Signal Processing and Piecewise Convex Estimation

Many problems on signal processing reduce to nonparametric function estimation. We propose a new methodology, piecewise convex fitting (PCF), and give a two-stage adaptive estimate. In the first stage, the number and location of the change points is estimated using strong smoothing. In the second stage, a constrained smoothing spline fit is performed with the smoothing level chosen to minimize the MSE. The imposed constraint is that a single change point occurs in a region about each empirical change point of the first-stage estimate. This constraint is equivalent to requiring that the third derivative of the second-stage estimate has a single sign in a small neighborhood about each first-stage change point. We sketch how PCF may be applied to signal recovery, instantaneous frequency estimation, surface reconstruction, image segmentation, spectral estimation and multivariate adaptive regression.

1. Signal Recovery

Techniques such as splines and wavelets are optimal for estimating an arbitrary function in a ball in function space. We claim that the “uniform” prior is unrealistic and that naturally occurring functions have very few inflection points. Our basic tenet is that the fitted curve should preserve the geometric fidelity of the unknown function by having the same number of inflections. Consider a signal, \( y_i = g(t_i) + \epsilon_i \), measured at \( t_i = i\delta, \ i = 1 \ldots N \), where \( \{\epsilon_i\} \) are independent Gaussian random variables: \( \epsilon_i \sim N(0, \sigma^2) \). Let \( g(t) \) have \( K \) change points of \( \ell \)-convexity with change points \( x_1 \leq x_2 \ldots \leq x_K \) if \( (-1)^{k-1}g^{(\ell)}(t) \geq 0 \) for \( x_k \leq t \leq x_{k+1} \). In practice, we take \( \ell = 2 \).

Our goal is to estimate \( g(t) \) while preserving the geometry of \( g \). A standard technique, kernel smoothers [10], estimates \( g(t) \) by a weighted local average: \( \hat{g}_h(t) = \frac{1}{Nh} \sum_{i=1}^{N} y_i K \left( \frac{t-t_i}{h} \right) \), where \( h \) is the kernel halfwidth that determines the amount of smoothing. As \( h \) increases, the random error (variance) in \( \hat{g} \) decreases, while the systematic error (bias) increases. In [8], the geometric faithfulness of kernel smoothers is examined in the limit as \( N \to \infty \) and \( h \to 0 \) with \( N\delta = 1 \). The halfwidth that minimizes the mean square error scales as \( N^{\frac{\nu}{2\nu+1}} \) for \( g \in C^m[0,1] \) provided that the kernel satisfies certain moment conditions. For \( \ell = m \) or \( m - 1 \), this halfwidth scaling, \( N^{\frac{\nu}{2\nu+1}} \), produces extra (artificial) \( \ell \)-change points with high probability. To eliminate the artificial inflection points with probability 1, the smoothing must be increased such that \( h >> N^{\frac{\nu}{2\nu+1}} \ln[N] \). Thus, the level of smoothing required for geometric fidelity is large enough to degrade the MSE. In [8], we propose a two-stage estimator.

Stage 1: Strongly smooth with \( h_N N^{\frac{\nu}{2\nu+1}} \ln N \to \infty \). Denote the empirical \( \ell \)-change points by \( \hat{x}_K \).

Stage 2: Perform a constrained smoothing spline fit by minimizing the penalized likelihood subject to the constraints that \( \hat{g}^{(\ell+1)}(t) \) does not change sign in the intervals, \( [\hat{x}_k - z_\alpha \delta_k, \hat{x}_k + z_\alpha \delta_k] \). The \( k \)-th empirical change point variance is \( \sigma^2_{\ell+1} = \frac{c^2}{|g_{\ell+1}(\hat{x}_k)|^2 N h^{2\nu+1}} \), where \( g_{\ell+1}(\hat{x}_k) \) is the estimate of \( g^{(\ell+1)}(\hat{x}_k) \) from the first stage. \( c \) is a constant that depends on the kernel shape. The confidence interval parameter, \( z_\alpha \), is the \( \alpha \)-quantile for the normal distribution.

