ON THE ESTIMATION OF SPECTRAL DATA: A GENETIC ALGORITHM APPROACH

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ABSTRACT

Spectral data estimation from image data is an ill-posed problem since (i) due to the integral nature of solid-state light sensors the same output can be obtained from an infinity of input signals and (ii) color signals are spectrally smooth in nature and therefore limit the number of linear independent equation that can be formulated for the identification problem. To enable the solution of these problems most methods relay on exact a priori knowledge, such as smoothness and modality, to formulate hard constraints. In this paper a new method based on an extended generalized cross-validation measure is introduced for this type of problems. The solution is obtained with a genetic algorithm that maximizes its prediction ability. The method does not require exact a priori knowledge on the solution, since it is able to extract this information from the input data.

1. INTRODUCTION

Spectral data estimation is an important issue in several image processing and computer vision tasks. Usually, it involves the estimation, for each wavelength λ (most often λ is confined to the visible spectrum), of some data distribution $X(\lambda)$. For instance, many radiometric camera calibration [1], demosaicing [2], color constancy [3] and spectral reflectance estimation methods [4] require the knowledge of the spectral distribution of the light sensor's sensitivities. Reflectance estimation is another typical situation where spectral data estimation has to be performed.

Spectral data estimation based on image data is an ill-posed problem, since (i) due to the integral nature of todays light sensors, the same sensor output can be obtained from an infinity of input signals, and (ii) it is observed that colors can be well approximated with just a few basis functions [4], which imposes an upper limit on the number of linear independent equations for the estimation problem. Fortunately, there are some assumptions that can be made on the solution that enable solving these type of problems. The most commonly applied constraints are the solution's (i) positivity and (ii) its smoothness [4][5][6][7], although other types of constraints can be found in literature (for instance, Finlayson [7] suggests using modality constraints, while local maxima are constrained in [5]).

Spectral data estimation can usually be formulated in therms of a least squares with linear inequality constraints problem [5][6][7]. In this paper the following formulation will be assumed: let $X \in \mathbb{R}^{n\times 1}$ be a discrete version of $X(\lambda)$ such that $X_i \equiv X(\lambda_i)$, $\lambda_i = \lambda_0 + (i-1)\Delta\lambda$, $i = 1...n$, and $\Delta\lambda$ is the sampling interval. It is seen that X can be computed from

$$\min\left\{\frac{\Delta\lambda}{m\sigma^2}\|AX-B\|^2+\frac{\alpha}{\Delta\lambda^4}\|DX\|^2\right\} \quad (1)$$

$$\text{subject to } CX \le H \quad (2)$$

where $AX = B$ ($A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times 1}$, $D \in \mathbb{R}^{(n-2)\times n}$, $C \in \mathbb{R}^{q\times n}$, $H \in \mathbb{R}^{q\times 1}$) are the m equations (usually $m \ll n$) that can be obtained from the sensor's outputs, and $\alpha \in \mathbb{R}^+$ is a regularization gain that controls the trade-off between the roughness of the solution as measured by $\|DX\|^2$ ($\Delta\lambda^{-2}DX$ approximates the second derivative of X) and the infidelity to the data as measured by $\|AX-B\|^2$. In (1) it is assumed that B is subject to uncorrelated white noise, i.e., $B+\varepsilon$:$\varepsilon_i\sim\mathcal{N}(0,\sigma)$. If distinct noise variances are present in B then (1) still holds if the following transformations are performed: let the noise associated to equation i, $i = 1...m$, be $\varepsilon_i \sim N(0,\sigma_i)$,then $A \equiv diag(\sigma/\sigma_i)A$ and $B \equiv diag(\sigma/\sigma_i)B$.

In practice, C, H and α are defined based on exact a priori knowledge on X [5][6][7], being the solution very dependant on these values. In fig.1 bottom the continuous curves show the sum squared errors (SSE), as a function of the regularization gain, obtained for several CCD spectral sensitivity estimation problems with $C = -I$ and $H = 0$. As can be observed, the quality of the solution is highly dependant on the quality of the a priori knowledge (in this

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case, the smoothness), which in most cases is difficult or even impossible to obtain.

