

After semilandmarks

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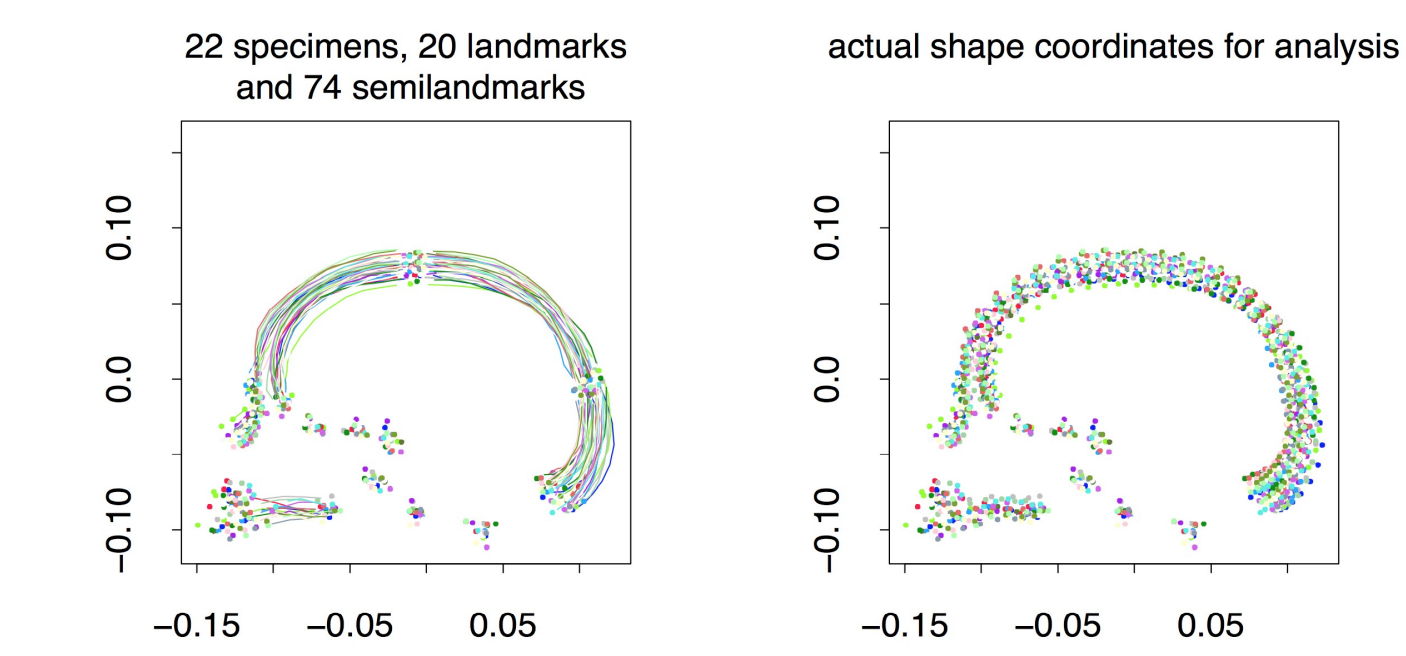
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Summary. For problems that are truly **bio**-logical, the geometric morphometric methods have proved a Procrustean bed. They amputate too much of the actual scientific context in the quest for methodological tidiness. To transcend this dilemma will require new biomathematical structures, not just tinkering with matrix algebra.

In the 2005 proceedings volume that derived from the predecessor of today's symposium, I plotted an alternate biometrical future "after landmarks" that freed the bioscientist from many severe restrictions of that formalism by instead emphasizing semilandmarks (SL's), which incorporate more anatomical realism than what is possible via the classic anthropometric notion of the landmark point. Today it is time for the same iconoclasm regarding that presumptive successor method, which, like the Procrustes/thin-plate-spline workbench for landmarks, has become canonical prematurely.

I will review two domains where optimism about the SL methods may be warranted: allometry and bilateral symmetry. But I will take more space exposing contexts into which I think the extension of the SL tools will NOT be justified without massive investments in deeper biomathematics. These all involve the articulation of the SL methods to domains like physiology, bioengineering or biotechnology dominated by scalar summaries such as kinetic, chemical, or elastic energy that have no tidy relationship to either of the two principal scalars of the Procrustes approach. Functional anatomy turns out to center in one of these domains.

