delta)} - \overline{f}||)$ can be selected such that there is a unique*

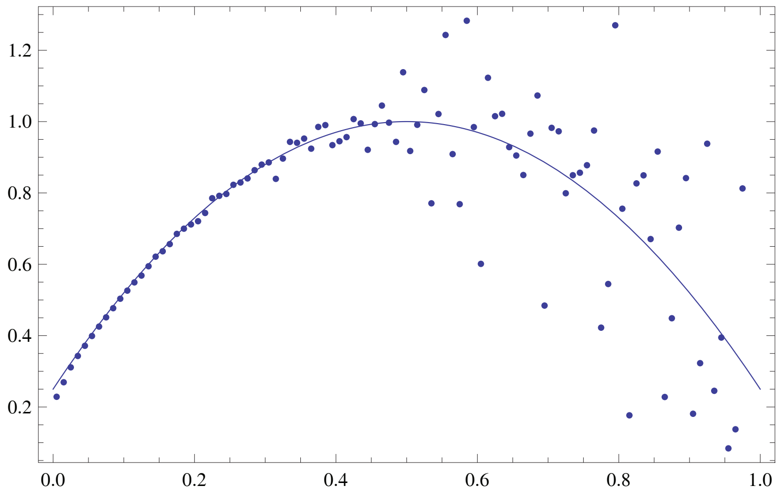

FIGURE 1. Example 1a. Solution obtained with $N = 100$, $\alpha = 1$, $\beta = 1$ and 0.03% relative noise in the observed g^δ.

solution $x^\delta_{\alpha(\delta),\beta(\delta)} \in L_\infty(0,1)$ *of the regularized equation* (11) *associated with perturbed data* $f^\delta_{\beta(\delta)}$ *which depends continuously on* $f^\delta_{\beta(\delta)}$. *Further,*

$$x^\delta_{\alpha(\delta),\beta(\delta)} \longrightarrow \overline{x}$$

as $\delta \to 0$.

5. Numerical examples. To illustrate local regularization methods for deconvolution of appearance potential spectra, we present a numerical equation using $k(s) = 1/(1 + (\pi s)^2)$, a normalized Lorentzian kernel. That is, we wish to solve

$$\int_0^t k(t-s)(x * x)\, ds = g(t)$$

for x.

In the figures, the true solution $\overline{x} = 1 - 3(t - 1/2)^2$ is plotted as a solid curve, and the regularized approximation $x^\delta_{\alpha(\delta),\beta(\delta)}$ is plotted as points. The collocated discretization is based on subdivision of the interval

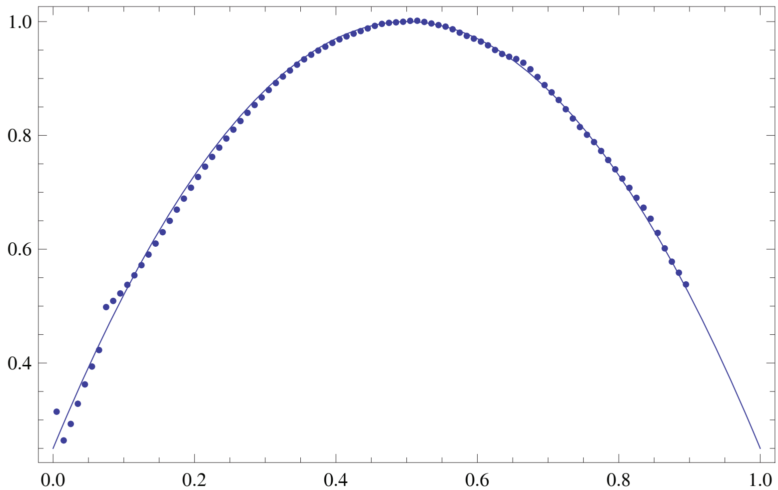

FIGURE 2. Example 1b. Solution obtained with $N = 100$, $\alpha = 7$, $\beta = 3$ and 0.03% relative noise.

$[0, 1]$ into $N = 100$ subintervals, α is the number of data points used for autoconvolution regularization and β is the number of data points used for the linear regularization. Thus, local regularization intervals are given by $[0, \alpha/N]$ and $[0, \beta/N]$ for the inside autoconvolution problem and the outside linear Volterra problem, respectively. The measures $\eta(\rho)$ and $\eta_\beta(\rho)$ are both the simple Lebesgue measure.

We present several illustrative examples.

5.1. Example 1. In Figure 1, the solution is obtained with no regularization at all ($\alpha = 1$ and $\beta = 1$), and despite a low relative noise in g^δ of 0.03%, the reconstruction shows the great instability characteristic of inverse problems. In fact, any more noise, and the numerical reconstruction fails altogether.

In Figure 2, by contrast, the noise is the same, but regularization is used on both the inside autoconvolution problem and the outside linear Volterra problem, with $\alpha = 7$ and $\beta = 3$. Compared to Figure 1, the smoothing effect of the regularization is apparent.

Several general characteristics of the double regularization are also worth noting.

