

## Notes 11: Numerical Methods I

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### Motivation

Efficient numerical schemes are usually critical in solving many optimization problems within a reasonable time. Often instead of having exact solutions one is satisfied with a good approximation.

## 1 Linear equations

We want to solve a classical large linear equation:

$$Ax = b, \tag{1}$$

where  $A$  is  $n \times n$  matrix and  $x$  and  $b$  are column vectors:

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ & \dots & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \dots \\ b_n \end{pmatrix}.$$

In the classical way, to get an exact solution we need an order of  $O(n^3)$  (to invert the matrix). Iterative methods can often attain a good approximation much faster (each iteration is linear in the data)

Let us decompose  $A$  into three matrices  $D$ ,  $L$  and  $U$  such that

$$A = D + L + U, \tag{2}$$

where  $D$  is the *Diagonal matrix*:

$$D = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ & \dots & & \\ 0 & 0 & \dots & a_{nn} \end{pmatrix}, \tag{3}$$

and  $L$  and  $U$  are the strictly *Lower triangle* and *Upper triangle*, respectively:

$$L = \begin{pmatrix} 0 & 0 & \dots & 0 \\ a_{21} & 0 & \dots & 0 \\ & \dots & & \\ a_{n1} & a_{n2} & \dots & 0 \end{pmatrix}, \quad U = \begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ 0 & 0 & \dots & a_{2n} \\ & \dots & & \\ 0 & 0 & \dots & 0 \end{pmatrix}. \quad (4)$$

## 1.1 Gauss-Seidel

We define the matrix  $L^*$  as the sum of the lower triangle and the diagonal  $L^* = L + D$ . Then we can write Eq. (1) as:

$$L^*x = b - Ux.$$

The idea is to split the solution into two parts. The right part is based on the previous iteration of  $x$  and the left part is updated, relying on the fact that a triangular matrix can be easily solved. The algorithm is iterative. One starts with some initial guess on  $x^{(0)}$  (like  $x_i^{(0)} = 0$ ,  $1 \leq i \leq n$ ) and performs the following iterations until convergence (when the change between consecutive iterations is below some tolerance threshold):

$$L^*x^{(k+1)} = b - Ux^{(k)}. \quad (5)$$

The analytic solution is  $x^{(k+1)} = (L^*)^{-1}(b - Ux^{(k)})$ , but instead of inverting  $L^*$  one goes sequentially through the equations from  $i = 1$  to  $i = n$  computing directly the solution for each element  $x_i^{(k+1)}$  by:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left( b_i - \sum_{j<i} a_{ij}x_j^{(k+1)} - \sum_{j>i} a_{ij}x_j^{(k)} \right). \quad (6)$$

## 1.2 SOR - Successive Over-Relaxation

This is a variant of Gauss-Seidel, which usually converges faster. One introduces a constant relaxation factor  $\omega > 1$ . Eq. (1) can be written as:

$$(D + \omega L)x = \omega b - (\omega U + (\omega - 1)D)x.$$

The iterations are

$$(D + \omega L)x^{(k+1)} = \omega b - (\omega U + (\omega - 1)D)x^{(k)}. \quad (7)$$

and the update of element  $x_i^{(k+1)}$  is

$$x_i^{(k+1)} = (1 - \omega)x_i^{(k)} + \frac{\omega}{a_{ii}} \left( b_i - \sum_{j<i} a_{ij}x_j^{(k+1)} - \sum_{j>i} a_{ij}x_j^{(k)} \right). \quad (8)$$

When  $A$  is symmetric and positive definite convergence is guaranteed for the range  $0 < \omega < 2$ . However, as for  $0 < \omega < 1$  we get slower convergence than Gauss-Seidel, this range is usually not used.

## 2 PDE's

This part follows the very well explained and accessible review of Weickert et al in [9] on efficient implementation methods for nonlinear PDE-based filtering.

The initial discussion is in 1D, then we see how it can be generalized to any dimension. We would like to discretize the evolution equation:

$$u_t = \partial_x (g(|\partial_x u|^2) \partial_x u), \quad (9)$$

with Neumann boundary conditions and initial condition  $u|_{t=0} = u_0$ . This can be discretized by

$$\frac{u_i^{k+1} - u_i^k}{\tau} = \sum_{j \in \mathcal{N}(i)} \frac{g_j^k + g_i^k}{2h^2} (u_j^k - u_i^k), \quad (10)$$

where  $\mathcal{N}(i)$  is the set of neighbors of pixel  $i$ , in the 1D case it is just the two adjacent pixels, where for boundary pixels we have only one neighbor.  $h$  is the spatial step ( $h = 1$  for most images) and  $\tau$  is the time step. The equation above is the explicit realization and  $k$  is the iteration number.