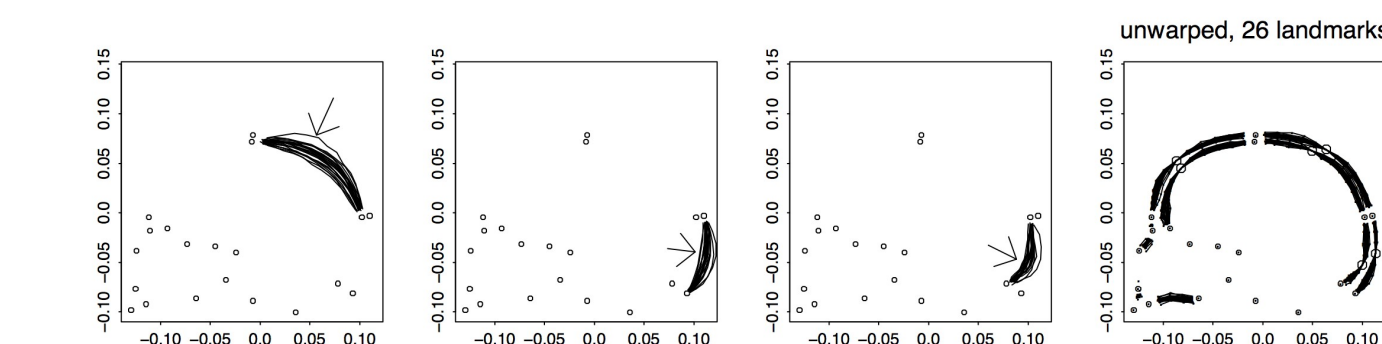
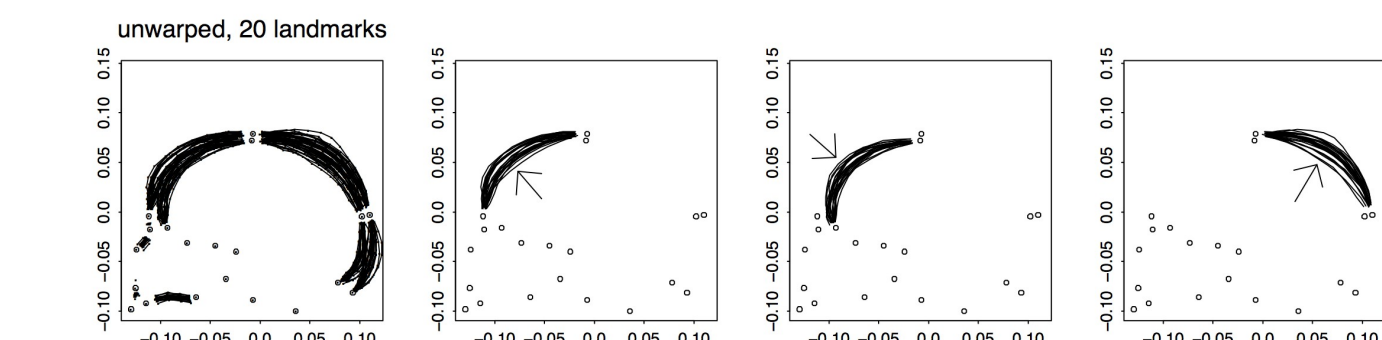
I will conclude that the fundamentals of today's most widely-installed notion of semilandmarks are biomathematically incoherent, so much so as perhaps to be unsalvageable for applications outside the current range of taxonomy and forensics. It will require rebuilding from the ground up if our theme --- the reduction of curving form to linearizable data --- is to remain part of the 21st-century biometrical canon. As this was D'Arcy Thompson's main theme already a century ago, it is hard to argue that we have made enough progress over that interval to feel as confident of our competences as we apparently do.



Mostly successful story I. Allometry at and between landmarks

These are the midsagittal data of Bookstein et al., 1999, as extended to more semilandmarks by Gunz et al., 2003.

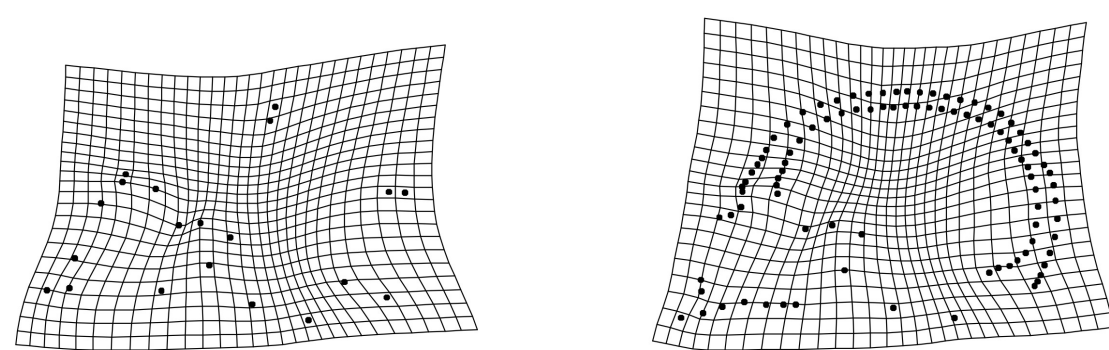
We see that each curve is represented effectively enough by one single additional point, which I have arbitrarily located near the midpoint of the arcs.



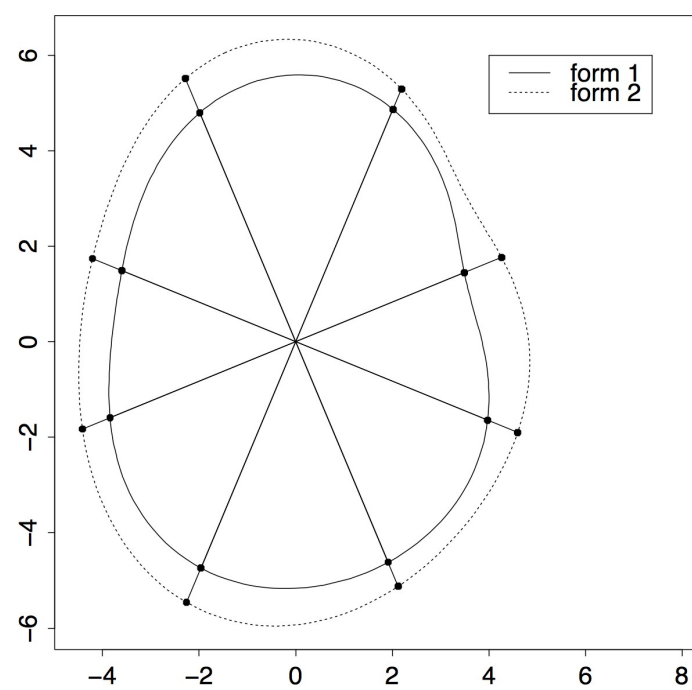
It can be shown to follow that the effect on molar descriptors, such as the first relative warp below, is itself local and limited in visual impact.