To motivate this two-stage estimator, consider the smoothing dilemma: If the smoothing level is optimized for MSE, there tends to be too many \( \ell \)-change points (wiggles). If the smoothing is chosen to eliminate the artificial change points (suppress wiggles), then the MSE suffers. Our two-stage estimate provides the best of both worlds! In [8], we show that this two-stage estimator achieves the optimal rate of convergence for functions in the Sobolev space \( W_{\nu,2} \), while suppressing artificial inflection points in the neighborhood where they are likely to occur.

In practice, we choose the second-stage smoothing parameter, \( \lambda_{\text{stage 2}} \), by generalized cross-validation while we scale the first-stage smoothing as \( h_{\text{stage 1}} = \epsilon(N) h_{GCV} \), where \( \epsilon(N) \equiv \log^2(N) N^\alpha \) with \( \alpha = \frac{1}{2\nu+1} - \frac{1}{2} \). Unconstrained smoothing splines can be used in first stage with the smoothing parameter, \( \lambda \), scaled with the correspondence: \( \lambda = h_{\text{eff}}^{2\nu+1} \), with \( h_{\text{eff}} \sim (\log N)^2 N^{\frac{\nu}{2\nu+1}} \).

When \( \ell = m - 1 \), the stage 2 minimization reduces to a finite dimensional convex minimization in the dual formulation. A simple implementation is that of Villabos and Wahba (VW) [14], who add pointwise constraints on the sign of \( \hat{g}^{(m)}(z_m) \) with \( z_m \) chosen in the constraint regions. The goal is to select \( \{z_j, j = 1, M\} \) such that the constraints are satisfied everywhere even though they are imposed only at a finite number of points. An important advantage of our two-stage estimator is that we impose constraints only in small regions about \( \hat{x}_k \). Since the constraint regions are small, the number of \( z_j \) that are necessary in the VW scheme is small. Thus, our two-stage estimator can be interpreted as a pilot estimator to determine where to place the \( \{z_j\} \) in the VW scheme.

The VW implementation of the second stage estimator reduces to a quadratic programming problem with linear inequality constraints. The number of constraints is bounded by \( (m \cdot k + \# \text{ of data points in constraint regions}) \).

The B spline representation gives a banded structure to the programming problem. The minimization may be
solved exactly using “active set” methods in quadratic programming or may be solved approximately using projected successive over-relaxation (PSOR) iterations. The PSOR method uses the band structure of convexity constraints while active set programs require modification to take advantage of the tridiagonal structure. In both cases, the dual formulation is easier to implement since positivity constraints are substituted for inequality constraints.

2. Adaptive regression splines
An alternative to smoothing splines is adaptive regression splines [3]. At each step, a new knot is added to the fit. The number and locations of the new knots are chosen by minimizing a Loss of Fit (LoF) function, $d_N(\hat{f}, \{y_i\})$. Let $\hat{\sigma}^2$ be a measure of the average residual error: $\hat{\sigma}^2(\hat{f}, \{y_i\}) = \frac{1}{N} \sum_{i=1}^{N} [y_i - \hat{f}(t_i)]^2$, or its $L_1$ analog. Typical discrepancy functions are

$$d_N(\hat{f}, \{y_i\}) = \frac{\hat{\sigma}^2}{[1 - (\gamma_1 p + m)/N]} \quad \text{and} \quad d^B(\hat{f}, \{y_i\}) = \frac{\hat{\sigma}^2[1 + (\gamma_2 p + m) \ln(N)/N]}{1 - (\gamma_1 p + m)/N},$$

(1)

where $p$ is the number of knots in the fit and $m$ is the spline degree. Friedman proposed $d^B_N$ with a default value of $\gamma_1 = 3$, while $d^B$ is the Bayesian/Schwartz information criterion when $\gamma_2 = 1$. For a nested family of models, $\gamma_2 = 1$ is appropriate while $\gamma_2 = 2$ corresponds to a nonnested family with $2\binom{N}{k}$ candidate models at the $k$th level [2]. In very specialized settings in regression theory and time series, it has been shown that LoF functions like $d^B_N$ are asymptotically efficient while those like $d^B$ are asymptotically consistent. In other words, using $d^B_N$-like criteria will asymptotically minimize the expected error at the cost of not always yielding the correct model. In contrast, the Bayesian criteria will asymptotically yield the correct model at the cost of having a larger expected error.