In this paper a new method is introduced which is able to learn the needed knowledge from the input data. The method uses an extended generalized cross-validation measure function GCV_{IC} to measure the prediction ability of the solution X for a particular set of constraints C, H and parameter α (section 2). The prediction ability is then maximized using a genetic algorithm (section 3). Results obtained with this method for light sensor sensitivity estimation problems are introduced and discussed in section 3.1. Finaly, in section 4, some main conclusions are presented.

2. THE PREDICTABILITY MEASURE

Equation (1) corresponds to the estimation of a spline in the general sense [8]. Hence, it can be tested how well the estimated spline predicts the data for different roughness penalty values γ and constraints C and H. This idea was first applied by Wahba [8] and lead to the introduction of the GCV (generalized cross-validation) measure for the unconstrained fitting problem. In this work, the GCV is extended to linear inequality constrained fitting problems. This extension results in a new GCV measure, the GCV_{IC}. The fitting problem in (1) and (2) can be rewritten as in (3).

$$\min\left\{\|A^*(\gamma)X - B^*\|^2\right\}, \text{subject to } CX \leq H \quad (3)$$

$$\gamma \equiv \frac{m\alpha\sigma^2}{\Delta\lambda^5}, A^*(\gamma) \equiv \begin{bmatrix} A \\ \sqrt{\gamma}D \end{bmatrix}, B^* \equiv \begin{bmatrix} B \\ 0 \end{bmatrix}$$

From the active set theory [9] it is known that the solution to the problem in (3) is equivalent to solve an equality constrained problem with the subset of constraints which, for a particular solution, are active, i.e., are verified with equality. Let $C^* \subseteq C$ and $H^* \subseteq H$ be the subset of linear independent constraints verified with equality for a particular solution, then the same solution can be found using the following theorem:

Theorem 1 *The best approximate solution to the equality constrained problem in (4) is (5). (for proof see [9])*

$$\min_x \|AX - B\|^2 \text{ subjected to } C^*X = H^* \quad (4)$$

$$X = \sum_{i=1}^{p}\left(\widetilde{d}_i/\beta_i\right) z_i^* + \sum_{i=p+1}^{n} \widetilde{b}_i z_i^* \quad (5)$$

where $A = W_A \begin{bmatrix} D_A^T & 0 \end{bmatrix}^T Z$, $C^* = W_C \begin{bmatrix} D_C & 0 \end{bmatrix} Z$ *are the generalized singular value decompositions of* A *and* B, $\widetilde{b} = W_A^T B$, $\widetilde{d} = W_C^T H^*$, $Z^{-1} = \begin{bmatrix} z_1^* & \cdots & z_n^* \end{bmatrix}$, $D_A = diag(\alpha_1, \ldots, \alpha_n)$ *and* $D_C = diag(\beta_1, \ldots, \beta_p)$.

Corollary 2 *Let* X *be the solution to (3) using the active set theory. Then, if* $C^*X = H^*$ *are the subset of active constraints,* X *verifies*

$$X = \Omega + \Theta B \quad (6)$$

with $\Omega = Z_1 D_C^{-1} W_C^T H^*$, $\Theta = Z_2 W_{21}$, Z, W_C, D_C, W_A *defined as in theorem 1, and*

$$W_A^T = \begin{bmatrix} \overbrace{W_{11}}^{m} & \overbrace{W_{12}}^{n-2} \\ W_{21} & W_{22} \\ W_{31} & W_{32} \end{bmatrix} \begin{matrix} p \\ n-p \\ m-2 \end{matrix}, Z^{-1} = \begin{bmatrix} \overbrace{Z_1}^{p} & \overbrace{Z_2}^{n-p} \end{bmatrix}$$

Proof is immediate by taking theorem 1 and the formulation in (3) and some simple algebraic manipulations.

Let $X^{[k]}$ denote the estimate of X using all but the kth data point in B. The OCV function measures the overall predictability of data points by the estimate $X^{[k]}$ and is defined by [8] (B_k - kth element of vector B; A_k - kth row vector of matrix A):

$$OCV_{IC} = \frac{1}{m}\sum_{k=1}^{m}(B_k - A_k X^{[k]})^2 \quad (7)$$

To derive the GCV_{IC} function from (7) some theorems have to be introduced.