RW 1, 22 specimens, 20 landmarks only

RW 1, 22 specimens, also with 74 semilandmarks



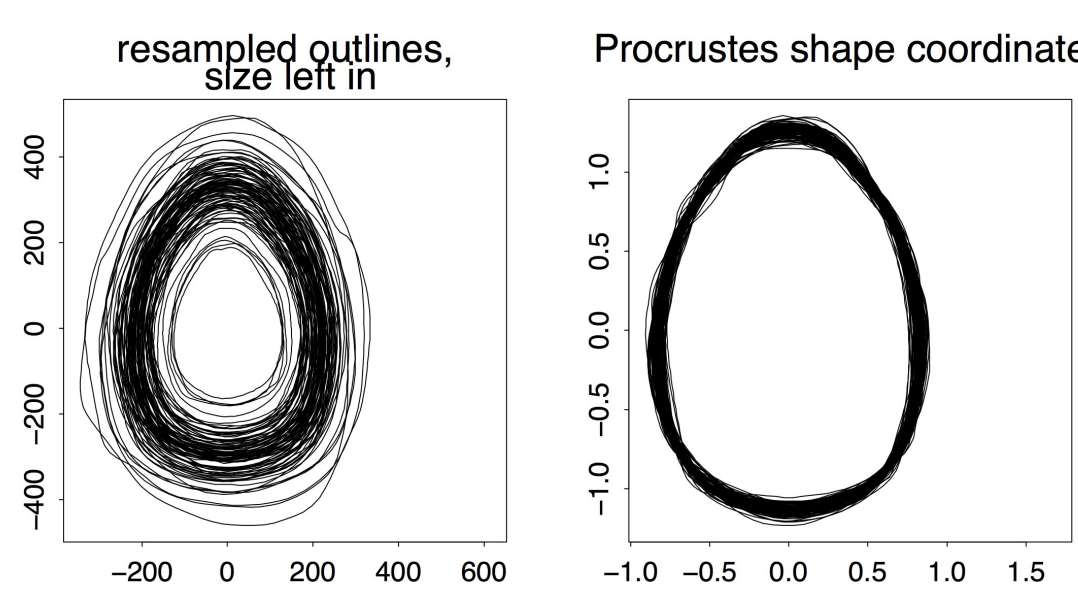
full resampled data set



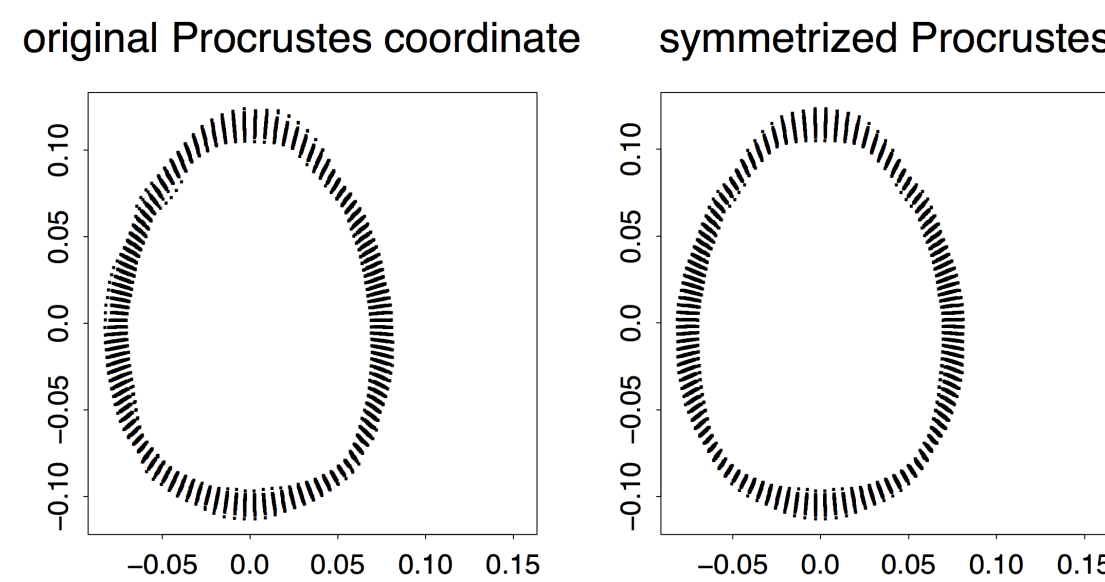
Mostly successful story II. Modifying Procrustes analysis for bilaterally symmetric outlines without landmarks.

This is an excerpt from Bookstein and Ward, 2013. The data were 99 video-extracted sections of *Baculites* from pre-KT Baja California. The analysis replaces the usual Procrustes method by an alternation between azimuthal sectioning and centering/orienting of the resulting vertices.