Our goal is to consistently select the number of convexity change points and efficiently estimate the model subject to the change point restrictions. Therefore, we propose the following new LoF function:

$$PCIC = \sigma^2(g, \{y_i\}) \left[ 1 + \gamma_2 K \ln(N)/N \right]$$

(2)

where $K$ is the number of convexity change points and $p$ is the number of knots. PCIC stands for Piecewise Convex Information Criterion. In selecting the positions of the $K$ change points, there are essentially $2\binom{N}{K}$ possible combinations of change point locations if we categorize the change points by the nearest measurement location. Thus, our default values are $\gamma_1 = 3$ and $\gamma_2 = 2$.

We motivate PCIC: to add a change point requires an improvement in the residual square error of $O(\sigma^2 \ln(N))$, which corresponds to an asymptotically consistent estimate. If the additional knot does not increase the number of change points, it will be added if the residual error decreases by $\gamma_1 \sigma^2$. Presently, PCIC is purely a heuristic principle. We conjecture that it consistently selects the number of change points and is asymptotically efficient within the class of methods which are asymptotically consistent with regards to convexity change points.

3. Instantaneous Frequency and Time-frequency representations
Much effort has been devoted to finding joint time-frequency representations of a signal whose frequency is being slowly modulated in time. The canonical example is a “chirp”: $y_t = \cos(at + bt^2)$, where the instantaneous frequency is $\omega_0(t) = a + 2bt$. In [7], we proposed using the WKB (eikonal/geometric optics) representation for signals whose amplitude and frequency are being slowly modulated in time:

$$y_t = A(\delta t) \cos \left[ \int_0^t \omega(s)ds \right] + \epsilon_t,$$

(3)

where $\epsilon_t$ is white noise and $\delta$ is a small parameter. The characteristic time scale for amplitude and frequency modulation is $1/\delta$. In [7], we propose estimating $A(\delta t)$ and $\omega(\delta t)$ using data adaptive kernel smoothers. The instantaneous frequency corresponds to a first derivative estimate. We represent the signal in the time-frequency plane as the curve, $A(t, \hat{\omega}(t))$. Since we expect the phase to be piecewise convex, we replace the adaptive kernel estimate of $\cos[\phi(t)]$ with PC fitting. The circular statistics require a penalized likelihood functional of the form:

$$\sum_{i=1}^{N} \left[ \frac{y_i}{A(t_i)} - \cos \left[ \int_{0}^{t_i} \hat{\omega}(s)ds \right] \right]^2 + \lambda \int |\hat{A}''(t)|^2 + |\hat{\omega}''(t)|^2 dt.$$  

(4)

Eq. (4) may also be used in for a smoothing spline fit without PC constraints. The first term in Eq. (4) differs from Katkovnik [4] by placing $A(t)$ in the denominator instead of the numerator.

4. Spectral Estimation
Consider a stationary time series, $\{x_t\}$, with an unknown spectral density, $S(f)$. A standard method to estimate $S(f)$ is to multiply the data by a spectral window, compute the windowed periodogram, and then smooth the windowed periodogram or its logarithm with a data-adaptive kernel smoother or smoothing splines. In [11-13], we show that a better estimate replaces the single spectral window with a family of orthonormal spectral windows.
The multiple window estimate reduces the broad band bias while making a variance stabilizing transformation of the log-periodogram. When we use the sinusoidal tapers of [11], \( v_i^{(k)} = \frac{2}{N + 1} \sin\left(\frac{kt}{N + 1}\right) \), the multi-window estimate reduces to

\[
\hat{S}_{MW}(f) = \frac{\Delta}{K} \sum_{k=1}^{K} |y(f + k\Delta) - y(f - k\Delta)|^2, \text{ where } \Delta = 1/(2N + 2).
\]

From [12], we recommend \( K = (N/2)^{8/15} \). Instead of kernel smoothing \( \ln[\hat{S}_{MW}(f)] \), we now advocate using the two-stage piecewise convex fitting procedure. Piecewise convex fitting should prove particularly advantageous to spectral estimation because it will suppress the \( 1/N \) oscillations that arise from discrete time sampling.

