Author’s response to E. de Kemp’s interactive comment on “Monte Carlo Simulations for Uncertainty Estimation in 3D Geological Modeling, A Guide for Disturbance Distribution Selection and Parameterization”.

An important study in developing uncertainty models for 3D geological modelling. The study focuses on a specific data perturbation method (MCUM) used in previous work but narrows in on how models can be calculated assuming that the constraining inter-face and orientation data has a predictable error (uncertainty) distribution. The work highlights the critical value in converting scalar orientation data to vector pole format (surface normals) for orientation measures. Some work on this topic, not in uncertainty modelling, has been done previously, as well as using quaternions (see De Paor 1995 C1(Quaternions, raster shears, and the modeling of rotations in structural and tectonic studies (1995) Geol Soc. Amer. Abs. with Prog., 27 (6), p. A72.), Karney 2007) to spherically rotate (perturb)the observation set. Also, highligts the value in assessing and transforming heteroscadastic data. Only 2 case studies were used to make the point that using poles versus dip/direction scalar values enhances uncertainty reduction. Probably does for the most part but could have demonstrated this more systematically and dramatically with a sphere of orientation measures. A considerable mathematical expose was done making the case for Baysian approach to developing priors for the distributions but this was hard to follow from a practical point of view. This section could use some more explanatory context such as when local or global priors are being estimated and how this is being done from the field point of view. Multi-observation sites to calculate local distributions? By regions? A major assumption sampling/disturbing ie. at K=100 the vMF distribution for orientation measures is that underlying natural variability is randomly concentrated on a spherical cluster. This is rarely the case in nature as there is generally a process dependant geometric bias such as deformation that controls rotation parameters. To capture this more work would need to be done. Perhaps part 2 but this will become important. Quaternions are potentially a way to do this as they are rotations about a vector which could be a population or local mean (E3 - eigenvector for example). At least moving from scalar orientation to poles is a great start. What about polarity? A near vertical stratigraphic interface needs to be managed with components for the pole to have direction to allow for overturning. Has this been considered when the disturbance is conducted? Overall a good and important study but could be made clearer and appealing for a wider audience if some more context and practical implications could be given.

Author’s answer:

The author’s agree that the manuscript is too abstract, some work was done in the introduction and discussion sections to make the topic more tangible in the geological world.

The number of case studies was voluntarily limited given that many mathematical concepts needed to be laid out in section 3 prior to any practical demonstration. In this sense, the case studies actually serve as proof of concepts rather than hard application case studies. More in-depth case studies will be the topic of subsequent publications.

Using K=100 for the vMF distribution falls in line with recent metrological work on geological compass’ measurement uncertainty (Allmendinger et al. 2017, Novakova et al. 2017). Anisotropy about the pole vector cluster may be addressed by switching to the Kent distribution that is mentioned in the discussion section of the paper. Note however, that parameterizing the Kent distribution is difficult and requires much more in depth metrological work because the Kent distribution has five parameters while the vMF distribution has two. Consequently, fitting data to the Kent distribution is not always possible and almost always less robust than fitting it to the vMF distribution.

Polarity, when dealing with poles to planes, is implicit (e.g. the Cartesian pole of a normal horizontal plane is [0, 0, 1] while its reversed counterpart is [0, 0, -1]).

Page 1, line 15-16:

E. de Kemp’s comment:

Assumption here is that the entire uncertainty distribution results from input data accuracy?

Author’s answer:

Not necessarily, the present paper does focus solely on this aspect although any kind of quantifiable source of input uncertainty (to include natural variability for example) could be included into the disturbance distributions. It is always possible to compound disturbance distributions further to account for new sources of uncertainty.

Changes to the paper:

…input data [*measurement*] uncertainty…

Page 3, line 20:

E. de Kemp’s comment:

What are interpolation ambiguities? Do you mean estimate the unknown variables at unsampled locations?

Author’s answer:

In implicit 3D geological modelling each series’ interfaces are modelled separately (n.b. in our case there is only one interface per series) and therefore "ignores" all other interfaces. The topological rules exist to solve which unit intersects which and therefore, which interface stops on which.

Changes to the paper:

The mention to “interpolation ambiguities” was removed as it doesn’t add significant meaning to the sentence.

