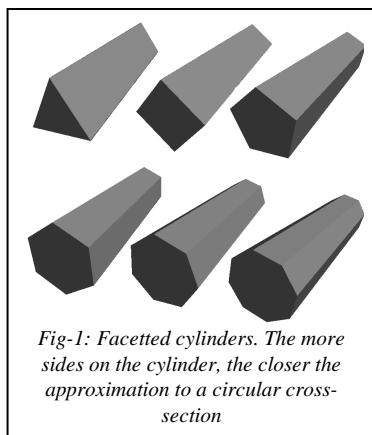


# A hexagon is a circle

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## Introduction

Models for generating synthetic data for diffusion MRI often model white matter fibres as cylinders arranged in parallel [1]. The cross section of these cylinders is commonly chosen to be circular [1], but cylinders with square cross-section have also been used [2][3]. Implementing such perfectly circular cylinders is possible using analytical surfaces, but simulations with polygonal cross-section (see Fig-1) are simpler to implement than truly cylinders with perfectly circular cross-section, for which reflection and intersection calculations are more complicated. The problem is worse for more complex surfaces, where faceted approximations offer significant computational and implementational advantages.

Here we compare synthetic diffusion-weighted signals from diffusion inside parallel, impermeable cylinders with circular cross section to those from faceted cylinders. Using the synthetic signals from diffusion in perfectly circular cylinders as a gold standard, we synthesise data for parallel cylinders with 3-20 facets. Corners of the polygon cross-sections of faceted cylinders are placed on the circumference of the circle being approximated. Each simulation compared with the gold standard contains only cylinders with a single number of facets (i.e. each simulation has cylinders with  $n$  facets, rather than a mixture of cylinders).

## Methods

Using a Monte-Carlo model of diffusion, we simulate 40000 spins executing random walks on a periodic substrate of cylinders regularly placed on a square lattice. Cylinders have radius  $1\mu\text{m}$  (corresponding to the distance of each facet vertex to the centre of the cylinder for faceted cylinders) separated by  $3\mu\text{m}$ . Trajectories for each spin contain 2500 steps and have a total duration of 0.1s (simulation time). Trajectories on each substrate are used to generate synthetic measurements using the

method of [1] for all physically allowed combination of diffusion time  $\Delta \in [0.01, 0.05]\text{s}$ , pulse duration  $\delta \in [0.005, 0.05]\text{s}$  and gradient strength  $G \in [0.005, 0.05]\text{Tm}^{-1}$ . In all simulations  $\delta < \Delta$  parameter combinations breaking this condition are not considered. Each parameter is incremented 6 times across the range. Synthetic diffusion-weighted signals were synthesised in 50 directions perpendicular to the cylinder axis. The ground truth data is compared to data synthesised from substrates for each of the faceted cylinder types. A similar set of experiments is possible with approximation of the sphere. In this case we can approximate spheres using the Platonic solids: the tetrahedron, cube, octahedron, dodecahedron and icosahedron. We calculate the standard deviation of the synthetic data over direction at a particular combination of scan parameters. This is a measure of departure from isotropy. A good approximation to the sphere will be isotropic and hence have a low standard deviation, whereas a poor approximation will exhibit anisotropy and

## Results

Fig-2 shows the mean and max squared difference between faceted cylinders and the circular ground truth. We observe that the differences drop off quickly as number of sides is increased. A cylinder with 6 facets is a good approximation of a circle.

Fig-3 shows the mean and max of the standard deviation over direction for each platonic solid, averaged over the same combinations of scan parameters used in the first set of experiments. All solids have a low standard deviation. The tetrahedron has the smallest maximum standard deviation, and the cube the largest.

## Discussion

These results illustrate that a faceted cylinder whose cross section is a regular polygon with 6 sides approximates a circular cylinder well enough for to generate synthetic diffusion-weighted MR signals over a wide range of parameters. We observe that the maximum values are 3 orders of magnitude larger than the means, suggesting that the differences between cylinders are mostly very small, with a few outliers in certain directions and parameter combinations. Max values tend to occur for high  $b$  value, in particular for high gradient strengths and long diffusion times. This combination of parameters would tend to suppress the relatively free diffusion in the extra-cellular compartment, favouring the signal intracellular compartment and thus being more discriminating of structural differences in substrate.

Approximating smooth geometric objects with faceted or mesh-like objects considerably simplifies implementation of complex geometrical models of diffusion and reduces the runtime of such simulations. Further work will assess the sphere more fully, as well as comparing simulation results to analytical solutions for diffusion signal in restricting geometries.

Our work suggests that the, in general, it is preferable to construct restricting geometries from faceted surfaces, rather than using more complicated primitives like smooth surfaces and spheres.

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## References

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