

ERROR BOUNDS FOR SPECTRAL ENHANCEMENT WHICH ARE BASED ON VARIABLE HILBERT SCALE INEQUALITIES

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ABSTRACT. Spectral enhancement—which aims to undo spectral broadening—leads to integral equations which are ill-posed and require special regularization techniques for their solution. Even when an optimal regularization technique is used, however, the errors in the solution, which originate in data approximation errors, can be substantial and it is important to have good bounds on these errors in order to select appropriate enhancement methods. A discussion of the causes and nature of broadening provides regularity or source conditions which are required to obtain bounds for the regularized solution of the spectral enhancement problem. Only in special cases do the source conditions satisfy the requirements of the standard convergence theory for ill-posed problems. Instead we have to use variable Hilbert scales and their interpolation inequalities to get error bounds. The error bounds in this case turn out to be of the form $O(\varepsilon^{1-\eta(\varepsilon)})$ where ε is the data error and $\eta(\varepsilon)$ is a function which tends to zero when ε tends to zero. The approach is demonstrated with the Eddington correction formula and applied to a new spectral reconstruction technique for Voigt spectra. In this case $\eta(\varepsilon) = O(1/\sqrt{|\log \varepsilon|})$ is found.

1. Introduction. One of the computational challenges in spectroscopy is the separation of overlapping spectral lines. This separation can be achieved by computationally narrowing the spectral lines and thus enhancing the resolution or correcting the spectrum. The class of methods of resolution enhancement considered here is based on the solution of linear Fredholm integral equations of the first kind using observed data for the right hand side. The basic approach was first analyzed in [2] but it goes back in principle to work by Stokes [47]. The effect of data errors has to be analyzed carefully, especially since

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the enhancement problem is ill-posed. This analysis is performed in the following using variable Hilbert scales [23, 24]. A more traditional error analysis which can be found in [21] is not directly applicable here as the source conditions are non-standard. However, in contrast to many other ill-posed problems here the underlying physical model does suggest specific source conditions. If f is the enhanced spectrum and f_α an (optimal order) regularized approximation of f , then bounds of the form

$$\|f - f_\alpha\| \leq \varepsilon^{1-\eta(\varepsilon)}$$

are found where ε is the residual of f_α . In the classical case the $\eta(\varepsilon)$ is constant; in contrast, it is shown here that this exponent slowly decreases with $\varepsilon \rightarrow 0$.

A new enhancement method based on Lorentz kernels for Voigt spectra is shown to provide good performance compared to more traditional methods like the Eddington correction as it capitalizes more on the smoothness of the data and does not require any advanced knowledge of the proportions of the Gaussian and Lorentzian components in the Voigt spectrum. If a spectrum contains a Gaussian component the error bound is of order $O(\varepsilon^{1-c/\sqrt{|\log \varepsilon|}})$ and the convergence rate thus grows with $\varepsilon \rightarrow 0$. For very small ε one can find very close to $O(\varepsilon)$ convergence; however, this depends on the level of enhancement required. Experiments show that this method leads to a reduction of linewidth of more than a factor of two in the case of a 5 percent data error.

In the remaining parts of this section a brief review of broadening mechanisms is given, in addition to a short discussion of a least squares method to determine the location and strength of spectral lines. In Section 2 we present the integral equation framework for resolution enhancement and illustrate this with the Eddington correction formula and Stokes correction by partial Gaussian deconvolution. In Section 3 the method using Lorentz deconvolution for Gaussian and Voigt spectra is discussed in terms of the errors. Section 4 then provides some demonstrations of the enhancement properties of this Lorentz deconvolution which in particular illustrates the broadening effects of noise and regularization. In the concluding Section 5 related and open problems are considered.

1.1. Models of spectra and broadening. In the natural sciences, a spectrum is a distribution of photon counts over energy

or frequency. Since Fraunhofer's work in 1814 it is well known that this distribution is concentrated along lines, both for emission and absorption spectra. The existence of these *spectral lines* was later confirmed by quantum mechanics. Their importance is due to the fact that they provide information about the energy levels of the electrons and thus insights into the structure and composition of the originating substrate. Spectroscopy has been for a long time one of the most important experimental tools in experimental science. A simple model for a spectrum based on the Fraunhofer spectral lines would consist of a probability measure with discrete support.

Almost simultaneously with Fraunhofer's discovery it was realized that spectral lines have a non-zero width. This broadening originates from many different physical effects and a discussion of spectral broadening can be found in a variety of different books and journals, see for example [6, 8–10, 14, 28, 31, 32, 45, 46]. In order to get a basic idea we review some of the most important mechanisms here.

A first type of broadening, termed *natural broadening*, occurs because the time of the transition between the two energy levels is finite. The spectral lines which have only been broadened by this type have a Lorentzian shape, i.e., have peaks of the form $1/(1 + x^2/s^2)$ where s is a width parameter. Usually natural broadening leads to very narrow lines. Much larger than natural broadening is the effect of *Doppler broadening* which occurs because the emitting (or absorbing) particles are in constant thermal motion which leads to a Doppler effect which shifts the energies of the photons. The shape of spectral lines which only have been Doppler broadened are Gaussian. While the width of the Doppler broadened lines is proportional to the energy we will neglect this here and assume a constant width approximation. Neighboring particles to the electrons emitting or absorbing the photons produce a third kind of broadening, the *pressure broadening*. One can show that in the case where only pressure broadening occurs the spectral lines are Lorentzian. Further broadening originates in the instrumentation and even discretization (or binning) of the spectrum produces a certain amount of broadening [15]. Finally the medium which the photons need to traverse before getting to the observer also produces some broadening. There are other effects which contribute to broadening and there are other distortions of spectra than broadening occurring.

This includes spectral shifts and the occurrence of extra peaks, so-called satellites [14].