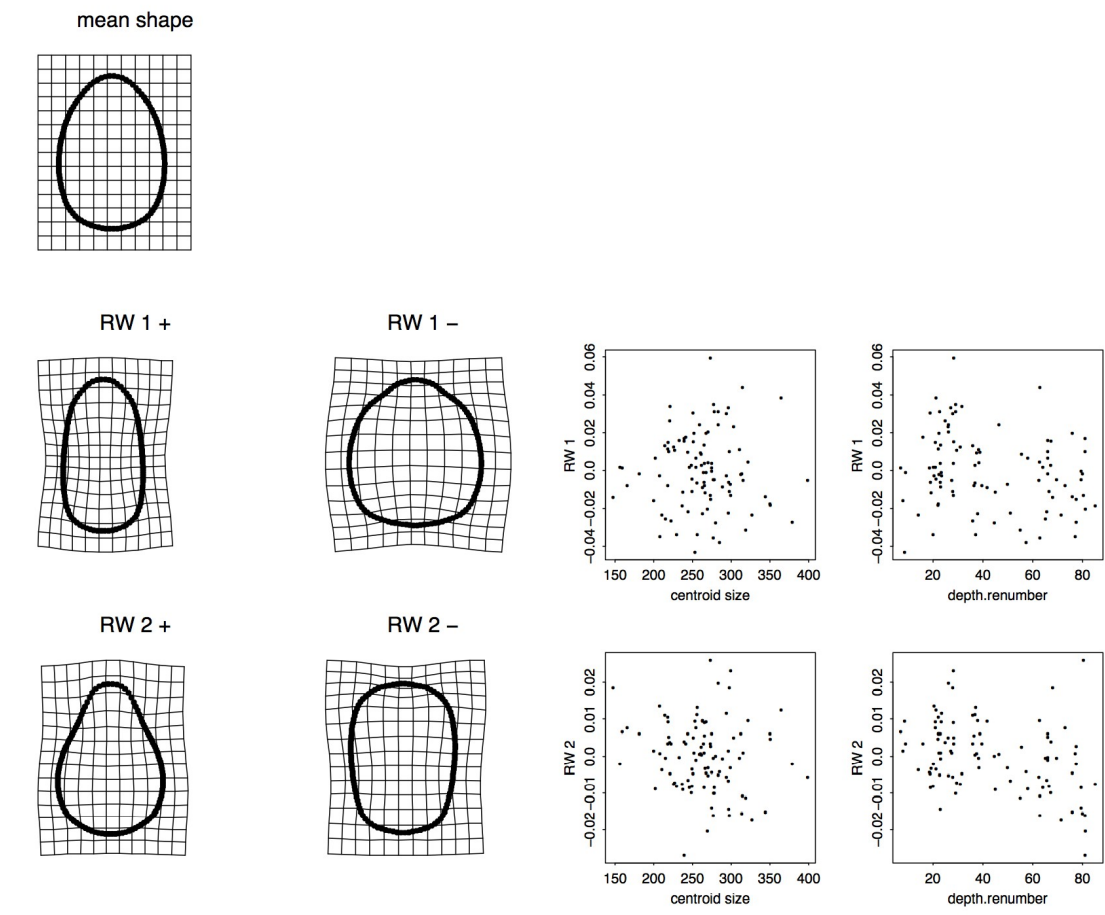
Everything else in the usual toolkit then goes forward quite well: size-standardization ...



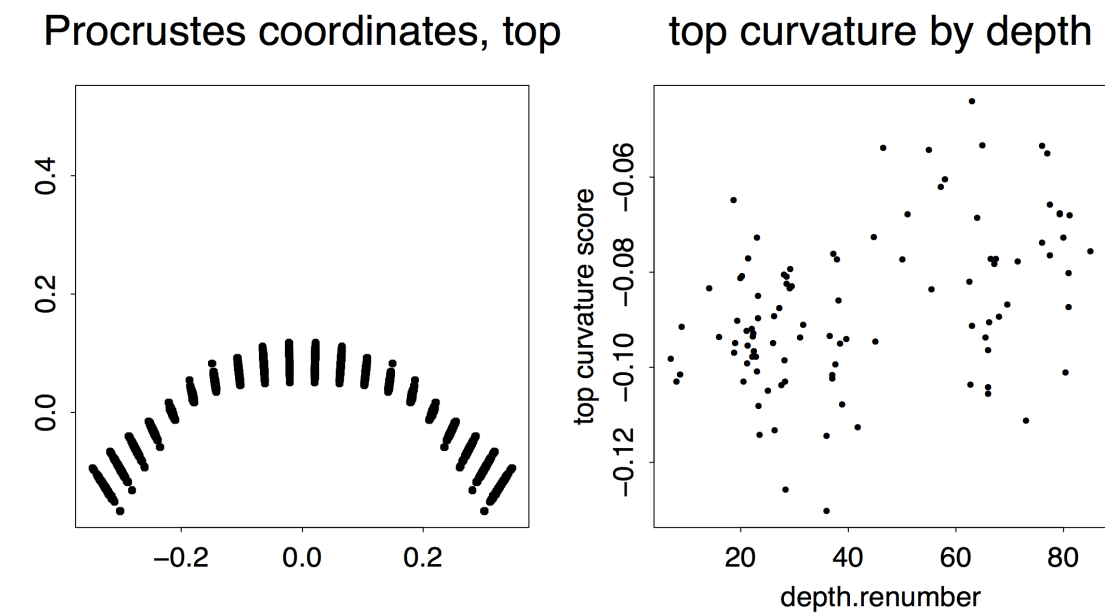
... standard bilateral symmetrization ...



... standard relative warps analysis ...



...and localization of the corresponding effect (evolution of a keel).



These examples were too easy

As soon as we begin to inquire into questions of integrative biology, current GMM methodology fails. I will concentrate on the domain where we have independent information about "the origins of form in force" (D'Arcy Thompson's explicit purpose of a century ago). We have a great advantage over him in access to the mathematics and especially the finite-element software that can either analytically or computationally predict the patterns we ought to be observing.

