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A note on approximation on the real line with nonnegative derivative constraints by Hermite interpolation using RBFs and convex quadratic programming

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A note on approximation on the real line with nonnegative derivative constraints by Hermite interpolation using RBFs and convex quadratic programming

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Problem formulation

In this note, we investigate a problem of approximating one-dimensional functional data with nonnegativity constraints on the function's derivative at given points. This is motivated by curve-fitting problems in High Dynamic Range Imaging (HDRI) in which we are interested in recovering suitably smooth nondecreasing functions from noisy measurements [Debevec and Malik, 1997].

Let us assume we are given measurements $(x_1, c_1), \ldots, (x_n, c_n) \in \mathbb{R} \times \mathbb{R}$ for which we seek a function $f : \mathbb{R} \to \mathbb{R}$ such that $f(x_i) \approx c_i$ and $f'(x_i) \geq 0$. The pointwise nonnegativity constraints are meant to hopefully recover a function which is nondecreasing close to the constraints' points. In order to try to recover a smooth function with little oscillation, we pose a constrained regularized weighted least-squares problem in which the regularizer is chosen to be the thin-plate energy (the L^2-norm of the function's second derivative):

$$\min_{f'(x_i) \geq 0} \left\{ \frac{1}{2n} \sum_{i=1}^{n} \rho_i \cdot \big(f(x_i) - c_i\big)^2 + \frac{\rho}{2} \cdot \int_{\mathbb{R}} f''(x)^2 dx \right\} \tag{1}$$

In order to solve this problem, we make a simple transformation which moves the function's values from the objetive to the constraints and decouples the function's derivatives from the nonnegativity constraints by introducing artificial variables $f_i, g_i \in \mathbb{R}$ for each given measurement. This results in the problem:

$$\min_{\substack{f(x_i) = f_i \\ f'(x_i) = g_i \\ g_i \geq 0}} \left\{ \frac{1}{2n} \sum_{i=1}^{n} \rho_i \cdot (f_i - c_i)^2 + \frac{\rho}{2} \cdot \int_{\mathbb{R}} f''(x)^2 dx \right\} \tag{2}$$

Since the only part of the objetive involving the sought function is the regularization term and the linear measurements in the constraints, we move these to an inner minimization problem resulting in the formulation:

$$\min_{\substack{\mathbf{f},\mathbf{g}\in\mathbb{R}^n \\ \mathbf{g}\geq 0}} \left\{ \frac{1}{2n}\sum_{i=1}^{n} \rho_i \cdot (f_i - c_i)^2 + \rho \cdot \left[\min_{\substack{f(x_i)=f_i \\ f'(x_i)=g_i}} \frac{1}{2}\int_{\mathbb{R}} f''(x)^2 dx \right] \right\} \tag{3}$$

Analyzing the inner problem first,

$$\min_{\substack{f(x_i)=f_i \\ f'(x_i)=g_i}} \frac{1}{2}\int_{\mathbb{R}} f''(x)^2 dx \tag{4}$$

we notice that it is a variational (first-order) Hermite interpolation problem in which the objetive functional is a Sobolev semi-norm. This problem is well-studied and its solution can be found elsewhere, in particular, in Duchon's seminal paper [Duchon, 1977] it is shown that the solution for an instance of this problem has the form (5) below, where the coefficients must satisfy the side-conditions (7) and (8):

$$f(x) = \sum_{j=1}^{n} \Big\{ \alpha_j \cdot |x - x_j|^3 - \beta_j \cdot 3(x - x_j)|x - x_j| \Big\} + \gamma x + \delta \tag{5}$$

$$f'(x) = \sum_{j=1}^{n} \Big\{ \alpha_j \cdot 3(x - x_j)|x - x_j| - \beta_j \cdot 6|x - x_j| \Big\} + \gamma \tag{6}$$

$$0 = \sum_{j=1}^{n} \Big\{ \alpha_j x_j + \beta_j \Big\} \tag{7}$$

$$0 = \sum_{j=1}^{n} \alpha_j \tag{8}$$

It is interesting to notice that the recovered function is a degree-one polynomial plus a linear combination of the simple "basis" functions in Figure 1.

The coefficients in the solution for this inner problem can be computed by solving a symmetric (indefinite) linear system of equations induced by both the interpolation constraints and the side-conditions above:

$$(5), (6), (7), (8), \ \begin{matrix} f\,(x_i) = f_i \\ f'(x_i) = f_i \end{matrix} \quad \Longrightarrow \quad A \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \\ 0 \\ 0 \end{pmatrix} =: b \tag{9}$$