A fairly general but simple broadening model would represent observed spectra as the effect of an integral operator on an underlying spectrum which might have been modified in other ways. Here this underlying spectrum u is assumed to be in $L_2(\mathbf{R})$ and so an observed spectrum g is of the form

$$g(x) = \int_{\mathbf{R}} a(x, y) u(y) dy$$

with some kernel a which in the simplest case is assumed to be a convolution kernel, i.e., $a(x, y) = \alpha(x-y)$ for some L_2 function α . More generally, an observed spectrum is modeled as the image of a product of several broadening operators A_1, \dots, A_n , i.e., as $g = A_1 \cdots A_n u$. In some cases, such a product can lead to a normal distribution because of the central limit theorem. Here we assume mostly that all the operators are convolutions and have Lorentzian or Gaussian shape (but different widths). As the operators commute and the convolution of Lorentzians is a Lorentzian and of Gaussians is a Gaussian, respectively, it is found that a good model is given by the Voigt shape which consists of a convolution of a Gaussian with a Lorentzian. In the following we call the integral equation $Au = g$ representing any kind of (linear) broadening the *broadening equation*.

1.2. Fitting the lines. While immediately appealing, the inversion of the broadening equation $Au = g$ is not feasible as it is typically severely ill-posed, the g has a substantial amount of observational error and u is typically not very smooth so that even a regularized solution cannot be expected to be a good approximation. Any feasible approximation will make use of the (approximate) Fraunhofer line structure of the u . The simplest model assumes that u is a measure with discrete support and intensities u_i so that the broadening equation takes the form

$$g(x) = \sum_{i=1}^{\infty} a(x, x_i) u_i.$$

The determination of the x_i and u_i from some data g_δ with $\|g - g_\delta\| \leq \delta$ can be done by minimizing the least-squares objective function

$$J(u) = \left\| \sum_{i=1}^{\infty} a(\cdot, x_i) u_i - g_{\delta} \right\|.$$

When the locations x_i of the spectral lines are known this amounts to a linear least squares problem. The determination of these locations, however, is a nonlinear problem. An interesting discussion of this problem from the perspective of Bayesian statistics can be found in [11].

In [20] Golub and Pereya discuss the *variable projection method* for the solution of the nonlinear problem above in the case of a finite number of nonzero u_i . Rather than minimizing the squared residual they first solve for the linear parameters u_i explicitly such that $u = A^+(x)g_{\delta}$ where $u = (u_1, \dots, u_n)$. They then use a nonlinear (typically Gauss-Newton) method to solve for the locations $x = (x_1, \dots, x_n)$ by minimizing the functional $\|A(x)A^+(x)g_{\delta} - g_{\delta}\|$. In a recent paper [41] the authors discuss the application of this method to spectroscopic problems and consider reasons for the success of the approach. In particular they point out the superior numerical conditioning and convergence of the Gauss-Newton method compared to the original optimization problem.

An important condition required by the variable projection method is that the matrix $A(x)$ has to have a fixed rank for x in some neighborhood of the minimum of the variable projection functional. This condition may be difficult to fulfill when one has two components of x which are very close. As two coinciding x_i will reduce the rank of $A(x)$, the neighborhood where the rank condition holds can be very small. It would certainly be difficult to find good initial conditions for the Gauss-Newton iteration which are in a neighborhood of the exact solution.

When the spectral lines are well separated then the variable projection method works very well. This is for example the case where the *baseline condition* holds in which case the functions $a(\cdot, x_i)$ have non-overlapping supports (at least numerically). It follows that the $a(\cdot, x_i)$ are pair-wise orthogonal, good starting values can be obtained and the rank condition can be maintained. A similarly favorable situation occurs if the *Rayleigh condition holds*. This motivates the development of methods which are able to enhance the spectrum so that the enhanced

spectral lines are better separated. A discussion of these aspects from a statistical perspective can be found in [1].

2. Resolution enhancement.

2.1. The enhancement equation. The resolution enhancement procedures considered here consist of algorithms which determine the *enhanced spectrum* f as a solution of an integral equation $Bf = g$ from the *observed spectrum* g_δ which satisfies $\|g_\delta - g\| \leq \delta$. The integral operator B is of the form

$$(1) \quad Bf(x) = \int_{\mathbf{R}} b(x, y)f(y) dy.$$

The integral equation

$$(2) \quad Bf = g$$

will be called the *enhancement equation*. The operator B is chosen such that the enhanced spectrum f has narrower lines than the original spectrum g . The main constraint in choosing B is that the enhancement equation should be solvable which means that g has to be in the range of B :

$$(3) \quad g \in \text{range}(B).$$

In the case where B is a convolution operator, the resolution enhancement is the *Stokes correction formula* [47]. The integral equation Ansatz for enhancement was introduced by Allen, Gladney and Glarum in their ground-breaking paper [2]. A simple precursor to this type of enhancement is the *Eddington correction formula* [9, 17, 18] for the enhancement of spectra with Gaussian peaks using differentiation.

The careful choice of the operator B is essential to successful enhancement. Even if the range condition (3) holds, the solution of the enhancement equation (2) may show poor resolution and contain a large error. This is due to the ill-posedness of the enhancement equation. Its solution will require some form of regularization. When selecting B one has to trade-off the amount of enhancement achievable by B against the regularization required for the solution of the enhancement equation.

While the theory of resolution enhancement is based on the general theory for the solution of integral equations, there is one important difference: When solving integral equations, the operator is given while for resolution enhancement, the operator B is chosen. In both cases, one needs to choose the regularization method.

There is a large literature on regularizers, a concise and short reference is still the book by Groetsch [21]. In this book, convergence rates of regularizers are given, provided that a *source condition* of the form $g \in \text{range}((BB^*)^s)$ holds for some integer $s > 1$ and where B^* denotes as usual the adjoint of the operator B . Here we will use a more general theory based on *variable Hilbert scale inequalities* [23, 24]. This framework has since been used in [33–36]. In the analysis literature, the variable Hilbert scale interpolation is called interpolation with a function parameter¹, see, for example [13, 39, 40]. In the analysis of partial differential equations, a related generalized Hölder inequality has been applied in [7]. Source conditions are very important in the analysis of convergence of regularization and some newer work which includes the application to nonlinear problems can be found in [16, 27, 33, 49]. The recovery of $f = B^{-1}g$ from g_δ is the main topic of the book [22] by Groetsch. The specific case of singular convolutions are covered in a paper by Sushkov [48].