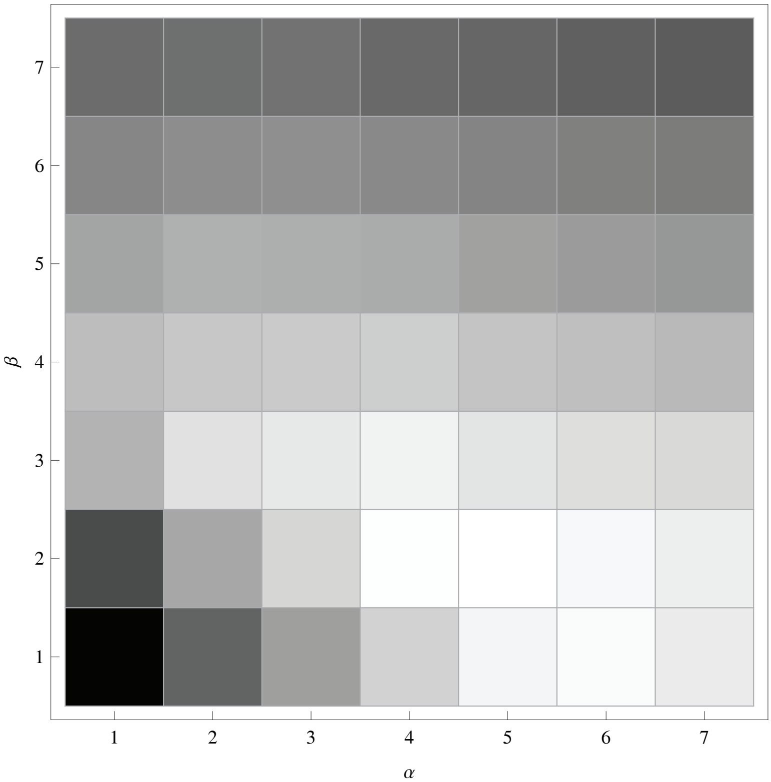

FIGURE 3. Error in the reconstructed solution with varying α and β, on $N = 100$ subintervals and 0.01% relative noise. Darker boxes represent larger errors. The worst is no regularization at all ($\alpha = 1, \beta = 1$), and the best is $\alpha = 5, \beta = 2$.

The first α reconstructed points are necessarily solved without regularization of the autoconvolution. The nonlinear autoconvolution regularization begins only with the $(\alpha + 1)$-th point.

Second, the reconstruction, because both regularizations are forward looking, only produces $N - \alpha - \beta$ points, so there are no reconstructed data at the end of the interval. Larger choices of the regularization parameters will make this "gap" respectively larger.

5.2. Varying α and β. Figure 3 shows a measure of the error in reconstruction over a range of choices of α and β. In all cases, the

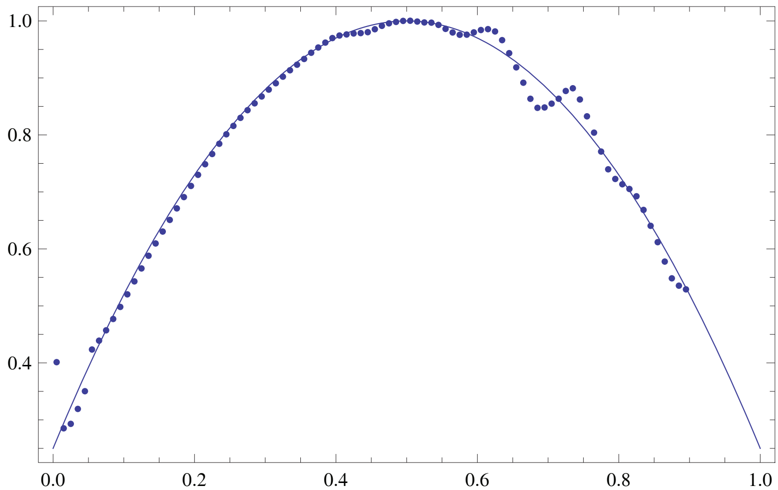

FIGURE 4. Example 2a. Solution obtained with $\alpha = 5$ and $\beta = 5$, on $N = 100$ subintervals and 0.1% relative noise.

noise was 0.01%. The best solution occurs with the choice of $\alpha = 5$ and $\beta = 2$.

Even for such low noise levels, a little regularization of either problem goes a long way towards smoothing the instability of the reconstruction. In the optimal choice, very little linear regularization is needed.

5.3. Example 2. Here the noise in g^δ is a bit more substantial $\delta = 0.1\%$, and several solutions are shown. In the first (Figure 4), the solution was obtained with significant regularization of both problems ($\alpha = 5$ and $\beta = 5$). The second (Figure 5) shows the result with only slight autoconvolution regularization ($\alpha = 2$ and $\beta = 5$), while the third (Figure 6) is obtained with only slight linear regularization ($\alpha = 5$ and $\beta = 2$).