Here are two success stories of numerically accurate simulations:

A diametrically compressed disk.

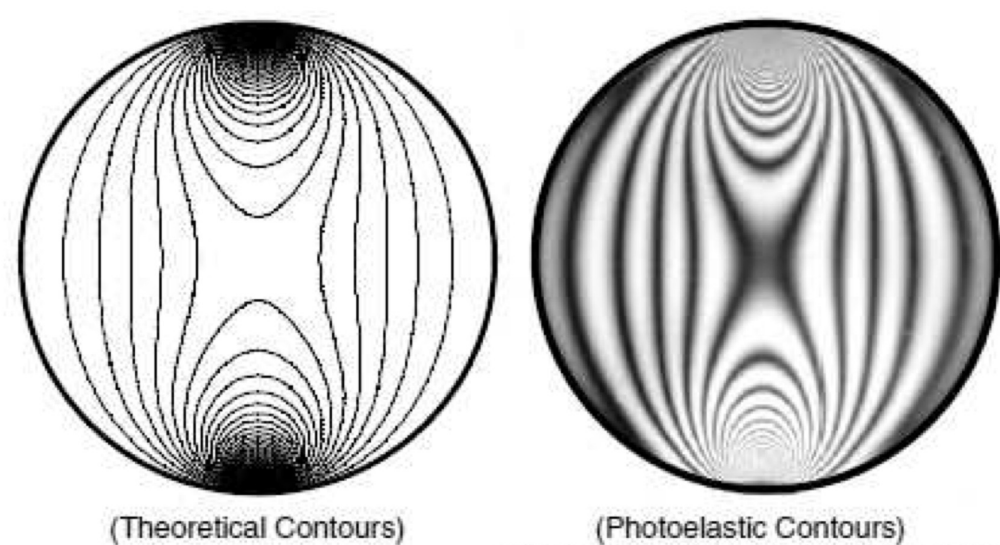


FIGURE 8-36 Maximum shear stress contours and corresponding photoelastic isochromatic for disk under diametrical compression.

A fishing rod under end load.

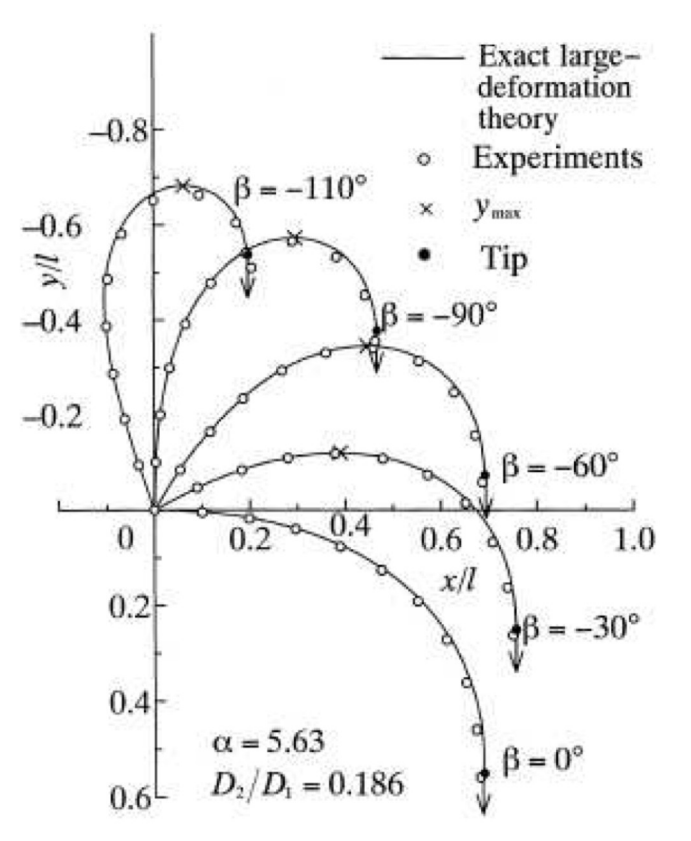
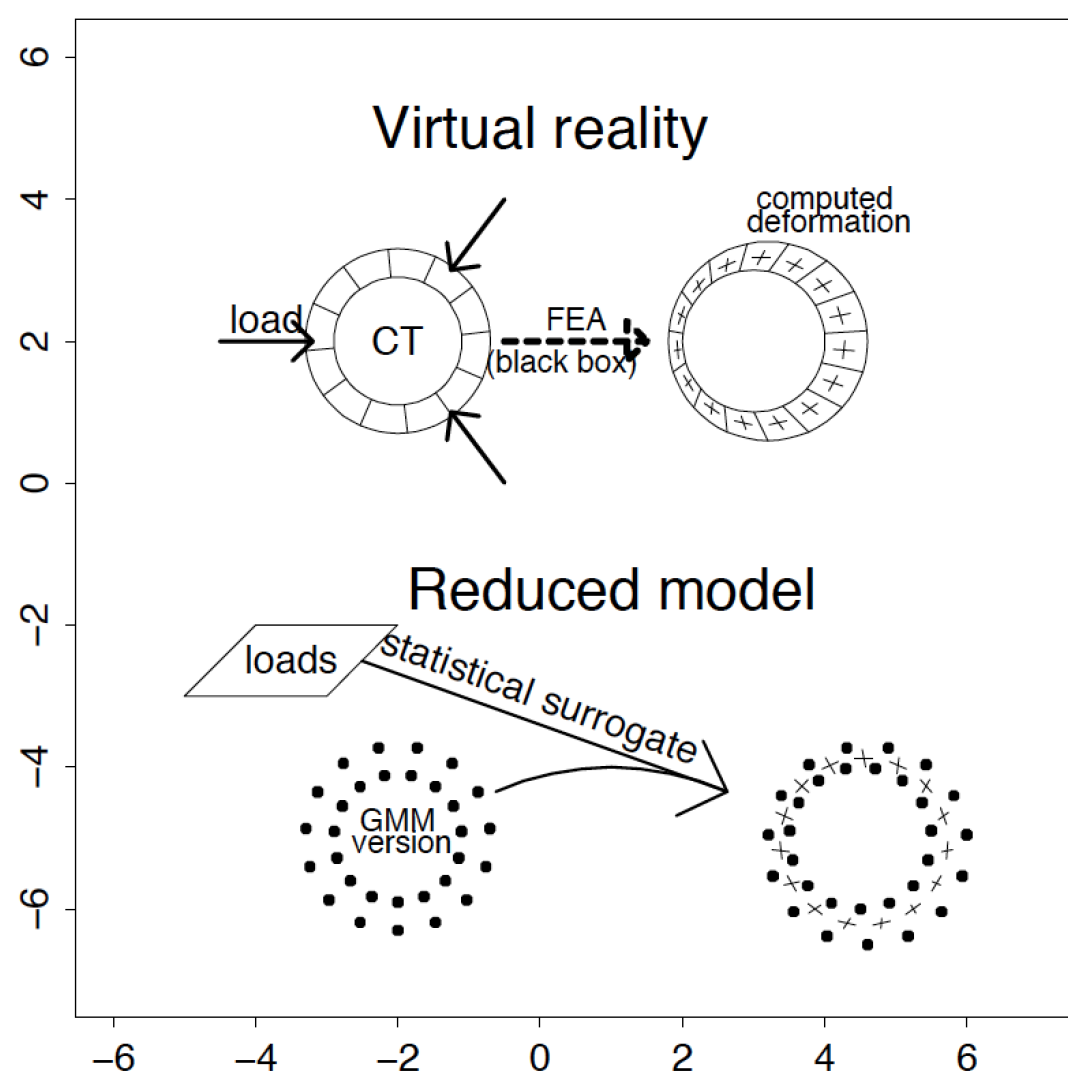