In the following we assume that B is injective so that the $B^{-1}g$ is well defined for any g in the range of B . We then set

$$\|g\|_B = \|B^{-1}g\|,$$

which turns the range of B into a Hilbert space which we call H_B . Furthermore let ψ be a continuous monotonically increasing function defined on $(0, \infty)$ and define $\psi((BB^*)^{-1})$ using the spectral decomposition of $(B^*B)^{-1}$ (like in [24]). Then let H_ψ be the Hilbert space containing all elements of $L_2(\mathbf{R})$ for which

$$\|g\|_\psi = (g, \psi((BB^*)^{-1})g)$$

is bounded.

In the following f_α will always denote a regularized solution of $Bf = g$. The next theorem provides a connection between the norm $\|Bf_\alpha - g\|$ of the residual and the norm of the error $\|f_\alpha - f\|$ where $Bf = g$. This

bound holds under an additional stability constraint $\|Bf_\alpha\|_\psi \leq C$. It can be seen that such a stability constraint naturally holds for many well-posed problems but for ill-posed problems this constraint needs to be imposed as part of the regularization method. A similar theorem used in the theory of numerical solvers for initial value problems is the Lax equivalence theorem. There convergence of methods which are consistent (which in our case translates to them having a small residual) follows if and only if a certain stability condition holds see, for example [5].

The next theorem is a direct consequence of earlier results [23, 24] and a similar proof can be found in [25]. In order to make the presentation here self-contained a sketch of this proof is provided which should be sufficient for a reader familiar with spectral theory.

Theorem 1. *Let $B : L_2(\mathbf{R}) \rightarrow L_2(\mathbf{R})$ be an injective, continuous linear operator. Furthermore, let ψ be a non-negative function which is monotonically increasing for non-negative arguments. Finally, let Ψ be a non-negative function such that $\Psi(\psi(\lambda)) \geq \lambda$ and Ψ is monotonically increasing and concave for all arguments $\lambda > 0$.*

If $f_\alpha \in H_\psi$ satisfies

$$(4) \quad \|Bf_\alpha\|_\psi \leq C, \quad \text{and}$$

$$(5) \quad \|Bf_\alpha - g\| = \varepsilon$$

then

$$(6) \quad \|f - f_\alpha\| \leq \varepsilon \sqrt{\Psi((C + \|g\|_\psi)^2 / \varepsilon^2)}$$

for all f and $g = Bf \in H_\psi$.

Proof. (Sketch). Recall that as B^{-1} is injective and ψ is linearly increasing the spaces H_B and H_ψ and their norms are well defined.

Let in the following the measure ν_r be defined by $d\nu_r(\lambda) = \|r\|^{-2} d(r, E(\lambda)r)$ for $0 \neq r \in L_2(\mathbf{R})$ where $E(\lambda)$ is the spectral family or resolution of the identity defined by the inverse $(B^*B)^{-1}$. One can see that ν_r is a probability measure on $(0, \infty)$.

By definition of the spectral measure $(r, E(\lambda)r)$ one has

$$\|B^{-1}r\|^2 = \|r\|^2 \int_0^\infty \lambda d\nu_r(\lambda).$$

for any $r \in H_B$. As $B r \in L_2(\mathbf{R})$ and we assume that $\lambda \leq \Psi(\psi(\lambda))$ holds one gets

$$\begin{aligned} \|B^{-1}r\|^2/\|r\|^2 &= \int_0^\infty \lambda \, d\nu_r(\lambda) \\ &\leq \int_0^\infty \Psi(\psi(\lambda)) \, d\nu_r(\lambda) \\ &\leq \Psi\left(\int_0^\infty \psi(\lambda) \, d\nu_r(\lambda)\right) \\ &= \Psi(\|r\|_\psi^2/\|r\|^2) \end{aligned}$$

from the (inverse) Jensen inequality. It follows that the interpolation inequality

$$\|r\|_B \leq \|r\| \sqrt{\Psi(\|r\|_\psi^2/\|r\|^2)}, \quad \text{for all } r \in H_\psi$$

holds.

Now we apply this inequality to the residual $r = Bf_\alpha - g$. As $g = Bf$ one has

$$\|r\|_B = \|Bf_\alpha - Bf\|_B = \|f_\alpha - f\|.$$

Furthermore, by the triangle inequality one gets

$$\|r\|_\psi = \|Bf_\alpha - g\|_\psi \leq \|Bf_\alpha\|_\psi + \|g\|_\psi$$

and, as Ψ is monotonically increasing, it follows that

$$\Psi(\|r\|_\psi^2/\|r\|^2) \leq \Psi((C + \|g\|_\psi)^2/\varepsilon^2).$$

Inserting this in the interpolation inequality gives the claimed bound. \square

In a practical computation, ψ might be unknown. In this case one may take a stronger norm for stabilization in a discrepancy method similar to the one discussed in [23]. For consistency one wants to make sure that ε is small. This is achieved indirectly by controlling the size of $\|Bf_\alpha - g_\delta\|$ and observing that

$$\|Bf_\alpha - g\| \leq \|Bf_\alpha - g_\delta\| + \|g - g_\delta\|$$

by the triangle inequality. In the following we call any (approximate) enhancement f_α which satisfies both conditions (4) and (5) a *spectrum which has been stably enhanced with B* .

Almost simultaneously with the establishment of the index functions and variable Hilbert scales in [23, 24] in 1992 and 1995 several related approaches appeared. The connections between the various approaches is currently an active area of research. Here we will not discuss this emerging research in detail but instead point out connections between some of the most closely related approaches. While Theorem 1 provides a bound of the error using the residual $\|Bf_\alpha - g\|$ an earlier paper by Nair et al. [42] gives a bound using the discrepancy $\|Bf_\alpha - g_\delta\|$ which is directly accessible. However, as by the triangle inequality

$$\|Bf_\alpha - g_\delta\| - \|g - g_\delta\| \leq \|Bf_\alpha - g\| \leq \|Bf_\alpha - g_\delta\| + \|g_\delta - g\|$$

bounds derived by one approach may be compared with bounds derived with the other approach. The discrepancy based approach in [42] is based on a paper [50] by Tautenhahn which appeared in 1998.

