Bakker and Poole

There are two levels of identification in Relational Data Problems:

1) identifying the objective function for purposes of finding the optima;

2) identifying the objective function for purposes of exploring it with Markov Chain Monte Carlo Methods.

For (1), the number of constraints is equal to s(s+1)/2. Namely, one point is placed at the origin for s constraints, a second point has s-1 coordinates placed at 0.0, a third point has s-2 coordinates placed at 0.0, etc. This fixes the rotation.

To see this consider s=2. Fix one point at the origin and then the rotation is fixed by selecting θ:

$$\Gamma = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \; 0 \le \theta \le 2\pi$$

This is equivalent to placing one coordinate of a second point at 0.0

For (2), we need s(s+2)/2 + 2^s -1 constraints. To see this, given a *specific* θ we have *four* rotation matrices:

$$\Gamma_1 = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \quad \Gamma_2 = \begin{bmatrix} -\cos\theta & \sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \quad \Gamma_3 = \begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{bmatrix} \quad \Gamma_4 = \begin{bmatrix} -\cos\theta & -\sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}$$

Or

$$\Gamma^* = \Delta\Gamma \text{ where } \Delta = \begin{bmatrix} \pm 1 & 0 \\ 0 & \pm 1 \end{bmatrix} \quad (14)$$

That is, given a specific θ, there are 2^s sign flips corresponding to the s columns of the rotation matrix. In practice we have placed s(s+1)/2 zeroes in the coordinate matrix and this arbitrarily selections *one rotation matrix*. Hence, there are 2^s -1 further possible rotation matrices corresponding to the remaining sign flips.