Lemma 3 *(extension of lemma 3.1 of Craven and Wahba) Let* $h(k, z)$ *be the solution to (3) with linear equality constraints and with the* k*th data point replaced by* z*, then* $h(k, A_k X^{[k]}) = X^{[k]}$ *. (Proof is immediate)*

Theorem 4 *The* OCV_{IC} *function for the problem defined in (3) with linear equality constraints is*

$$OCV_{IC} = \frac{1}{m}\sum_{k=1}^{m}\frac{(B_k - A_k X)^2}{(1-\rho_{kk})^2} \quad (8)$$

where ρ_{kk} *is the* kk*th element of* $\rho = A\Theta$ *and* Θ *is as defined in (6).*

Proof. To proof this theorem we will show that

$$B_k - A_k X = (1 - \rho_{kk})(B_k - A_k X^{[k]})$$

Let Ω_k^1 be the kth element of $A\Omega$. From the lemma 3, the above equation is equivalent to $(1 - \rho_{kk})(B_k - A_k h(k, A_k X^{[k]})) = B_k - A_k X$. Let $B_k^* \equiv A_k h(k, A_k X^{[k]})$. From the definition of h and using (6) it is seen that

$$B_k^* = \Omega_k^1 + \rho_k \begin{bmatrix} B_1 & \cdots & B_k^* & \cdots & B_m \end{bmatrix}^T \Longleftrightarrow$$
$$(1-\rho_{kk})(B_k - B_k^*) =$$
$$(1-\rho_{kk})B_k - \rho_k \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & I \end{bmatrix}^T B - \Omega_k^1 =$$
$$\begin{bmatrix} -\rho_{k1} & \cdots & 1-\rho_{kk} & \cdots & \rho_{km} \end{bmatrix} B - \Omega_k^1$$

On the other hand, $B_k - A_k X = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} B - \rho_k B - \Omega_k^1 = \begin{bmatrix} -\rho_{k1} & \cdots & 1-\rho_{kk} & \cdots & \rho_{km} \end{bmatrix} B - \Omega_k^1$. ■

Theorem 5 *The GCV_{IC} function for the problem defined in (3) with linear equality constraints is*

$$GCV_{IC} = \frac{\frac{1}{m}\|B - AX\|^2}{\left(\frac{1}{m} trace\,(I-\rho)\right)^2} \tag{9}$$

Proof. Proof is immediate by taking a weighted OCV_{IC} to account for non equally spaced data points, as suggested by Wahba [8]. It can be shown that ρ is symetric. Hence, following Wahba, it is possible to find a transformation Γ such that $\Gamma A \Gamma^T$ is circulant. Taking the OCV_{IC} on this new system, it is seen that the points are equally spaced and the transformation is equivalent to take the weights given by $w_k = \left[(1-\rho_{kk})/\frac{1}{m} trace(I-\rho)\right]^2$. Substituting this in (8), (9) is verified. ■

3. THE GENETIC ALGORITHM

The GCV_{IC} function usually exhibits several local minima. Further, it is seen that its gradient is not straightforward to compute explicitly. Therefore, given a search space $(\Delta C, \Delta H, \Delta\gamma)$, a genetic algorithm (GA) approach is applied to compute $\min\{GCV_{IC}\}$, since it is able to perform a parallel exploration of the search space [10][11], it does not suffer from local minimum problems and it does not require the computation of gradients. The implemented GA uses real coding and its population is composed by 45 chromosomes (C^i, H^i, γ^i), $i = 1, ..., 45$. Selection and sampling are performed with the ranking strategy and the universal stochastic sampling algorithm, respectively [10] [11]. Selection is based upon the GCV_{IC} measure for each of the chromosomes. The chosen genetic operators are the extended line recombination operator and the Breeder GA mutation operator with a mutation probability of 0.1. Generational reproduction is applied. Given a chromosome (C^i, H^i, γ^i) the algorithm computes $min_\gamma GCV_{IC}^i$ using (C^i, H^i) and γ^i as a starting point. This strategy can be implemented with a line search algorithm which does not require gradient computation. In the current implementation the golden section search algorithm is applied. This hybrid GA strategy exhibits some advantages compared to standard GA implementations:(i) the specified search interval $\Delta\gamma$ for the regularization gain serves only to specify starting points. Hence, if the optimal γ is outside the specified interval it is still achievable as long GCV_{IC} decreases at the interval limits. (ii) From our tests, it seems that it enables faster convergence than standard real coded GA.