In another related approach source sets of the form $M = \phi(B^*B)^{1/2}U_1$ are considered where U_1 is the unit ball in the Hilbert space. These source sets correspond to the unit ball in H_ψ which could be defined as $M = \psi((B^*B)^{-1})^{-1/2}U_1$. The advantage of the approach taken here is the relative ease with which error bounds like the one in Theorem 1 can be derived using this approach. The source conditions have been used to derive conditional stability estimates of the form

$$\|f\| \leq \beta(\|Bf\|), \quad f \in M,$$

see, e.g., [30]. In a recent paper [44] by Reginska and Tautenhahn the authors use this approach to obtain bounds on regularization errors. The proof uses Jensen's inequality and is similar to the proof of Theorem 1 or the corresponding theorems in [23, 24]. The structure of the conditional stability estimate appears to be very close to the interpolation inequality used in Theorem 1. However, the concise formulation of these connections is outside the scope of this paper.

In contrast to many earlier papers on variable Hilbert scale interpolation we here introduce a function Ψ like in [25]. In the earlier papers one has $\Psi = \psi^{-1}$. This function Ψ was introduced in a paper

by Bégout and Soria [7] where Hölder inequalities were found which are of the same form as the Hilbert scale interpolation inequalities in [23, 24]. We require Ψ to be monotonically increasing and concave and to be a generalization of an inverse of ψ in the sense that

$$(7) \quad \lambda \leq \Psi(\psi(\lambda)).$$

This covers in particular cases where ψ^{-1} itself is not concave or only concave for large enough λ . We are currently working on a general characterization of conditions under which the inequality (7) holds and Ψ is concave. We found that it is easier to find functions Ψ which are concave and satisfy inequality (7) for a given ψ than to find ψ which defines an appropriate Hilbert space H_ψ and then choosing $\Psi = \psi^{-1}$.

Theorem 1 is not only used for the analysis of spectral correction. Indeed it generalizes the discussion of the convergence of regularization methods as established in the standard textbooks on the topic of regularization. Since the corresponding theorems were established in [24, 25] they have been cited numerous times and used in many different contexts. A quick internet search using a common search engine gives over 100 hits for the term “variable Hilbert scales.” Here we provide a reformulation of the earlier results and a discussion of how these results can be used to understand the accuracy of numerical spectral enhancement procedures.

2.2. The Eddington correction formula. This early and still popular approach to the enhancement of Gaussian spectra uses derivatives and is of the form

$$f = g - \frac{g^{(2)}}{2} + \frac{g^{(4)}}{8} - \dots,$$

see [9, 17, 18]. It has been observed in [2] that correction formulas of this type may be viewed as solutions of integral equations of the form discussed in subsection 2.1. We can thus apply Theorem 1 to obtain an error bound for the Eddington correction. See also [38] for a discussion of their application in practice. Other procedures to spectral enhancement based on differentiation are discussed from the point of view of numerical differentiation in [4].

The k -th order Eddington correction f is defined as

$$(8) \quad f = \sum_{j=0}^k \frac{(-1)^j}{2^j j!} g^{(2j)}$$

where $g^{(2j)}$ denotes the derivative of order $2j$ of g . The Eddington correction formula now fits into the integral equation framework for resolution enhancement with enhancement equation $Bf = g$ and the enhancement operator B has a kernel

$$b(x, y) = \frac{1}{\pi} \int_0^\infty \left(\sum_{j=0}^k \frac{\omega^{2j}}{2^j j!} \right)^{-1} \cos(\omega(x-y)) d\omega.$$

In particular, for $k = 1$ one has

$$b(x, y) = \frac{1}{\sqrt{2}} e^{-\sqrt{2}|x-y|},$$

and for $k = 2$ the kernel is of the form

$$b(x, y) = \gamma e^{-\alpha|x-y|} \cos(\beta(|x-y| + \theta))$$

for some α, β, γ and θ .

In the following, let

$$a_G(x, y) = \frac{1}{\sqrt{2\pi}} e^{-(x-y)^2/2},$$

and let a spectrum g which has been broadened by a_G be called a *Gaussian spectrum*. In this case one has

$$(9) \quad g(x) = \int_{\mathbf{R}} a_G(x, y) u(y) dy,$$

for some $u \in L_2(\mathbf{R})$. The Eddington correction formula have been designed to reduce some of the broadening produced by a_G .

A motivation for this particular formula comes from the convolution theorem as

$$\widehat{g}(\omega) = \widehat{a}_G(\omega) \widehat{u}(\omega)$$

where $\hat{a}_G(\omega) = \exp(-\omega^2/2)$ and \hat{g} and \hat{u} are the Fourier transforms of g and u , respectively. By the Taylor theorem one then formally gets

$$\hat{u}(\omega) = \sum_{j=0}^{\infty} \frac{1}{2^j j!} \omega^{2j} \hat{g}(\omega).$$

Truncating this expansion and using the fact that multiplication with ω^2 in the Fourier domain corresponds to taking $-d^2/dx^2$ in the original domain gives the formula.

The following lemma provides the expressions and some properties for the ψ and Ψ which will be used to establish the error bound of the correction formula.

Lemma 1. *Let B be the enhancement operator² for the k -th order Eddington correction formula. Furthermore, let $t_k(\eta)$ be the k -th order Taylor polynomial for the exponential function for $k \geq 0$ and $t_k = 0$ for $k < 0$. Then*

(1) *Any Gaussian spectrum g is in H_ψ , the Hilbert space with the scalar product $(g, g)_\psi = (g, \psi((BB^*)^{-1})g)$ and where*

$$\psi(\lambda) = \exp(2t_k^{-1}(\sqrt{\lambda})), \quad \lambda \geq 1.$$

(2) *The inverse*

$$\Psi(\eta) = \psi^{-1}(\eta) = t_k(\log(\eta)/2)^2, \quad \eta \geq 1$$

is concave.