Page 3, line 29:

E. de Kemp’s comment:

briefly define 'disturbance distribution and relate it to natural phenomina i.e. a natural horizon deformation can be a summation of location translation, block rotation about an axis etc.

Author’s answer:

Definition added page 3, line 18.

Changes to the paper:

[*Essentially, a disturbance distribution quantifies the degree of confidence that one has in the input data used for the modeling such as the location of a stratigraphic horizon or the dip of a fault.*]

Page 4, line 9-14:

E. de Kemp's comment:

Concern here is that you start with afirming that sample points controlling fault geometry may be linearily biased but are still independant? They are apriori spatially dependant should the disturbance function somehow not take into consideration this bias by disturbing the direction of greatest likley variance? Chicken and egg problem as you may not know the prior fault feature continuity direction? More of this in the intro / discussion? The Fisher disurbance is also going to have some prior direction as planar features tend to be rotated preferentially around an axis (i.e. plunge direction).

Author's answer:

In the case where only measurement uncertainty is considered, the dispersion of the disturbance distributions is independent. That is not to say that dispersion is necessarily isotropic or homoscedastic (see Kent distribution in discussion section).

Of course, dispersion dependencies may be added afterwards to update the dispersion parameters. The sampling itself is independent for usual structural inputs regardless of spatial dependencies.

Changes to the paper:

None

Page 5, line 1:

E. de Kemp's comment:

Transposed mean unit vector?

Why do you say transposed just because you use the norm?

Author's answer:

That is the standard form of the vMF distribution. The vector is transposed in order to compute the dot product of x and gamma which directly quantifies their angle on the unit sphere because both are unit vectors.

Changes to the paper:

None

Page 5, line 5:

E. de Kemp's comment:

...and if K ~ 1 or = 1 what does that represent? Many geological surfaces locally have vMF distributions that are near 1.

Author's answer:

On the vMF distribution:

- $\kappa = 0$ corresponds to a 95% confidence interval ≈ 170 degrees half angle.
- $\kappa = 1$ corresponds to a 95% confidence interval ≈ 150 degrees half angle.
- $\kappa = 10$ corresponds to a 95% confidence interval ≈ 37 degrees half angle.
- $\kappa = 100$ corresponds to a 95% confidence interval ≈ 11 degrees half angle.

Changes to the paper:

None

Page 5, line 9:

E. de Kemp's comment:

where is v in this equation?

Perhaps an example in the appendix?

Author's answer:

Equation updated.

Changes to the paper:

Equation 3 changed from

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^{p/2} I_{p/2-1}(\kappa)},$$

to

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^{p/2} I_{v=p/2-1}(\kappa)},$$

Page 5, line 21:

E. de Kemp's comment:

I think you are trying to say it is better to encourage multi-observations per site to come up with a local set of statistics for both location and orientation so that in the end you have the freedom to have many site specific disturbance distributions? If so try to say that in non-statistical language.

Author's answer:

It is a fact that multi observations yield lower dispersion (higher quality) disturbance distributions as a consequence of the usage of the Bayesian framework. Although, no specific recommendation is made at this point of the paper given that demonstration has not been made yet of this enhanced utility. Mention of this specific subject is made in the discussion page 23, line 18.

Changes to the paper:

…makes metrological work [*and multi-observations per site*] ~~a~~ mandatory ~~step~~ to any form of modeling…

Page 5, line 24:

E. de Kemp's comment:

clarify why the distribution is not just described by the population mean and standard deviation? The true mean = population mean AND true dispersion is the standard deviation? Not exacly clear if this is a local sample set or global population you are describing.

Author's answer:

That is so because the true parameters refer to a population whereas observers deal with finite samples.

Changes to the paper:

true mean and dispersion [*of the population*], respectively.

Page 6, line 18:

E. de Kemp's comment:

true if all priors are independent...

Author's answer:

True, however, for repeated measurements made at the same sampling site, the relevant priors are independent.

Changes to the paper:

None

Page 7, line 23:

E. de Kemp's comment:

That is not at all clear ...

Author's answer:

Explanation added.

Changes to the paper:

underestimation of dispersion [*because* $\sigma^2 \geq \frac{\sigma^2}{n}$ *and* $\kappa \leq \frac{\kappa R}{1+R}$.]