3.1. Application to light sensor sensitivity estimation

In this section it is shown how the GVC_{IC} measure can be applied to the light sensor spectral sensitivity estimation problem. As as been observed in [5], for small values of γ, the solution to this problem tends to exhibit large values of SSE due to its oscillation. As γ is increased, oscillation is eliminated. However, local maxima of the solution tend to be flatten due to the increased importance of the smoothness component in the objective function. This leads to increases of SSE values. Hence, the solution to this problem can be improved if local maxima are constraint [5]. Therefore, C and H are build such that the following constraints are defined: (i) (positivity constraint) $X_i \geq 0$, $i = 1, ..., M-2, M+2, ..., n$, and (ii) (maxima constraint) $X_M = \widehat{X}_M$, $X_{M-1} \leq \widehat{X}_M, X_{M+1} \leq \widehat{X}_M$, where $\widehat{X}_M$ is the unknown amplitude of the local maxima of the solution. As for the GA's search interval $\Delta\widehat{X}_M$ for $\widehat{X}_M$, an extension to the method introduced in [5] is applied: let $\widehat{X}_M(\gamma_1)$ be the estimated local maxima obtained with the regularization gain γ_1, such that γ_1 is the lower limit of the identified stable regularization gain interval (gains which do not induce oscillation of X). The search interval for local maxima is defined by $\Delta\widehat{X}_M = [\max\{0, |\widehat{X}_M(0) - \delta\widehat{X}_M - \widehat{X}_M(\gamma_1)|\}, \widehat{X}_M(0) + \delta|\widehat{X}_M(0) - \widehat{X}_M(\gamma_1)|], \delta \in [1, \infty[$, where $\widehat{X}_M(0)$ is the estimated maxima with the algorithm introduced in [5]. Parameter δ is not critical, since it simply establishes a search range for local maxima. In the shown tests, δ was fixed to 2, but, larger values can be applied. However, it should be noted that very large values for δ enlarge the search space and increase, therefore, the computational load. The required search interval of regularization gains was fixed to $\Delta\gamma = [0.01, 5]$. To measure the performance of the described method a simulation program was developed as described in [5]. The shown test results are (i) for an asymmetrical Gaussian model for the spectral sensitivities (these are typical sensitivity curves for some cameras such as the Sony DXC-930 color video camera [6]) and (ii) for the spectral sensitivity curves from a Kodak DCS200 camera as described in [2]. These two types of sensitivity functions were chosen to evaluate the method's performance for curves with distinct smoothness and modality. In these testes 24 ($m = 24$) patches of the MacBeth-Color Checker map were applied. Finally, the sampling step was fixed to $\Delta\lambda = 2nm$, $\lambda_0 = 400nm$, $\lambda_n = 700nm$ ($n = 150$) and the SSE (Sum Squared Error) values were computed by $SSE = \|X^{\text{real}} - X\|^2$ (X^{real} represents the real function). Table 1 summarises the applied conditions and achieved results. A comparison between the described estimation method based on the GCV_{IC} measure and by arbitrating γ with $C = -I$ and $H = 0$ are depicted in fig. 1. As can be observed the GCV_{IC} technique enables the estimation of suboptimal solutions in the vicinity of the global optimums. This is in accordance with Craven and Wahba's theorem 4.2 [8], since the global optimum is not achievable, given that the "expectation efficiency" is usually less than 1. Further, the method is able to estimate X_M (see table 1). An

Channel	$\Delta\widehat{X}_M$	X_M^{real}	$\widehat{X}_M$	SSE
GR	[0.0102,0.0139]	0.0133	0.0132	1.29E-6
GG	[0.0102,0.0108]	0.0107	0.0107	2.91E-6
GB	[0.0114,0.0128]	0.0126	0.0122	2.25E-6
KR	[0.00643,0.00881]	0.00804	0.00839	2.61E-6
KG	[0.00594,0.00598]	0.00594	0.00598	6.25E-7
KB	[0.00360,0.00374]	0.00377	0.00373	2.02E-6

Table 1. Simulation conditions and results. Legend for first column: GX - Gaussian curves; KX - Kodak DCS200; X (R-red, G-green, B-blue).

interesting result is the one obtained for the red channel of the gaussian curve. As can be observed, the computed solution exhibits a SSE which is more than 300% lower than the best SSE that can be obtained by varying γ. This is possible because this method ever comes near to estimate correctly the real maxima, while GCV_{IC} enables its identification.