Proof. (1) The B -norm is by Parseval's theorem

$$\|g\|_B^2 = \|B^{-1}g\|^2 = \int_{\mathbf{R}} t_k(\omega^2/2)^2 |\hat{g}(\omega)|^2 d\omega.$$

As $\psi(t_k(\omega^2/2)^2) = \exp(\omega^2)$ by definition one gets

$$\|g\|_\psi = (g, \psi((BB^*)^{-1})g) = \int_{\mathbf{R}} \exp(\omega^2) |\hat{g}(\omega)|^2 d\omega,$$

which is equal to $\|u\|^2$ if g is a Gaussian spectrum with

$$g(x) = \int_{\mathbf{R}} a_G(x, y)u(y) dy.$$

It follows that $\|g\|_\psi$ is a norm on the set of Gaussian spectra which provides a Hilbert space structure for this space.

(2) As $dt_k(\zeta)/d\zeta = t_{k-1}(\zeta)$ one has $d\Psi(\zeta)d\zeta = t_{k-1}(\zeta)$ and consequently

$$\frac{d^2\Psi}{d\zeta^2} = -\frac{1}{2\zeta^2} \left(\frac{1}{k!} \left(\frac{\log(\zeta)}{2} \right)^k t_{k-1} + \frac{1}{(k-1)!} \left(\frac{\log(\zeta)}{2} \right)^{k-1} t_k \right)$$

which is non-positive and so $\Psi(\zeta)$ is concave for $\zeta \geq 1$. \square

We now get the main theorem which provides bounds on how well one can evaluate the Eddington correction.

Proposition 1. *Let f_α be a stably enhanced spectrum using B the k -th order Eddington enhancement for Gaussian spectra and $\psi(\lambda) = \exp(2t_k^{-1}(\sqrt{\lambda}))$. Then there exists a $C > 0$ independent of ε such that*

$$(10) \quad \|f - f_\alpha\| \leq C\varepsilon |\log(\varepsilon)|^k.$$

Proof. By Theorem 1 and Lemma 1 one has for $1/\varepsilon \geq C + \|g\|_\psi$:

$$\begin{aligned} \|f - f_\alpha\| &\leq \varepsilon \sqrt{\Psi((C + \|g\|_\psi)^2/\varepsilon^2)} \\ &\leq \varepsilon t_k(2 \log(C + \|g\|_\psi) - 2 \log(\varepsilon)) \\ &\leq \varepsilon e^{2k} (\log(C + \|g\|_\psi) - \log(\varepsilon))^k \\ &\leq \varepsilon e^{4k} (-\log(\varepsilon))^k \\ &\leq C\varepsilon |\log(\varepsilon)|^k, \end{aligned}$$

as $t_k(\lambda) \leq e\lambda^k$ for $\lambda \geq 1$. \square

A consequence of this lemma is that the ill-posedness of the problem is really an issue for very high derivatives only. However, it is necessary

to use regularization nonetheless as otherwise the data errors would remove any advantage of the resolution enhancement and typically render the so “enhanced” spectrum useless. Allen et al. [2] provide similar correction formulas to the Eddington formula for Lorentz spectra and also provide other correction formulas determining the coefficients in different ways, see also [26]. The accuracy of so enhanced spectra can be analyzed in exactly the same way as the Eddington formula.

In order to compare the above error bound for the Eddington correction formula with the ones which we will obtain for other enhancement methods, one could restate it as

$$\|f - f_\alpha\| \leq C\varepsilon^{\eta(\varepsilon)}$$

where the exponent is

$$\eta(\varepsilon) = 1 - k \frac{\log |\log(\varepsilon)|}{|\log(\varepsilon)|}.$$

The formula is valid asymptotically and we assume that $0 < \varepsilon \leq 1/e$. It can be seen that the smallest exponent is now obtained for $\varepsilon = e^{-e}$ as

$$\eta_{\min} = 1 - k/e,$$

and consequently

$$\|f - f_\alpha\| \leq C\varepsilon^{1-k/e}.$$

It follows that for $k = 1, 2$ one gets an error bound which is similar to the one obtained for an enhancement obtained through sharpening, see [25]. One can also get similar bounds for larger k a necessary condition on the error in this case, however, is

$$\frac{\log |\log(\varepsilon)|}{|\log(\varepsilon)|} < 1/k$$

and while first and second order Eddington corrections (with second and fourth derivatives) should work well even in the case of larger errors, for higher order derivative corrections one does require smaller data errors.

2.3. Stokes enhancement with a Gaussian kernel. By using Fourier transforms, Stokes [47] was able to introduce more general

spectral correction formulas which amount to general deconvolutions. An example of such a formula would use a Gaussian kernel of the form

$$(11) \quad b(x, y) = \frac{1}{\sqrt{2\pi\kappa}} \exp\left(-\frac{(x-y)^2}{2\kappa^2}\right).$$

One can see that a resolution enhancement using this kernel reduces the width of a unit Gaussian spectral line from equation (9) from one to $\sqrt{1-\kappa^2}$. The enhanced spectrum is again a Gaussian with no other local maxima and no local minima. While such an approach can be generalized to other than Gaussian spectra (see [23]) it does require the knowledge of the spectrum. As Gaussian spectral lines are very smooth, using this type of enhancement for less smooth non-Gaussian spectra will lead to meaningless results as the range condition is not satisfied in such a case.

For the Gaussian case, however, one has the following result about the error of a regularized enhancement f_α :

Proposition 2. *Let g be a Gaussian spectrum which has been enhanced by an operator with kernel b given in equation (11). Then the stable approximation f_α satisfies the error bound:*

$$(12) \quad \|f - f_\alpha\| \leq C\varepsilon^{1-\kappa^2}.$$

Proof. Using Fourier transforms and the Parseval equality one derives $\psi(\lambda) = \lambda^{1/\kappa^2}$. As $\kappa \in (0, 1)$ the inverse $\Psi(\eta) = \psi^{-1}(\eta) = \eta^{\kappa^2}$ is concave and the bound then follows from Theorem 1. \square

Note that in this case the source condition is of a classical form and thus the error bound may also be obtained using methods from [21].

