

CS 426 HW 3

1. For geometric hashing, the kind of transformation we allow determines the number of points needed to establish a reference frame. For example, for translation (i.e., no rotation, no scaling) in any dimension, we need just one point; this point is enough to determine the location of our reference frame's origin. For each of the following transformation types, determine the number of points needed to establish a reference frame.

- 2-dimensions, translation and scaling
- 2-dimensions, translation, rotation, and scaling
- 3-dimensions, translation and scaling
- 3-dimensions, translation, rotation, and scaling

2. Consider the following two sets of points. Determine the RMS distance between the two point sets under each of the following assumptions. The two sets are assumed to be ordered so that corresponding points are in the same position in each list. You may want to write a simple program to do the calculations or you may want to use Matlab. If you write a program, include it in your hw solution. If you use Matlab, include the commands you use in your hw solution.

Assume that the point sets are in fixed position (no rotation, no translation).

Assume that the point sets are allowed to translate, but not rotate. Find the translation that produces the minimum RMS distance. Report this translation and the resulting distance.

Point Set A:

0.9003	-0.3258	-0.2888
-0.5377	0.2196	-0.8140
0.2137	0.8614	-0.4608
-0.0280	-0.0740	-0.9969
0.7826	0.2782	0.5569
0.5242	-0.7065	0.4755
-0.0871	0.9154	-0.3929
-0.9630	0.2336	-0.1344
0.6428	-0.6475	0.4094
-0.1106	0.7801	-0.6158

Point Set B:

-0.8842	0.4649	0.0448
-0.2943	-0.0193	-0.9555
0.6263	-0.7336	0.2636
-0.9803	0.1798	-0.0821
-0.7222	-0.6759	0.1467
-0.5945	-0.7013	0.3934
-0.6026	0.4536	-0.6566
0.2076	-0.9660	-0.1540
-0.4556	0.2610	0.8511
-0.6024	-0.3751	-0.7046

3.

- (a) Enumerate all the possible conformations of a two dimensional self-avoiding polymer of 10 monomers embedded in a square lattice. The positions of the first two amino acids are fixed (say on $(0,0)$ and $(0,a)$ where “a” is the lattice constant).
- (b) How many conformations does the above polymer have? Write a computer program to generate and count all conformations.
- (c) Consider the sequence PPPHHHHPHP. Identify all of the lowest energy conformers. How many lowest energy conformations do you find?
- (d) Plot $P(E)$ the probability that a structure (of the polymer defined in (b)) picked at random will have an energy between E and $E+dE$ (where dE is a small energy interval).