IMAGE ANALYSIS AND PATTERN RECOGNITION

SPRING SEMESTER 2004

SOLUTIONS
TO
HOMEWORK # 4

Multi-resolution contour-based fitting of macromolecular structures

P. Chacon and W. Wriggers

Part B:

The ***Fourier Transform*** is used throughout the manuscript, both as a tool for effectively concolving 3D volumetric density maps and for acceleration of the translational search.

Convolution is used in the resolution lowering and filtering, both the resolution lowering and Laplacian filtering were performed in one step by convolving the Gaussian with the Laplace operator to yield a Mexican hat operator, then the atomic structure was concolved with the Mexican hat operator, whereas the electron microscopy map was convolved with the Laplace operator as it already was at low resolution. Also, the Fourier convolution theorem is used in the context of FFT acceleration.

FFT acceleration is used here in the context of the 6D rigid-body matching algorithm. FFT is used to rapidly scan the translation of a probe molecule relative to a fixed reference molecule. Note that there are 3 rotational and 3 translational degrees of freedom (DOF) in the problem (3D+3D=6D). FFT acceleration only accelerates the three translational DOF as described in the paper.

The ***Laplacian Filter*** is used here as an edge-detection filter to find the surface information or the contour of a molecule. Contour information was obtained by finding the edges of a 3D object. The Laplacian operator was defined as a finite difference approximation.

Template convolution is a term using in image processing for the matching of two images or for matching of objects in images (typically 2D). As explained in the class notes it is actually not a convolution but a correlation technique, but like the convolution it can be handled most efficiently in Fourier space by multiplying the Fourier transforms together, except (unlike in a true convolution) we use the complex conjugate of one of the

Fourier transforms. In the paper here this idea was extended to the matching of 3D objects.

Part C:

The main problem when going from 2D to 3D is not that the translational search has an additional DOF, but that the rotations are much more complex to handle. Instead of a simple angle (as in 2D) we now need to describe the orientation of a 3D object relative to another 3D object by three Euler angles. For an exhaustive search of orientations this involves a massive computational task. E.g. a sampling of the three rotational DOF with an orientational accuracy of 9^{o} produces 30,481 sets of Euler angles instead of just 40 9^{o}-steps in 2D orientational matching (one rotational DOF).

Part D:

D1

Effect of Laplacian on the performance of template convolution for matching low-resolution 3D EM data:

Laplacian filtering allows for the matching to be accurate in the range of 0-25Å resolution of the volume data, whereas standard matching with the unfiltered density is only accurate from 0-10Å.

D2

Application of Laplacian operator in direct space is identical to multiplying in Fourier space with a harmonic function (a parabola, see the suggested handout).

D3

Laplacian is a high pass filter because the multiplication with a parabolic function attenuates (reduces) low frequencies and amplifies high frequencies. Actually, the Laplacian does more than just allowing high frequencies to pass through, since it is multiplying with an ever increasing parabola, it is amplifying the very high frequencies that are typically corrupted by noise.

D4

In direct space, the Laplacian acts as the second derivative. Thresholding is effective at eliminating noise below a cutoff density level, but it introduces a hard boundary of the density (step). The first derivatives at the step will be discontinuous, it is zero in the flat thresholded region, but corresponds to the density gradient in the non-thresholded region. Due to the discontinuity of the first derivative, the second derivative (Laplacian) applied to a thresholded density will show singularities (i.e. the values will be extremely high at the boundary), distracting from the desired matching of the filtered object densities. To get correct matching results using the cross-correlation, it is therefore necessary to mask out the extremely high values of the Laplacian at the thresholded boundary. This can be done by a simple erosion operation after applying the Laplacian, or by applying a relaxation procedure inside the thresholded region that modifies the thresholded densities such that the Laplacian (and not the density values themselves) are zero in the region.