As the spectral enhancement reduces the width by a factor $\sqrt{1-\kappa^2}$ it follows for example that a reduction of the width by a factor two is obtained by solving an integral equation of the first kind with error $O(\varepsilon^{1/4})$ if a stable method is used and ε is the data error.

3. Enhancing Voigt spectra with unknown line shape. While it is known that many spectra are of Voigt type, i.e., they contain a

mixture of Gaussian and Lorentz broadening it is often unknown, how much of both types are current in any particular spectrum. We will now present an enhancement procedure which utilizes a Lorentz kernel for the enhancement of a Voigt spectrum.

The enhancement equation $Bf = g$ providing the enhancement is an integral equation with a Lorentz kernel of the form

$$(13) \quad b(x, y) = \frac{1}{\kappa\pi} \frac{1}{1 + (x - y)^2/\kappa^2}.$$

Thus Bf is again a convolution and the Fourier transform is

$$\widehat{b}(\omega) = \exp(-\kappa|\omega|).$$

The width parameter κ has to be chosen similar to the width parameter for the Gaussian sharpening discussed in subsection 2.3 or the order of the Eddington correction formula of subsection 2.2. In this choice one considers the trade-off between the enhancement obtained through the narrower lines in the spectra and the error from the solution of the integral equation.

Before discussing the general case of a Voigt spectrum we provide a bound for the error of the Stokes correction with Lorentz kernel of a Gaussian spectrum.

Lemma 2. *Let B be the enhancement operator for the Stokes correction formula with a Lorentz kernel with width κ . Then a Gaussian spectrum is in the space H_ψ (based on B) with $\psi(\lambda) = \exp((\log(\lambda)/(2\kappa))^2)$. Furthermore, the inverse $\Psi(\eta) = \psi^{-1}(\eta) = \exp(2\kappa\sqrt{\log(\eta)})$ is concave if $\kappa \leq \sqrt{2}$ or if $\eta \geq (\kappa/2) + \sqrt{(\kappa/2)^2 - 1/2}$.*

Proof. We use the Fourier transforms of the kernel of BB^* which is $\exp(-2\kappa|\omega|)$ and AA^* which is $\exp(-\omega^2)$ and the Parseval equality to get ψ .

The second derivative of Ψ is then

$$\frac{d^2\Psi}{d\eta^2} = -\frac{\kappa (2 \log \eta - 2 \sqrt{\log \eta} \kappa + 1) e^2 \sqrt{\log \eta} \kappa}{2 \eta^2 (\log \eta)^{3/2}},$$

and it follows that Ψ is concave if $2 \log \eta - 2 \sqrt{\log \eta} \kappa + 1 \geq 0$. The conditions then follow directly. \square

It then remains to apply Theorem 1 to get the following error bound:

Proposition 3. *The error of a stably computed enhancement f_α of a Gaussian spectrum using the Stokes correction formula with a Lorentz kernel is bounded by*

$$\|f_\alpha - f\| \leq \varepsilon^{1-2\kappa/\sqrt{|\log \varepsilon|}}$$

for $0 < \varepsilon < \varepsilon_0$ and some $\varepsilon_0 > 0$.

Proof. By Theorem 1 and Lemma 2 one has for $\varepsilon > 0$ and some C which satisfy

$$\frac{1}{\varepsilon} \geq C + \|g\|_\psi \geq \sqrt{\kappa/2 + \sqrt{(\kappa/2)^2 - 1/2}}$$

the bounds

$$\begin{aligned} \|f - f_\alpha\| &\leq \varepsilon \sqrt{\Psi((C + \|g\|_\psi)^2/\varepsilon^2)} \\ &\leq \varepsilon \exp(\kappa \sqrt{\log((C + \|g\|_{\psi_i})^2/\varepsilon^2)}) \\ &\leq \varepsilon \exp(2\kappa \sqrt{|\log \varepsilon|}) \\ &\leq \varepsilon^{1-2\kappa/\sqrt{|\log \varepsilon|}}. \quad \square \end{aligned}$$

Note that here κ is not the width of the enhanced spectrum but a parameter which controls how much enhancement is done. Thus a larger κ corresponds to more enhancement and $\kappa = 0$ to no enhancement. For example, if one has $\varepsilon \approx 10^{-3}$ and $\kappa = 0.7$ one gets an error of approximately $O(\varepsilon^{1/2})$.

As discussed in the introduction many spectra have undergone broadening both with Gaussian and with Lorentz kernels. The resulting class of spectra are the Voigt spectra. We assume here that we know that a given spectrum is in this class; however, we do not assume that we know

how much each of the two components has contributed to the broadening. This is why we suggest a Stokes correction with Lorentzian kernels.

Specifically, let the Lorentz kernel be

$$a_L(x, y) = \frac{1}{\sqrt{2\pi}} \frac{1}{1 + [(x - y)^2/2]}$$

with Fourier transform

$$\widehat{a}_L(\omega) = \exp(-\sqrt{2}|\omega|).$$

The Voigt spectrum (with mixing parameter θ) is then defined by its Fourier transform

$$\widehat{a}_V(\omega) = \widehat{a}_G(\omega)^\theta \widehat{a}_L(\omega)^{1-\theta},$$

and the kernel is thus

$$a_V(x, y) = \frac{1}{2\pi} \int_{\mathbf{R}} e^{i\omega(x-y)} \widehat{a}_V(\omega) d\omega.$$

A Voigt spectrum is then of the form

$$g(x) = \int_{\mathbf{R}} a_V(x, y) u(y) dy$$

for some $u \in L_2(\mathbf{R})$ and $0 < \theta \leq 1$. One then has

Lemma 3. *Let B be the enhancement operator for the Stokes correction formula with a Lorentz kernel with width κ . Then a Voigt spectrum with parameter θ is in the space H_ψ (based on B) with $\psi(\lambda) = \exp(\theta(\log(\lambda)/(2\kappa))^2 + \sqrt{8}(1 - \theta)\log(\lambda)/(2\kappa))$. Furthermore, the inverse $\Psi = \psi^{-1}$ is defined by*

$$\Psi(\eta) = \exp\left(\frac{2\kappa}{\theta} \left(\sqrt{2(1 - \theta)^2 + \theta \log(\eta)} - \sqrt{2}(1 - \theta)\right)\right)$$

and is concave if $\kappa \leq \sqrt{2}\theta^{3/2}$ or if $\eta \geq \eta_0$ for some $\eta_0 > 0$.