With insufficient regularization of either problem, the solution obtained is sub-optimal. In both cases a kind of oscillatory behavior is apparent in the reconstruction, although it appears worse when the linear problem is insufficiently regularized.

The final, Figure 7, shows that significant improvement is still possible by increasing the autoconvolution regularization by just one more point ($\alpha = 6$).

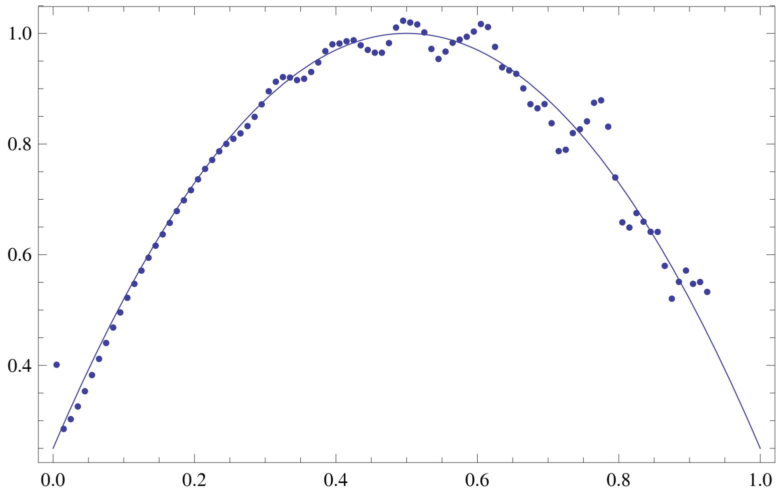

FIGURE 5. Example 2b. Solution obtained with $\alpha = 2$ and $\beta = 5$, on $N = 100$ subintervals and 0.1% relative noise.

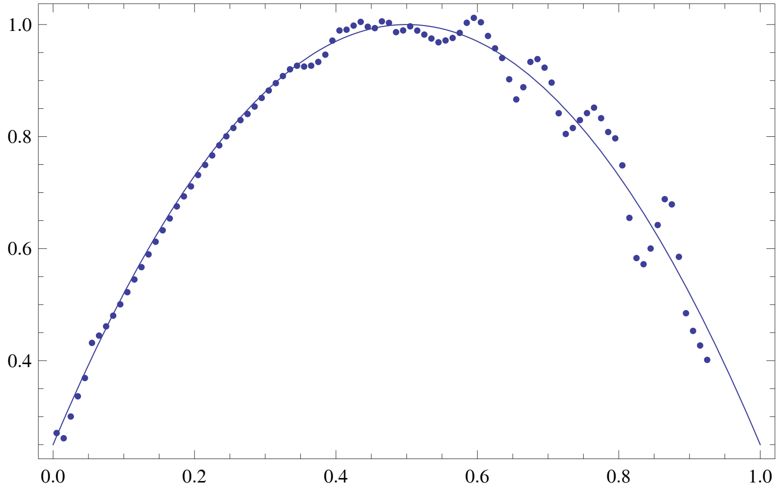

FIGURE 6. Example 2c. Solution obtained with $\alpha = 5$ and $\beta = 2$, on $N = 100$ subintervals and 0.1% relative noise.

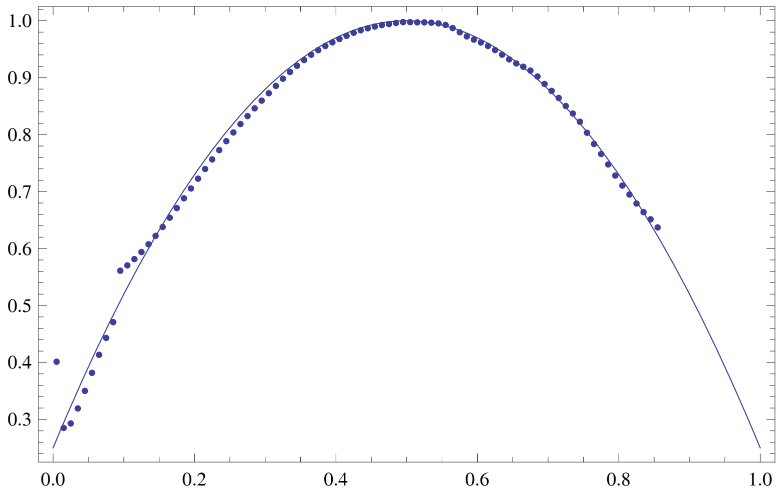

FIGURE 7. Example 2d. Solution obtained with $\alpha = 6$ and $\beta = 5$, on $N = 100$ subintervals and 0.1% relative noise.

The observations here stand in contrast to the error results in the previous section, where the optimal choice was just a little linear regularization and much more autoconvolution regularization. We have observed that, as the noise level changes, the optimal choices for the regularization parameters α and β change too.

We have not yet produced any model for making optimal choices of α and β, but numerical experience perhaps supports our hypothesis that α should generally be larger than β, because the linear problem is only 1-smoothing, and therefore not as ill-posed. A formal model awaits further research.

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