Figure 5: Effect of the supporting angles, β , on large deformation of a rod.

But today's GMM can come nowhere near this degree of validation accuracy.



This is easy to show with toy examples.

We have known ever since Galileo that real beams clamped at one end and loaded vertically at the other end do this:

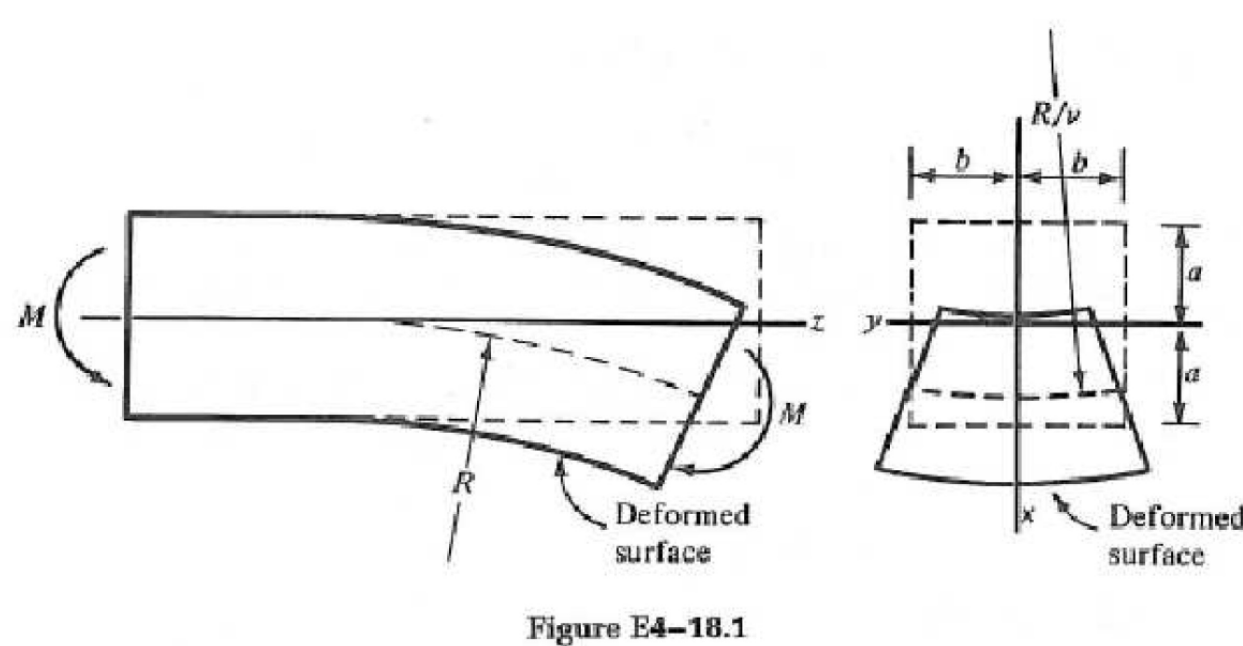
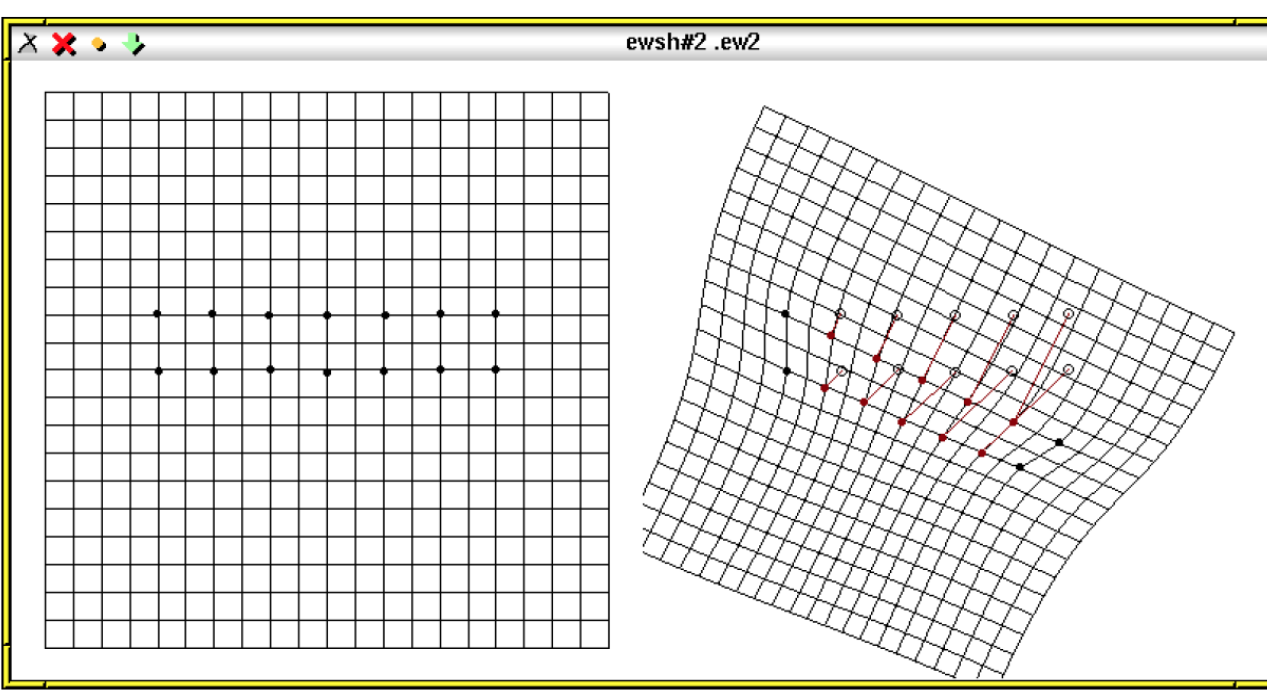
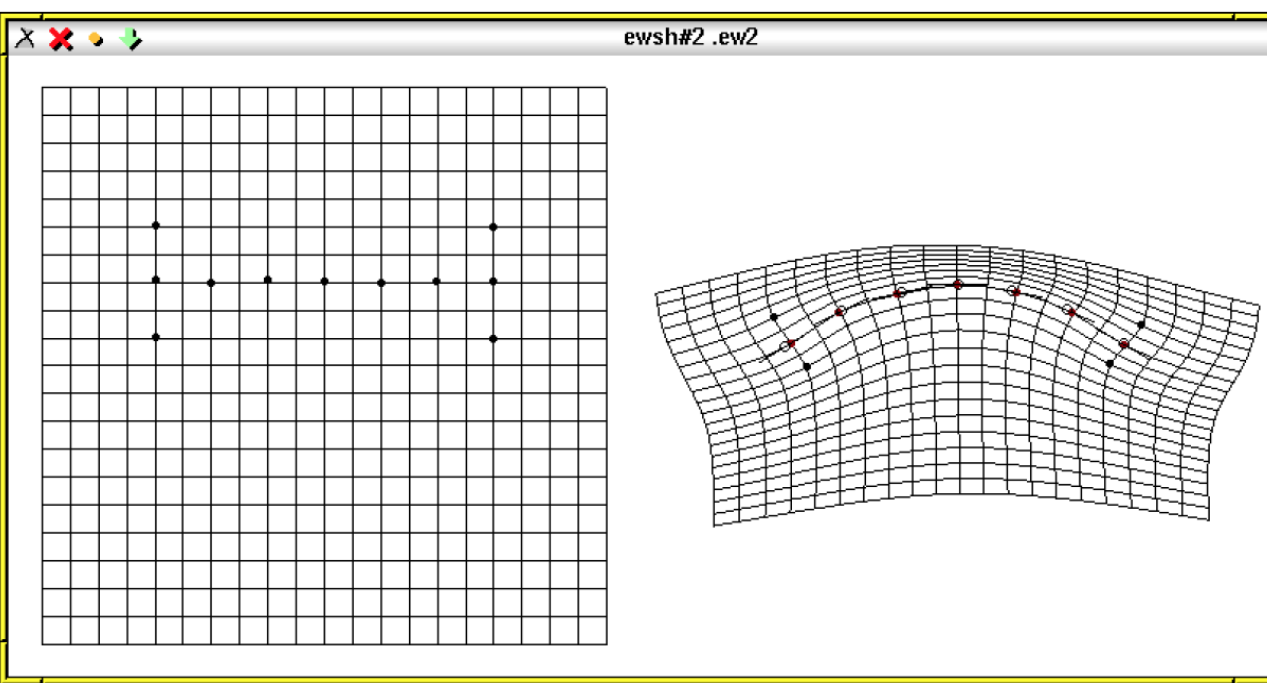