Proof. We use the Fourier transforms of the kernel of BB^* which is $\exp(-2\kappa|\omega|)$ and AA^* which is $\exp(-\theta\omega^2 - \sqrt{8}(1-\theta)|\omega|)$ and the Parseval equality to get ψ .

With $\zeta(\eta) = \sqrt{\log(\eta) + b}$, $a = 2\kappa\theta^{-3/2}$ and $b = 2(1-\theta)^2\theta$, one then has for the second derivative of Ψ

$$\exp(\sqrt{2}(1-\theta)) \frac{d^2\Psi}{d\eta^2} = -\frac{ae^{a\zeta(\eta)}}{4\eta^2\zeta(\eta)^3} (2\zeta(\eta)^2 - a\zeta(\eta) + 1).$$

One gets convexity for Ψ if $2\zeta(\eta)^2 - a\zeta(\eta) + 1 \geq 0$ which happens if $\kappa \leq \sqrt{2}\theta^{3/2}$, or for $\eta > \eta_0$ and large enough η_0 . \square

Then an application of Theorem 1 provides again an error bound:

Proposition 4. *The error of a stably computed enhancement f_α of a Voigt spectrum with width parameter θ using the Stokes correction formula with a Lorentz kernel is bounded by*

$$\|f_\alpha - f\| \leq \varepsilon^{1-2\kappa/\sqrt{\theta|\log\varepsilon|+(1-\theta)^2}}$$

for $0 < \varepsilon < \varepsilon_0$ and some $\varepsilon_0 > 0$.

Proof. By Theorem 1, Lemma 3 and the monotonicity of Ψ one has for $\varepsilon > 0$ satisfying $\varepsilon(C + \|g\|_\psi) \leq 1$ the bounds

$$\begin{aligned} \|f - f_\alpha\| &\leq \varepsilon\sqrt{\Psi((C + \|g\|_\psi)^2/\varepsilon^2)} \\ \|f - f_\alpha\| &\leq \varepsilon\sqrt{\Psi(\varepsilon^{-4})} \\ &\leq \varepsilon \exp\left(\frac{\kappa}{\theta} \left(\sqrt{2(1-\theta)^2 + 4\theta|\log\varepsilon|} - \sqrt{2}(1-\theta)\right)\right) \\ &= \varepsilon^{1-\eta(\varepsilon)} \end{aligned}$$

where

$$\begin{aligned} \eta(\varepsilon) &= \frac{\sqrt{2}\kappa}{\theta} \left(\frac{\sqrt{(1-\theta)^2 + 2\theta|\log(\varepsilon)|} - (1-\theta)}{|\log\varepsilon|} \right) \\ &= \sqrt{2}\kappa \frac{2}{\sqrt{(1-\theta)^2 + 2\theta|\log\varepsilon|} + (1-\theta)} \\ &\leq \frac{2\kappa}{\sqrt{\theta|\log\varepsilon| + (1-\theta)^2}}. \end{aligned}$$

As $0 < \varepsilon < 1$ an upper bound for $\eta(\varepsilon)$ will lead to an upper bound for the error. \square

4. Enhancing a Gaussian peak. We provide some simple experiments which show how resolution enhancement modifies a single Gaussian peak. In Figure 1 a Lorentz correction formula is applied with different values of the parameter κ . Comparing the widths at height 0.5 one sees that for κ ranging from $\sqrt{2}$ to 4 one gets reductions of the widths between a factor of 1/2 to almost 1/5. Note that resolution enhancement comes at a cost which grows with κ in the sense that side bands start to occur. From the plot it appears that the peaks of the side bands are at the level of the original (unenhanced) spectrum but can be negative.

To illustrate the (broadening) effect of noise and regularization we consider the solution of the enhancement equation $Bf = g$ from some data g_δ using Tikhonov regularization where f_α is the minimizer of the functional

$$\Phi_\alpha(f) = \|Bf - g_\delta\|^2 + \alpha\|BA^{-1}f\|^2$$

where the operators A and B correspond to the convolution with Lorentzian (equation (13) with $\kappa = 2$) and Gaussian (equation (11) with $\kappa = 1$) kernels, respectively. The regularization term $\alpha\|BA^{-1}f\|^2$ assumes that it is known that the observed spectrum g is Gaussian with peaks described by elements of the range of A . This is an optimal situation and in practice one may not have this information available and other choices will have to be made. As this example only serves to illustrate broadening by regularization we will not discuss this issue further here. The actual computations were done using Fourier transforms. In Figure 2 the case of zero data error was considered. One can clearly see the oscillations and the broadening which are caused by regularization.

Finally, Figure 3 considers the same regularization method and parameters for the case of data with error. Here a data error of 5 percent has been assumed. One sees that the effect of the error on the enhanced signals is some additional broadening but most noticeably are oscillations away from the main peak—especially for the cases of small regularization parameter α .

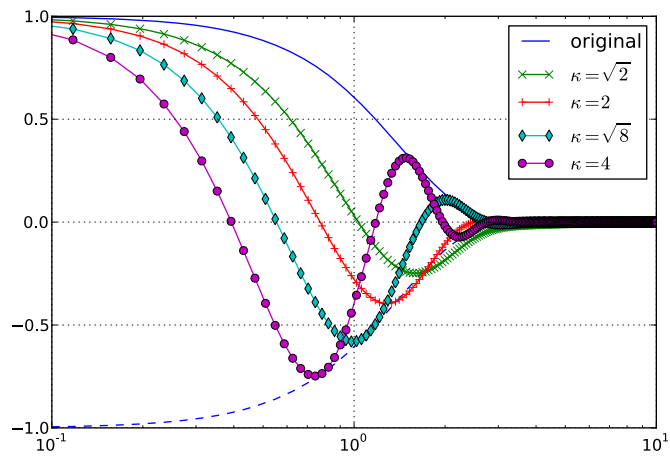


FIGURE 1. Lorentzian correction of a Gaussian.

