Exercise 08: Spatial Smoothing at Scale

Laplacian Smoothing:

(A)

$$A \text{ is of the form } A = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ a_{21} & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix} \text{ where } a_{ij} = \begin{cases} 1, & \text{if } \exists \{i, j\} \\ 0, & \text{if } \not\equiv \{i, j\} \end{cases}$$

 $A \text{ is of the form } A = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ a_{21} & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix} \text{ where } a_{ij} = \begin{cases} 1, & \text{if } \exists \{i, j\} \\ 0, & \text{if } \not \equiv \{i, j\} \end{cases}$ $W \text{ is of the form } W = \begin{bmatrix} w_{11} & 0 & \cdots & 0 \\ 0 & w_{12} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{nn} \end{bmatrix} \text{ where } w_{ii} = \# \text{ of neighbours of vertex } i.$

$$L = W - A = \begin{bmatrix} w_{11} & -a_{12} & \cdots & -a_{1n} \\ -a_{21} & w_{12} & \cdots & -a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n1} & -a_{n2} & \cdots & w_{nn} \end{bmatrix}.$$

Therefore, l_{ii} is the # of neighbours of vertex i, and l_{il} is negative the # of adjacency.

Therefore,
$$t_{ii}$$
 is the $\#$ of heighbours of vertex i , and t_{il} is negative the $\#$ of adjacency.

$$D = D_{m \times n} = \begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1n} \\ d_{21} & d_{22} & \cdots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{m1} & d_{m2} & \cdots & d_{mn} \end{bmatrix}, \text{ where } d_{ij} = \begin{cases} 0, & \text{if } \nexists \text{ adjacency for } j \\ 1, & \text{if } \exists \{j, k\} \text{ and } j \leq k \\ -1 & \text{if } \exists \{k, j\} \text{ and } j > k \end{cases}$$

Therefore, D^TD is a $m \times m$ matrix and the ij^{th} element of D^TD is $dd_{ij} = \sum_{k=1}^n d_{k,i}d_{k,j}$.

If
$$i \neq j$$
, then $dd_{ij} = \begin{cases} 0, & \text{if } \nexists \{i, j\} \\ -1, & \text{if } \exists \{i, j\} \end{cases}$;

If i = j, then $dd_{ii} = \sum_{k=1}^{n} d_{k,i} d_{k,i} = \#$ of edges from/to (just for the sake of notation. There is no direction in the graph though.) node i.

It is easy to see that dd_{ij} is exactly the same as l_{ij}

(B)

The Laplacian smoothing problem becomes:

$$\underset{x \in \mathbb{R}^n}{minimize} \ \tfrac{1}{2} \|y - x\|_2^2 + \tfrac{\lambda}{2} \|Dx\|_2^2$$

Let
$$F(x) = \frac{1}{2} ||y - x||_2^2 + \frac{\lambda}{2} ||Dx||_2^2 = \frac{1}{2} (y - x)^T (y - x) + \frac{\lambda}{2} x^T D^T D x$$

By FOC, $\frac{\partial}{\partial x} F = (x - y) + \lambda D^T D x = (1 + \lambda D^T D) x - y = 0$
 $\Rightarrow (1 + \lambda L) \hat{x} = y$

(C)
Solve
$$C\hat{x} = b$$
, where $C = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix}$, $b = \begin{bmatrix} b_1 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}$

Gauss-Seidel method:

$$C = L_* + U, \text{ where } L_* = \begin{bmatrix} c_{11} & 0 & \cdots & 0 \\ c_{21} & c_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix}, U = \begin{bmatrix} 0 & c_{12} & \cdots & c_{1n} \\ 0 & 0 & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

Therefore, the equation becomes $L_*x = b - \bar{U}x$, $x^{t+1} = L_*^{-1}(b - Ux^t)$

Step 1. Set initial value x^0 , and t = 1;

Step 2. Repeat until converges:

(i) For
$$i = 1, \dots, n$$
, set $x_i^{t+1} = \frac{1}{c_{ii}} (b_i - \sum_{j=1}^{i-1} c_{ij} x_j^{t+1} - \sum_{j=i+1}^{n} c_{ij} x_j^t)$
(ii) $t = t+1$

Step 3. Get final estimation $x^{t_{final}}$

The convergence properties of the GaussSeidel method are dependent on the matrix C. Namely, the procedure is known to converge if either:

- C is symmetric positive-definite;
- C is strictly or irreducibly diagonally dominant.