4. CONCLUSIONS

In this paper a new spectral data estimation technique is introduced. The method is based on an extended generalized cross-validation measure which, given a particular solution, measures its prediction ability. No exact a priori knowledge on the data characteristics are required, since the method is able to extract the needed constraints from the input data. This is a relevant result because, in practice, exact a priori knowledge is often difficult or even impossible to obtain with the required accuracy. Due to the nonlinearity of the extended generalized cross-validation measure, a hybrid genetic algorithms is described for its minimization.

The described method is tested on light sensor spectral sensitivity estimation problems with unknown smoothness and maxima locations. The obtained results show that the GCV_{IC} based GA enables the identification of suboptimal solutions in the vicinity of the global optimum.

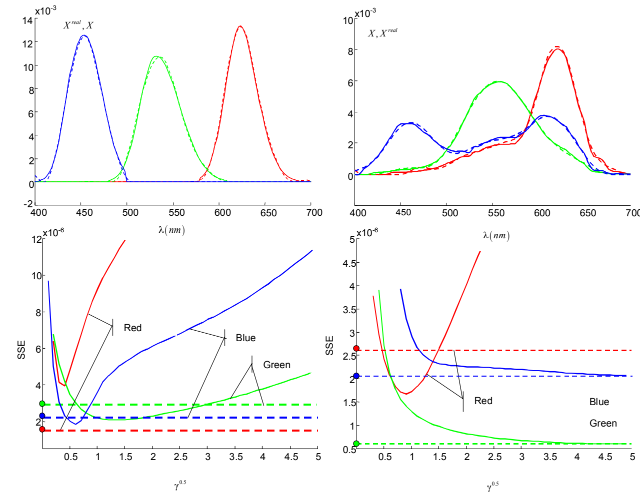

Fig. 1. Top: Continuous curves - X^{real}; dashed curves - estimated X with GCV_{IC}. Bottom: SSE evolution with γ. Continuous curves - SSE of the solution for $C = -I$, $H = 0$. Dashed curves - obtained SSE with GCV_{IC} (γ not shown).

5. REFERENCES

[1] Y.-C. Chang and J. F. Reid, "RGB calibration for color image analysis in machine vision," *IEEE Trans. on Image Processing*, vol. 5, no. 19, pp. 1414–1422, 1996.

[2] P. Vora, J. Farrell, J. Tietz, and D. Brainard, "Digital color cameras - 2 - spectral response," Tech. Rep. HPL-97-53, Hewlett-Packard Lab., 1997.

[3] K. Barnard, "Computational color constancy: Taking theory into practice," M.S. thesis, Simon Fraser University, 1995.

[4] J. Farrell, J. Cupitt, D. Saunders, and B. Wandell, "Estimating spectral reflectances of digital artwork," in *Chiba Confernce on Multispectral Imaging*, 1999.

[5] P. Carvalho, A. Dourado, and B. Ribeiro, "Improving error stability in spectral camera calibration for color inspection with maxima constraints," in *6th Int. Conf. On Control, Automation, Robotics and Vision*, 2000.

[6] K. Barnard and B. Funt, "Camera calibration for color research," in *Proc. SPIE Electronic Imaging IV*, 1999.

[7] G. Finlayson and S. Hordley, "Recovering device sensitivity with quadratic programming," in *IST/SID's Color Imaging Conf.: Color Science, Systems and Applications*, 1998, pp. 90–95.

[8] P. Craven and G. Wahba, "Smoothing noisy data with spline functions," *Numer. Math.*, vol. 31, pp. 377–403, 1979.

[9] P. Ciarlet and J. Lions, *Handbook of Numerical Analysis*, Elsevier-North Holland, 1990.

[10] Z. Michalewicz, *Genetic Algorithms+Data Structures=Evolution Programs, Third Revised and Extended Edition*, Springer Verlag, 1996.

[11] A. Santos and A. Dourado, "Global optimization of energy and production in process industries: A genetic algorithm application," *Control Engineering Practice*, vol. 7, no. 4, pp. 549–554, 1999.