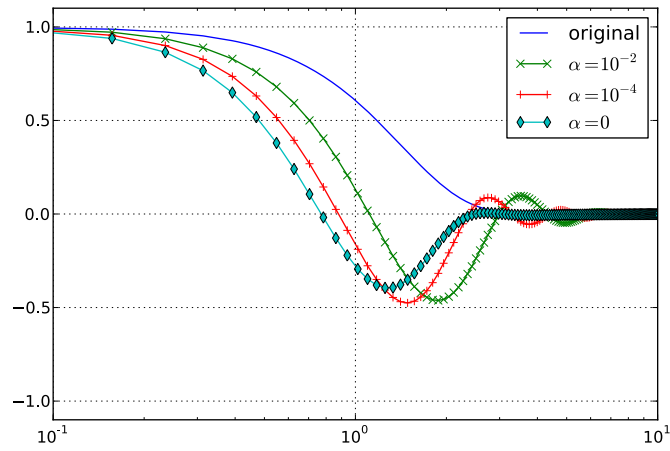


FIGURE 2. Regularized Lorentzian correction of a Gaussian.

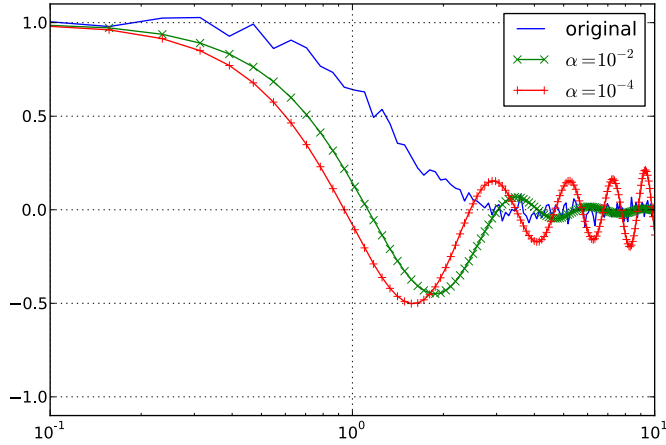


FIGURE 3. Regularized Lorentzian correction of a Gaussian with 5 percent data error.

5. Conclusion. From the physics of spectral broadening one obtains the broadening equation $Au = g$. For various reasons including the severe ill-posedness of the equations, the fact that A might not be known, and that u might not be sufficiently smooth, the solution of $Au = g$ is typically not feasible. However, this equation provides a regularity or source condition for the solution of enhancement equations $Bf = g$ which are essential for obtaining error bounds or regularization methods. As typically A^*A is not a power of B^*B the standard convergence theory for ill-posed problems cannot be used. Instead we apply the variable Hilbert scale theory and obtain convergence results for Eddington correction and Lorentz deconvolution of Gaussian and Voigt spectra in particular. Knowing these error bounds provides some insight into the choice of the enhancement operators B which goes beyond the range condition $\text{range}(A) \subset \text{range}(B)$.

By a change of perspective one interprets resolution enhancement as an application of an unbounded operator R . In the case of this paper, $R = B^{-1}$ for the integral operator B . Another larger class of such enhancements is obtained when R is a differential operator. The theory of the application of such operators is covered in the recent book [22] by Groetsch. A specific algorithm for numerical differentiation based on

averaging and differences which converges with the size of the sampling with is analyzed in [3]. The important question of the choice of the amount of differentiation for enhancement is discussed in [4].

If the broadening operator is known explicitly and is a convolution a different approach to resolution enhancement is based on the dilation (or rather contraction) of the spectral lines. Error bounds can also be obtained and a variant of variable Hilbert scales, the *dilational Hilbert scales* has been introduced to perform this analysis in [23]. The approach has a particular appeal in practice as it does not introduce any satellite maxima. Such maxima might still occur, however, when data errors are large and regularization has to be used.

There is a substantial practical literature on separating overlapping line-shapes which cannot be covered here in any detail. As an example of a method which uses extra information, i.e., the ratio of the heights of two lines and the distance between them is the Rachinger correction formula [43]. This formula allows the determination of the corresponding line strengths u_i even without knowledge of the shapes $a(\cdot, x_i)$. In a sense, this is also what spectral enhancement methods attempt to achieve—but without any extra information.

Related to the problem of spectral enhancement is the statistical problem of deconvolution of a density. Convergence rates have been found for several such problems in [12]. These problems are often much more severely ill-posed and very slow convergence rates are obtained. The reason for this is that one can only assume that the underlying density is k times differentiable. While the authors did not use spectral theory nor the variable Hilbert scale interpolation inequality for their results one can obtain similar results with these more modern tools. This work has been continued and practical estimators are discussed (also for less severely ill-posed problems) in [19]. An interesting adaptive approach to these statistical problems is discussed in [51] where similar convergence results are obtained as in our discussion but using different techniques for analysis and different algorithms, see also [29, 37]. It would certainly be of interest to investigate these approaches from an ill-posed problem perspective using variable Hilbert scales.

Maybe the most important limitation of the above discussion relates to the fact that all the operators occurring are convolutions. As

outlined in the discussion of the models on broadening, the Doppler broadening is not a convolution and one can see that the operator may be factorized into diagonal operators and a convolution. The next natural step would be to utilize norm equivalences (possibly using wavelets) with the variable Hilbert scale interpolation theory to deal with such more general source conditions.

Acknowledgments. This paper is dedicated to Chuck Groetsch who made an important contribution to the original variable Hilbert scale paper [23] by encouraging the author at a crucial point in the process.

ENDNOTES

1. Thanks to M. Hansen and S. Kuehn for pointing this out to me.
2. Sometimes the inverse B^{-1} is called enhancement operator.

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