Page 8, line 2:

E. de Kemp's comment:

such as when what is done in practice ? Try to relate the statistical concepts to real world for the reader? Not clear yet how a disturbance distribution would be BEST derived practically or which practice you favor.

Author's answer:

Explanation added.

Changes to the paper:

[*Incorrect informative priors have low dispersion (high precision, 'self-confident') and high bias (low accuracy, 'off target'). This results in an inability of standard Bayesian schemes to update these priors regardless of the strength of the evidence.*] ~~Prior uncertainty distributions are then inappropriate disturbance distributions~~ To avoid this detrimental effect, ~~and~~ one should sample…

Page 8, line 3:

E. de Kemp's comment:

somehow this is not being communicated well. It should be obvious not just from the math but also from descriptions of what is occuring to the disturbance estimates as one uses priors. Maybe this comes out later in teh case studies?

Author's answer:

More of this is indeed described in the case studies and very visible in Figures 8 and 10.

Changes to the paper:

See above changes.

Page 8, line 18:

E. de Kemp's comment:

uncertanty and error are used here as equivalent. Is this true?

Author's answer:

Yes.

Changes to the paper:

and their uncertainty[*/error*] to be possible (Fig. 4).

Page 8, line 27:

E. de Kemp's comment:

...how could this be done given the operational requirements for geological field studies.

Author's answer:

This is typically metrological lab work, reference to recent work on this topic added.

Changes to the paper:

[*(Allmendinger et al., 2017; Cawood et al., 2017; Novakova and Pavlis, 2017)*]

Page 10, line 16:

E. de Kemp's comment:

no mention of polarity issues? Using bi-direction data as dip vector or poles gives ambiguity as well for near vertical orientations.

Author's answer:

Polarity issues for non-pole based perturbation are mentioned page 10, line 20. More added.

Changes to the paper:

Conversely, poles to planes carry information about polarity implicitly (e.g. the Cartesian pole of a normal horizontal plane is [0,0,1] while its reversed counterpart is [0,0,-1]).

Page 11, line 8:

E. de Kemp's comment:

a sandstone ? Is it unconsolodated? Gives reader and idead of spatial continuity. How deformed ?

Author's answer:

Details added.

Changes to the paper:

…siliceous detritic type [*ranging from mildly deformed sandstones to siltstones and shales*].

Page 11, line 24:

E. de Kemp’s comment:

what does this mean? Can you clarify this as it is not a common term even though work has been done to define it by Wellman etc.

Author’s answer:

Explanations added.

Changes to the paper:

…entropy uncertainty models. [*Information entropy is a concept derived from Boltzmann equations (Shannon 1948) that is used to measure chaos in categorical systems. Because of this, it is possible to use information Entropy as an index of uncertainty in categorical systems.*].

Page 13, line 2:

E. de Kemp’s comment:

Try to state the topic and/or concept so the reader is not always forced to go back to the quoted section. Discussions should be easy to read, and flow from the more rigorous body of the paper. Should not be an back index or summary of the paper.

Author’s answer:

Section updated, unnecessary references to previous sections removed, added paragraph page 13, line 25.

Changes to the paper:

[*Note that it is acceptable to use preexisting metrological studies to define the priors (Allmendinger et al., 2017;Cawood et al., 2017;Novakova and Pavlis, 2017) provided that the measurement device and procedure used are similar to that of the studies. To gather multi observations per site is strongly recommended as this practice sharply increases the quality of the disturbance distributions. From a practical point of view this would require field operators to perform several measurements onto the same outcrop. If that is not possible one may group measurements of clustered outcrops together provided that the scale of the modeled area compared to that of the cluster allows it. The authors recommend not grouping clusters that are spread out more than 3 orders of magnitude below the model size (e.g. for a 10km model, clusters of size higher than 10m shall not be grouped).*]

Page 29, line 1:

E. de Kemp's comment:

Dip vectors are green? pole vectors are blue and red data (a,c,e) and vMF distributions of K=100 (b,d,f) ? Need to clarify colours as it is pretty confusing.

Author's answer:

Description added.

Changes to the paper:

[*Correct (pole perturbed) dip vectors are green, incorrect (dip perturbed) dip vectors are red and blue vectors are the poles.*]