Quick Distance Calculation over Periodic Dimensions via Fourier Transform

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Let $\mathbf{u}(\mathbf{x},\mathbf{y})$ and $\mathbf{v}(\mathbf{x},\mathbf{y})$ be two fields that are periodic in dimensions $\mathbf{x}$ and non-periodic in dimensions $\mathbf{y}$. Notice that, for any $\delta\mathbf{x}$,

$$\begin{aligned} \|\mathbf{u}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\|^2 &= \langle \mathbf{u}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y}), \mathbf{u}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\rangle \\ &= \|\mathbf{u}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\|^2 + 2\langle \mathbf{u}(\mathbf{x},\mathbf{y}), \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\rangle \\ &= \|\mathbf{u}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{v}(\mathbf{x},\mathbf{y})\|^2 + 2\langle \mathbf{u}(\mathbf{x},\mathbf{y}), \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\rangle. \end{aligned} \tag{1}$$

Hence, if we can compute the inner product $\langle \mathbf{u}(\mathbf{x},\mathbf{y}), \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\rangle$ quickly, we can compute $\|\mathbf{u}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\|^2$ quickly. The norms $\|\mathbf{u}(\mathbf{x},\mathbf{y})\|$ and $\|\mathbf{v}(\mathbf{x},\mathbf{y})\|$ do not depend on $\delta\mathbf{x}$ and must be computed only once.

Using Plancherel's Theorem,

$$\int \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x} = \int \overline{F(\mathbf{k})} G(\mathbf{k}) d\mathbf{k},$$

where capital letters denote the Fourier transform, e.g.,

$$G(\mathbf{k}) = \mathcal{F}\left[g(\mathbf{x})\right],$$

we find that

$$\begin{aligned} \langle \mathbf{u}(\mathbf{x},\mathbf{y}), \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y})\rangle &= \int\int \overline{\mathbf{u}(\mathbf{x},\mathbf{y})} \cdot \mathbf{v}(\mathbf{x}-\delta\mathbf{x},\mathbf{y}) \; d\mathbf{x} \; d\mathbf{y} \\ &= \int\int \overline{\mathbf{U}(\mathbf{k},\mathbf{y})} \cdot \left(e^{-i\mathbf{k}\cdot\delta\mathbf{x}} \mathbf{V}(\mathbf{k},\mathbf{y})\right) \; d\mathbf{k} \; d\mathbf{y} \\ &= \int e^{-i\mathbf{k}\cdot\delta\mathbf{x}} \left(\int \mathbf{U}(\mathbf{k},\mathbf{y}) \cdot \mathbf{V}(\mathbf{k},\mathbf{y}) \; d\mathbf{y} \right) \; d\mathbf{k} \\ &= \mathcal{F}^{-1}\left[\int \mathbf{U}(\mathbf{k},\mathbf{y}) \cdot \mathbf{V}(\mathbf{k},\mathbf{y}) \; d\mathbf{y} \right] \end{aligned}$$

Hence, the pseudo code for the quick algorithm is as follows:

1. compute the norms of $\mathbf{u}$ and $\mathbf{v}$.
2. compute their FFTs, $\mathbf{U}$ and $\mathbf{V}$.
3. integrate $\mathbf{U} \cdot \mathbf{V}$ over all non-periodic dimensions, $\mathbf{y}$.
4. compute the inverse Fourier transform of the resulting field, over all periodic dimensions, $\mathbf{x}$. This computes $\langle \mathbf{u}(\mathbf{x}, \mathbf{y}), \mathbf{v}(\mathbf{x} - \delta\mathbf{x}, \mathbf{y}) \rangle$ as a function of $\delta\mathbf{x}$.
5. compute $\|\mathbf{u}(\mathbf{x}, \mathbf{y}) - \mathbf{v}(\mathbf{x} - \delta\mathbf{x}, \mathbf{y})\|^2$ from Equation 1.

NOTE that the FFT in Matlab is normalized oddly, so you will have to make sure that the "inner product" induced by Matlabs FFT agrees with the norm used to compute $\|\mathbf{u}\|$ and $\|\mathbf{v}\|$.

Here is a Matlab implementation of the method in 1D:

```
function F = fftdistance(u,v)

% finds the best l the minimizes ||v(x)- u(x-l)||

F = conj(fft(u)).*fft(v);
F = ifft(F,'symmetric');

F = F*numel(F); % takes care of FFT normalization
F = sqrt(dot(u,u)+dot(v,v)-2*F);

% due to roundoff error when the distance is near zero
    you may want to run
F = real(F);

end
```