The GaussSeidel method sometimes converges even if these conditions are not satisfied.

Jacobi Iterative method:

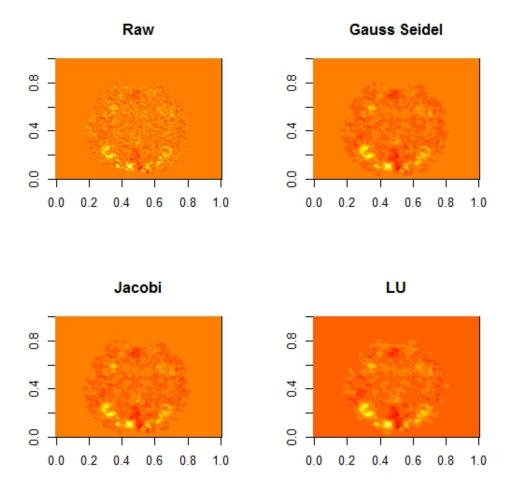
$$C = D + R, \text{ where } D = \begin{bmatrix} c_{11} & 0 & \cdots & 0 \\ 0 & c_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_{nn} \end{bmatrix}, \text{ and } R = \begin{bmatrix} 0 & c_{12} & \cdots & c_{1n} \\ c_{21} & 0 & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \cdots & 0 \end{bmatrix}$$

$$Dx = b - Rx, x^{t+1} = D^{-1}(b - Rx^t)$$

The standard convergence condition (for any iterative method) is when the spectral radius of the iteration matrix is less than 1.

A sufficient (but not necessary) condition for the method to converge is that the matrix A is strictly or irreducibly diagonally dominant.

Comparison:



The original problem is to minimize

$$\underset{x \in \mathbb{R}^n}{minimize} \frac{1}{2} ||y - x||_2^2 + \lambda |Dx|_1$$

Rewrite the problem as

$$\begin{aligned} & \underset{x \in \mathbb{R}^n}{minimize} \frac{1}{2} \|y - x\|_2^2 + \lambda |r|_1 \\ & \text{subject to } Dx = r \end{aligned}$$

Rewrite the problem as $\underset{x,r}{minimize} \frac{1}{2} \sum_{i=1}^{n} \frac{\eta_i(y_i - x_i)^2}{2} + \lambda |r|_1 + I_C(x,r)$,

where $I_C(x,r)$ takes the value 0 whenever $(x,r) \in C$, and ∞ otherwise. C is the convex set C = x, r : Dx = r.

Introduce 2 sets of slack variables (z for x, s for r). This yields another new problem:

$$\begin{aligned} & \underset{x,z,r,s}{minimiz} e^{\frac{1}{2} \sum_{i=1}^{n} \frac{\eta_{i}(y_{i}-x_{i})^{2}}{2}} + \lambda |r|_{1} + I_{C}(z,s) \\ & \text{subject to } x = z \in \mathbb{R}^{n} \ \& \ r = s \in \mathbb{R}^{m} \end{aligned}$$

We now have a constrained optimization in four sets of primal variables x, z, r, s. Let u be the scaled dual variable corresponding to the constraint x = z, and let t be the scaled dual variable corresponding to the constraint r = s. We can write the augmented Lagrangian of problem in scaled form as

$$L_x(x, z, r, s, t, u) = \frac{1}{2} \sum_{i=1}^n \frac{\eta_i(y_i - x_i)^2}{2} + \lambda |r|_1 + I_C(z, s) + \frac{a}{2} ||x - z + u||_2^2 + \frac{a}{2} ||r - s + t||_2^2$$
. Here a is the step-size parameter.