## 5. Additive Models, Projection Pursuit and MARS

Many classes of models attempt to fit multi-dimensional functions as sums of one-dimensional functions. In each case, we can replace the standard nonparametric estimation methods with piecewise convex fitting. Additive growth curve models [9] fits models of the form \( g(t,x_1 \ldots x_m) = f_0(t) + \sum_{j=1}^{m} f_j(t)x_j \), where the \( x_j \) are determined by smooth splines (old method) or PC fitting (new method). The back fitting algorithm (corresponding to the Gauss-Seidel iteration) may be used to PC fit the \( f_j \) iteratively. The same remarks apply to projection pursuit [3]. In MARS (multivariate adaptive regression splines), a sum of products form: \( f(x_1, x_2 \ldots x_m) = \sum_{j,j'=1}^{M} g_j(x_j)h_j(x_j') \) is assumed. The knots are placed adaptively, in our case using PCIC (2).

## 6. Robust Estimation

At present, our understanding of the statistics of false inflection points is limited to Gaussian errors and linear estimators. In practice, it is often advantageous to replace both the residual errors and the penalty function with more robust analogs: \( \sum_{i=1}^{N} |y_i - \hat{g}(t_i)|^{q_i} + \lambda \int |\hat{g}^{(m)}(t)|^{q_i} dt \), where \( 1 \leq q_i \leq 2 \). Representation and duality theorems are given in [8] for \( q_i > 1 \). A heuristic scaling shows that the effective halfwidth of the robustified function satisfies \( h_{eff} \sim |\lambda f^{(m)}(t)|^{(q_i-2)/2} \). This bias error scales as \( g^{(m)}(t)h_{eff}^m \) while the “variance” is proportional to \( 1/Nh_{eff} \). The halfwidth that minimizes the MISE scales as \( h_{eff} \sim N^{-1/14} \), while the halfwidth to eliminate false change points of \( g^{(t)} \) with asymptotic probability one satisfies \( h_{eff}N^{1/14} \to \infty \). The optimal variable halfwidth kernel smoother has a kernel halfwidth proportional to \( |f^{(m)}|^{1/14} \). For \( 1 \leq q_i \leq 2 \), the effective halfwidth of the robustified function automatically reduces the halfwidth in regions of large \( |f^{(m)}(t)| \) just like a variable halfwidth smoother. When \( q_1 = q_2 = 1 \), the problem reduces to a linear programming problem for each predetermined set of constraints.

## 7. Image Segmentation

Image segmentation divides a digital picture into similar regions for further processing. The Mumford-Shah (MS) algorithm assumes that the image is piecewise constant, and that the boundaries of the regions are unknown [5]. The region boundaries are determined by minimizing the sum of the residual square fit error plus a penalty term proportional to the length of the boundary. If the boundary is parameterized as \( x(s) \), the penalty term is the total variation of \( x(s) \). We suggest modifying the MS algorithm by replacing the total variation penalty with a piecewise convex constrained fit using a robustified penalty function such as the \( L_1 \) integral of the boundary curvature. When using the PCIC (2), we use the arclength divided by the grid spacing as a proxy for \( N \), the number of data points.

## 8. Response Surface Estimation

We seek to estimate a smooth function, \( g(x_1, x_2) \), given \( N \) noisy measurements. The two dimensional analog of PC fitting is to divide the plane into regions where the Gaussian curvature (or more simply \( \Delta f \)) has a single sign. The boundaries between regions of positive and negative Gaussian curvature are free boundaries, which we require to be PC. In the first stage of the fit, we use a penalty function of the form \( \lambda \int |\Delta^{m/2}\hat{g}|^2 \), where we require that \( \lambda \sim 2/\log(N)N^{1/14} \). This scaling is heuristic since the statistics of false zeros of \( \Delta^{l/2}\hat{g} \) are unknown, as is the critical scaling of the smoothing parameter that avoids extra regions of incorrectly specified curvature. To answer these issues, a two-dimensional analog of the Cramer-Leadbetter formula is necessary.