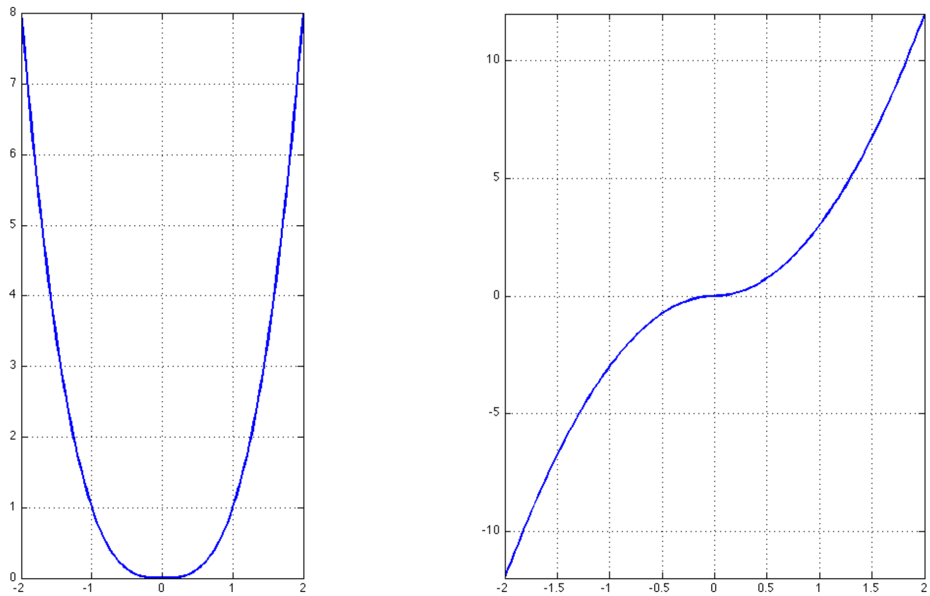

Figure 1: "Basis" functions: (left) actual RBF $|x|^3$; (right) its derivative $3x|x|$.

where the interpolation matrix $A \in \mathbb{R}^{(2n+2)\times(2n+2)}$ can be easily deduced from the above equations and has its derivation somewhat detailed (in another context) in the paper [Macêdo et al., 2010]. It can be shown that the optimal value of that variational problem is given by

$$\min_{\substack{f(x_i)=f_i \\ f'(x_i)=g_i}} \left\{ \frac{1}{2} \int_{\mathbb{R}} f''(x)^2 dx \right\} \quad = \quad \frac{1}{2} \langle A^{-1} b, b \rangle \tag{10}$$

which can be "plugged" into our original (outer) minimization to give the (finite-dimensional) convex quadratic programming problem:

$$\min_{\substack{\mathbf{f},\mathbf{g}\in\mathbb{R}^n \\ \mathbf{g}\geq 0}} \left\{ F(\mathbf{f},\mathbf{g}) := \frac{1}{2n} \sum_{i=1}^{n} \rho_i \cdot (f_i - c_i)^2 + \frac{\rho}{2} \cdot \langle A^{-1} b, b \rangle \right\} \tag{11}$$

bearing in mind that the vector $b \in \mathbb{R}^{2n+2}$ is a simple (affine) function of $(\mathbf{f}, \mathbf{g})$.

In order to numerically solve this convex-constrained optimization problem, we use the projected-gradient code described in [Birgin et al., 2001], which just requires us to be able to compute values and gradients of F at given pairs $(\mathbf{f}, \mathbf{g})$ and Euclidean projections of pairs like these in the feasible set. It is possible to show that such gradients as given by

$$\partial_{f_i} F(\mathbf{f},\mathbf{g}) = \frac{\rho_i}{n} \cdot (f_i - c_i) + \rho \cdot \alpha_i \tag{12}$$

$$\partial_{g_i} F(\mathbf{f},\mathbf{g}) = \rho \cdot \beta_i \tag{13}$$

while the projection operator P_C is defined by

$$C := \left\{(\mathbf{f}, \mathbf{g}) \in \mathbb{R}^n \times \mathbb{R}^n \mid \mathbf{g} \geq 0\right\} \tag{14}$$

$$\mathrm{P}_C(\mathbf{f}, \mathbf{g}) = (\mathbf{f}, \mathbf{g}^+) \tag{15}$$

$$(\mathbf{g}^+)_i := \max(0, g_i). \tag{16}$$

Our implementation uses a version of the projected-gradient solver coded in `C` and the computation of the objetive function's values and gradients employs the optimized linear algebra packages BLAS (for general vector operations) and LAPACK (for the LDL^T factorization of the interpolation matrix, as a pre-processing, and subsequent solutions of the linear system involving different right-hand sides b) [BLAS, 2011, LAPACK, 2011]. After solving for the optimal $\mathbf{f}$ and $\mathbf{g}$, we can recover the optimal f by solving the linear (Hermite) interpolation system reusing the LDL^T factorization of A in this task.

A couple illustrative experiments

To illustrate properties of our approach, we performed a couple experiments on a sequence of monotonic datasets varying the function values while holding fixed the measurement points. These experiments show also that our method allows for interpolation of exact data corresponding to the assymptotic case where the data-fitting weights go to infinity ($\rho_i \to +\infty$) leading to the "simpler" problem

$$\min_{\substack{f(x_i)=c_i \\ f'(x_i)\geq 0}} \frac{1}{2} \int_{\mathbb{R}} f''(x)^2 dx. \tag{17}$$

The results of these experiments are depicted in Figure 2. The most noteworthy properties and limitation depicted in these results are:

- analytic (closed-form) solution;
- smoothness of the reconstructed functions ($C^{1,1}$);
- reproduction of degree-one polynomials (noticed in the very middle figure);
- nonmonotone reconstructions from monotone data are still possible (as is easily visible in the first and last plots, but less noticeable in the second and the second from last ones).