Algorithm:

Updating x:

$$x^{t+1} = \underset{x}{argmin} \frac{1}{2} \sum_{i=1}^{n} \frac{\eta_i (y_i - x_i)^2}{2} + \frac{a}{2} ||x - z^t + u^t||_2^2.$$

This is separable in each component of $x_i^{t+1} = \frac{\eta_i y_i + a(z_i^t) - u_i^t}{\eta_i + a}$.

Updating r:

$$r^{t+1} = argmin\lambda |r|_1 + \frac{a}{2}||r - s + t||_2^2.$$

This is also separable in each component, with minimum given by the soft-thresholding operator:

$$r_i^{t+1} = S_{\lambda a}(s_i^t - t_i^t)$$
, and the soft thresholding operator is $S_a(x) = sign(x)|x - a|_+$

Updating (z,s):

The update in (z, s) must be done jointly. It is the only computationally demanding step of the algorithm. Specifically, we have

$$(z^{t+1}, s^{t+1}) = \underset{(z,s)}{\operatorname{argmin}} I_C(z,s) + \frac{a}{2} ||x - z + u||_2^2 + \frac{a}{2} ||r - s + t||_2^2$$

Equivalentely, $\underset{z,s}{minimize} \|z - w\|_2^2 + \|Dz - v\|_2^2$

subject to
$$s = Dz$$

Since s does not appear in the objective, we can just solve for z and then set s = Dz. The ordinary first-order optimality condition for z in the above optimization problem is $(I + D^T D)z^{t+1} = w + D^T v$, recalling that $w = x^{t+1} + u^t$ and $v = r^{t+1} + t^t$

Code for Laplacian Smoothing:

```
#### FMRI Data ####
fmri=read.csv( "C:/Users/Yuxin/Dropbox/Courses/2016 Fall/Stat Model for Big Data/Exercise
makeD2_sparse = function (dim1, dim2) {
require(Matrix)
D1 = bandSparse(dim1 * dim2, m = dim1 * dim2, k = c(0, 1),
        diagonals = list(rep(-1, dim1 * dim2), rep(1, dim1 *
            dim2 - 1)))
D1 = D1[(seq(1, dim1 * dim2)\%dim1) != 0,]
D2 = bandSparse(dim1 * dim2 - dim1, m = dim1 * dim2, k = c(0, dim1)
        dim1), diagonals = list(rep(-1, dim1 * dim2), rep(1,
        dim1 * dim2 - 1)))
return(rBind(D1, D2))
}
#### Gauss Seidel ####
GaussSeidel = function( x0=x0, b=y, C , maxiter, tol ){
0x=x
n= length(y)
t=1
L_star = tril(C)
U = triu(C, 1)
while(t<maxiter){</pre>
x.t = solve(L_star, b - U %*% x[,t])
```

```
x=cbind(x,x.t)
t=t+1
if( sum(abs(x[,t] - x[,t-1])) < tol){}
break
}
}
return( list( x=x , iter=t, x.final=x[,t] ) )
}
n= length(y)
x0=matrix(0, nrow=n, ncol=1)
lambda = 1
C = Diagonal(n) + lambda * L
x0=matrix(0, nrow=n, ncol=1)
fit.GaussSeidel=GaussSeidel(x0=x0, b=y, C=C, maxiter=50, tol=1e-4)
fit.GaussSeidel$iter
x.final.GaussSeidel=fit.GaussSeidel$x.final
x.Matrix.GaussSeidel = matrix(x.final.GaussSeidel, nrow = nrow(fmri))
#### Jacobi ####
Jacobi = function( x0=x0, b=y, C , maxiter, tol ){
0x=x
n= length(y)
```

```
t=1
D=Diagonal(x=diag(C))
R = C - Diagonal(x = diag(C))
while(t<maxiter){</pre>
x.t = solve(D, b - R %*% x[,t])
x=cbind(x,x.t)
t=t+1
if( sum(abs(x[,t] - x[,t-1])) < tol ){
break
}
}
return( list( x=x , iter=t, x.final=x[,t] ) )
}
```