In the second stage, we suggest imposing constraints on the sign of \( \partial_{normal}\Delta^{l/2}\hat{g} \) near the first-stage convexity boundaries. The stage 2 convexity boundaries, \( (x(s), y(s)) \), are free and need to be fit using a penalty function plus PC constraints on the curve shape. The numerical implementation appears tricky with a need for some elliptic analog of front tracking. Overall, the two-dimensional problem appears very challenging from both theoretical and numerical perspectives. Basic issues such as replacing \( \partial_{normal}\Delta^{l/2}\hat{g} \) with geometric invariants have not been addressed.
9. Evolutionary Spectra
A common model of nonstationary stochastic processes is \( x_t = \int_{-\pi}^{\pi} A(\omega, \delta t)dZ(\omega) \), where \( dZ(\omega) \) is a stochastic process with independent spectral increments \( E[dZ(\omega)dZ(\omega)'] = \delta(\omega - \omega')d\omega \). The representation is nonunique for Gaussian processes since \( A(\omega, t) \) corresponds to a square root of the covariance matrix. To resolve the nonuniqueness, we require that \( A(\omega, \delta t)e^{i\omega t} \) correspond to the Fourier transform of the positive definite square root of the covariance matrix. The evolutionary spectrum is \( S(\omega, t) = |A(\omega, t)|^2 \).

Let \( \lambda_f \) be the characteristic frequency scale length and \( \tau \) be the characteristic time scale of \( A \): \( A(f/\lambda_f, t/\tau) \), with the sampling rate = 1. In [6], we present an asymptotic expansion of the mean square error in estimating \( S(f/\lambda_f, t/\tau) \). We begin by evaluating the multi-window analog of the log-spectrogram on a two-dimensional time frequency lattice. The bias error is minimized by using a window length of \( N_w \sim \sqrt{\tau/\lambda_f} \). In [6], we estimate \( \hat{S}(\omega, t) \) using a two dimensional cross-product kernel smoother on the log-multi window spectrogram. The optimal halfwidths, \( h_t \) & \( h_f \), scale as \( h_t/h_f \sim \sqrt{\tau/\lambda_f} \) and \( h_fh_t \sim (\tau^2\lambda_f^2)^{-1/3} \), where \( h_t \) and \( h_f \) are the halfwidths in the \( t \) and \( f \) directions.

We now advocate replacing kernel smoothing with PC fitting the log multi-windowed spectrogram. This method should eliminate the spurious \( 1/N_w \) oscillations which occur due to the discrete sampling.

10. Wavelet thresholding: a wiggle enhancer
Wavelet algorithms for function estimation offer two advantages: 1) speed, the algorithms are often \( O(N \log(N)) \), 2) asymptotic minimax optimality in a number of decision theoretic settings [2]. The speed arises from separability: each wavelet coefficient is estimated separately without regard to geometric fidelity. The asymptotic optimality theory assumes that the unknown function is an arbitrary member of a function space, which makes function fits with ten or twenty inflection points as reasonable as fits with no inflection points. Essentially, function spaces contain too many “unphysical” functions. We prefer the “common sense prior” that the function has only a few inflection points with high probaability.

Both of these advantages of wavelets disappear when the more realistic assumption is made that the unknown function has only a small number of convexity change points. Wavelet thresholding has another intrinsic disadvantage when it comes to geometric fidelity: wavelets possess the complete oscillation property [1]. In contrast, B-splines have the antithetical and valuable property, total positivity.

11. Summary
Sections 1 & 2 describe nonparametric estimation methods that seek to exclude spurious oscillations with negligible sacrifice of fit quality. We have outlined a number of applications of our two-stage piecewise convex fitting method. The PCF methodology can be used to solve inverse problems.

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