Final remarks

In order to implement a prototype, the problem was stated in quite an abstract way which maybe somewhat far from the intended HDRI applications. These application usually have multiple measurements at the same approximation point x_i and usually are restricted to a fixed interval of interest (x_{min}, x_{max}) in which

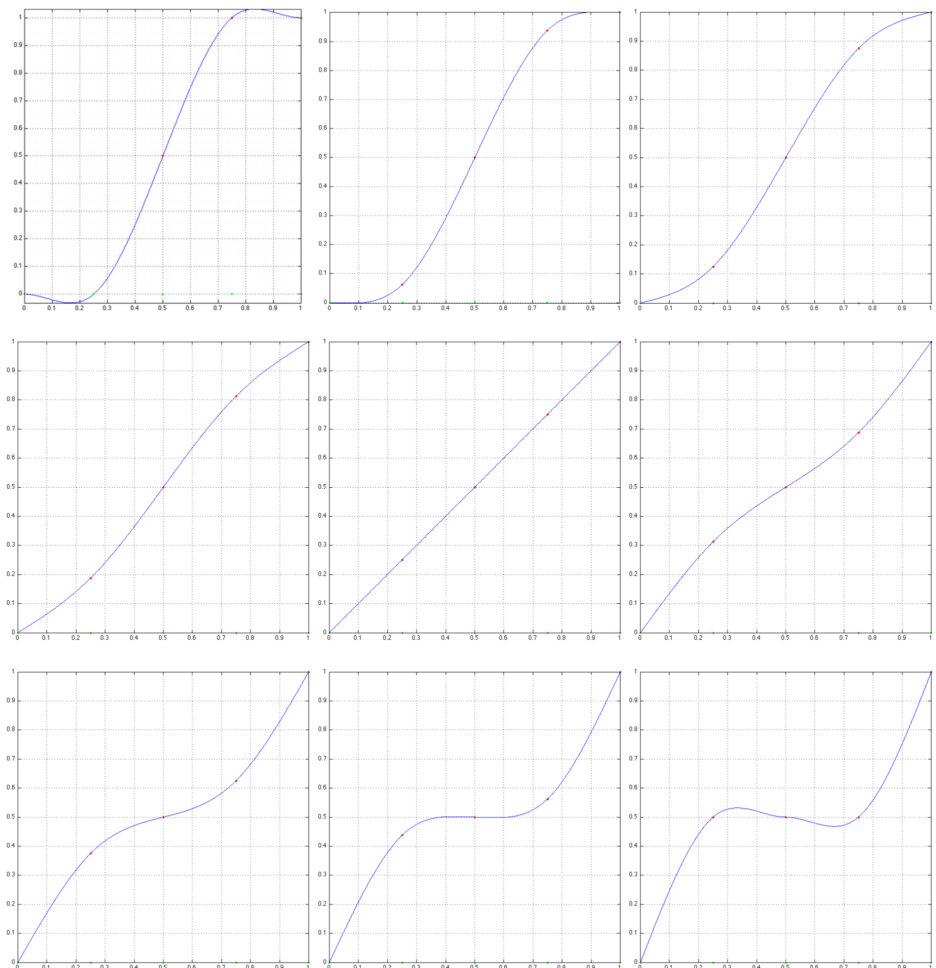

Figure 2: Reconstructions from nondecreasing datasets at 5 interpolation points.

the noisy measurements have varying confidence, usually represented by means of a positive weighting function $w : (x_{min}, x_{max}) \to \mathbb{R}_{++}$. The first difference is the easiest to tackle using our approach since the data-fidelity term in the original objective function can be replaced by a more general convex quadratic term as employed in [Debevec and Malik, 1997] and the final (outer) problem is can be modified almost verbatim. The weighting function is also somewhat simple to incorporate employing the weights ρ_i in our formulation. However, the second issue is more complicated to deal with in the regularization-term since the closed-form presented assumes the integral is taken in the whole real line. In this aspect, the second issue also relates to the third in that the formulation presented in [Debevec and Malik, 1997] incorporates the weighting function in the regularization term for which we wouldn't have a closed-form solution. In principle, the method we present has the same monotonicity issue as that of Devebec and Malik in that it cannot ensure that the recovered function is non-decreasing. However, we believe that the constrained optimization viewpoint we employed here can be used to enforce this monotonicity requirement to their formulation by running the optimization in the feasible set given by the (polyhedral) monotonicity cone $\{\mathbf{f} \in \mathbb{R}^m \mid f_{i+1} \geq f_i,\ i = 1, \ldots, m-1\}$. Projections onto this cone seem to have very special properties which might be exploited to design efficient and robust methods for these kind of applications.

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