The diffusivity  $g_i^k$  for pixel  $i$  can be approximated by

$$g_i^k = g \left( \sum_{p,q \in \mathcal{N}(i)} ((u_p^k - u_q^k)/(2h))^2 \right). \quad (11)$$

We can write Eq. (10) as

$$\frac{u^{k+1} - u^k}{\tau} = A(u^k) u^k, \quad (12)$$

where  $A(u) = a_{ij}(u)$  is defined by

$$a_{ij}(u) = \begin{cases} (g_i(u) + g_j(u))/(2h^2) & j \in \mathcal{N}(i), \\ -\sum_{n \in \mathcal{N}(i)} (g_i(u) + g_n(u))/(2h^2) & i = j, \\ 0 & \text{otherwise.} \end{cases} \quad (13)$$

Let  $I$  be the identity matrix. The three different time step discretization models can be summarized by:

*Explicit scheme:*

$$u^{k+1} = (I + \tau A(u^k))u^k. \quad (14)$$

*Semi-implicit scheme:*

$$(I - \tau A(u^k))u^{k+1} = u^k. \quad (15)$$

*Fully implicit scheme:*

$$u^{k+1} = u^k + \tau A(u^{k+1})u^{k+1}. \quad (16)$$

Both semi-implicit and fully implicit schemes are unconditionally stable for any time step  $\tau$  (in both cases, naturally, the approximation accuracy degrades with the growth of  $\tau$ ). However, the fully implicit scheme yields a nonlinear system of equations which is very hard to solve.

The semi-implicit method can be solved using any linear iterative solver (like Gauss-Seidel or SOR). However, one can exploit the specific tridiagonal structure of the matrix and get a fast noniterative solution using the Thomas algorithm (named after the British physicist Llewellyn Thomas). Note that in 1D, the only nonzero elements of  $A(u)$  are on the 3 center diagonals.

## 2.1 Thomas algorithm

We would like to solve  $Au = d$ . Let  $A$  be a tridiagonal matrix of the form

$$A = \begin{pmatrix} a_1 & b_1 & 0 & \dots & 0 \\ c_1 & a_2 & b_2 & \dots & 0 \\ & \dots & & & \\ & & \dots & c_{n-2} & a_{n-1} & b_{n-1} \\ 0 & \dots & 0 & c_{n-1} & a_n \end{pmatrix}. \quad (17)$$

We want to decompose it into a lower and an upper triangular matrices such that  $A = \hat{L}\hat{U}$ , where

$$\hat{L} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ \ell_1 & 1 & 0 & \dots & 0 \\ & \dots & & & \\ & & \dots & \ell_{n-2} & 1 & 0 \\ 0 & \dots & 0 & \ell_{n-1} & 1 \end{pmatrix}, \hat{U} = \begin{pmatrix} m_1 & u_1 & 0 & \dots & 0 \\ 0 & m_2 & u_2 & \dots & 0 \\ & \dots & & & \\ & & \dots & 0 & m_{n-1} & u_{n-1} \\ 0 & \dots & 0 & 0 & m_n \end{pmatrix}. \quad (18)$$

Comparing the coefficients we have  $u_i = b_i$  for all  $i$ , and  $m_i$  and  $\ell_i$  can be found by the following procedure:

- $m_1 = a_1$ .

- Do loop on  $i = 1, \dots, n$ . In each iteration  $\ell_i = c_i/m_i$ ;  $m_{i+1} = a_{i+1} - \ell_i b_i$ .

We solve  $\hat{L}\hat{U}u = d$  in two steps, first we solve  $\hat{L}y = d$  for  $y$  by forward substitution:

- $y_1 = d_1$ .
- Do loop on  $i = 1, \dots, n$ . In each iteration  $y_i = d_i - \ell_{i-1}y_{i-1}$ .

Having  $y$  we can now solve for  $u$  the problem  $\hat{U}u = y$  by backward substitution:

- $u_n = y_n/m_n$ .
- Do loop on  $i = n-1, n-2, \dots, 1$ . In each iteration  $u_i = (y_i - b_i u_{i+1})/m_i$ .

The whole scheme is very efficient and requires only about  $5N$  multiplications and  $3N$  subtractions.

## 2.2 AOS - Additive Operator Splitting

In any dimension, to solve the semi-implicit equation directly, one cannot use the Thomas algorithm, since the matrix  $A(u)$  is not tridiagonal any more. The idea of AOS is to split the problem into additive 1D problems.

In the case of  $m$  dimensions. We define a matrix  $A_l(u)$ ,  $l = 1, \dots, m$ , for each dimension, where  $A_l = (a_{ijl})_{ij}$  corresponds to derivatives along the  $l$ -th coordinate axis.

The standard discretization can be written as:

$$u^{k+1} = \left( I - \tau \sum_{l=1}^m A_l(u^k) \right)^{-1} u^k. \quad (19)$$

In AOS one replaces it by

$$u^{k+1} = \frac{1}{m} \sum_{l=1}^m (I - m\tau A_l(u^k))^{-1} u^k. \quad (20)$$

## 3 Functionals

We have learned explicit methods and mentioned Chambolle's projection algorithm for solving ROF [3] and later for solving TV-G [1] and TV-L1 [2] as well as their nonlocal counterparts [6]. In recent years very powerful schemes were proposed to solve  $L^1$  and TV-type functionals.

**Split Bregman:** This scheme, suggested by Goldstein and Osher in [7], stems from Augmented Lagrangian and ADMM (Alternating direction method for multipliers) methods, see a review on this in [5]. More details can be found in the original paper [7].

**Chambolle-Pock:** This is another very strong and general recent algorithm for solving various nonlinear optimization problems. The algorithm initiated by Pock-Cremers-Bischof-Chambolle for the Mumford Shah functional [8]. Later it was analyzed and generalized in [4].

## References

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