Figure 14-18.1

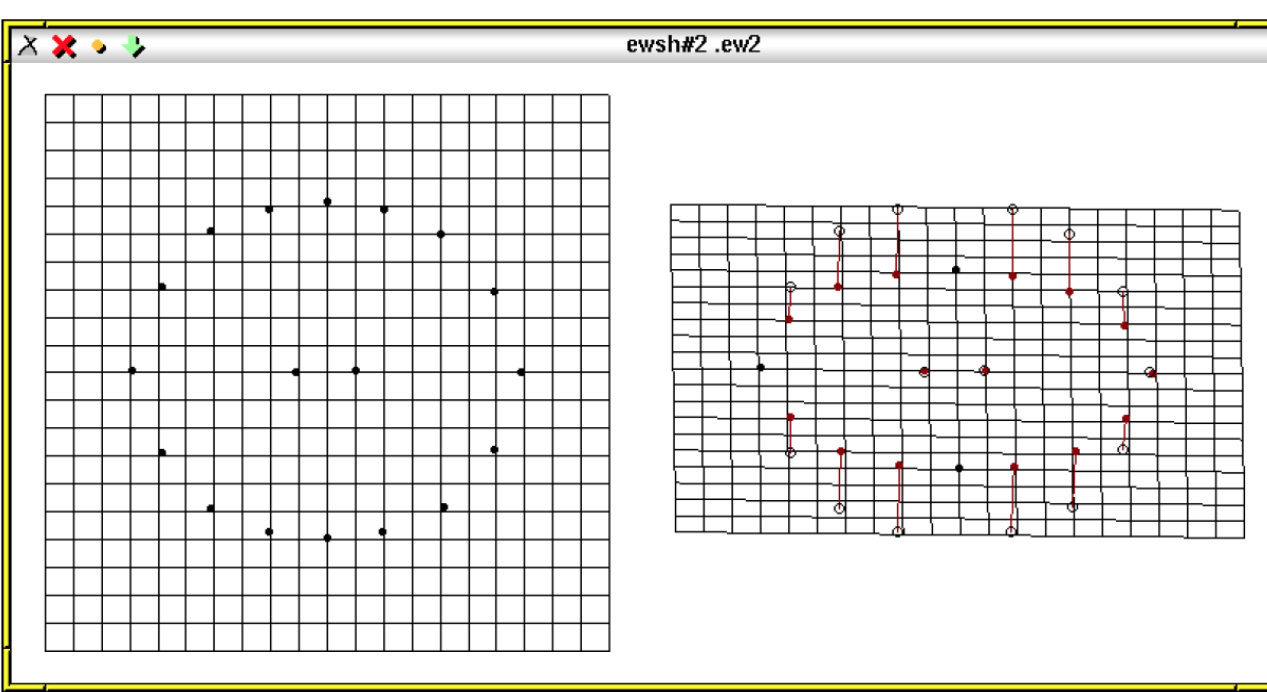
But GMM sees it this way instead:



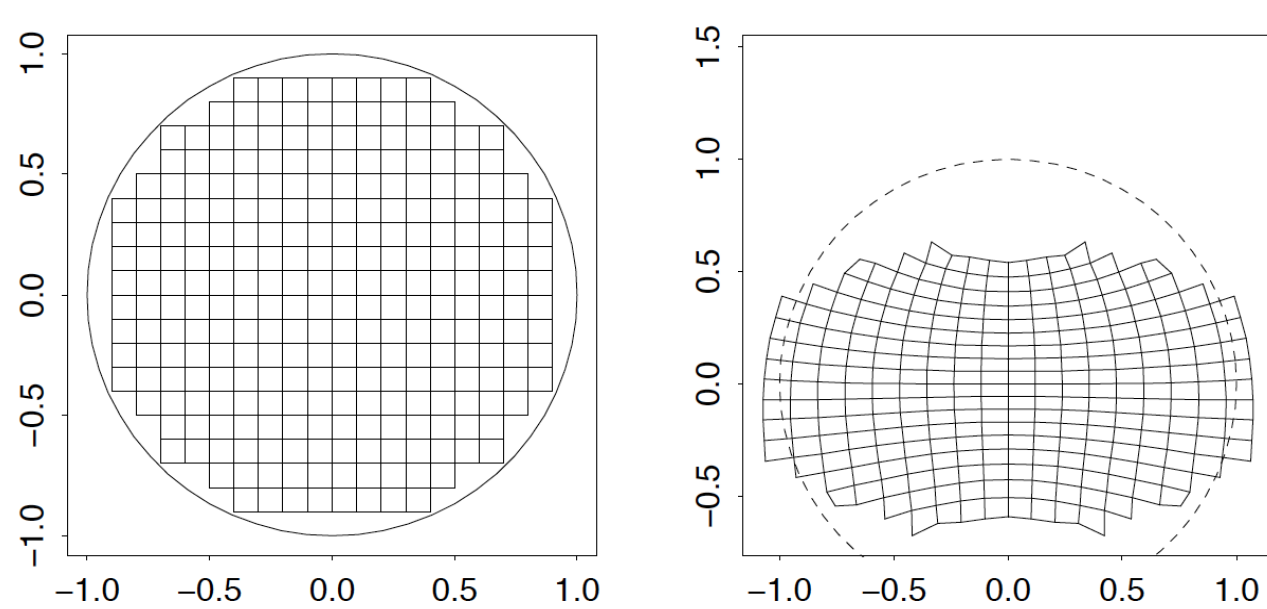
And if we try to enforce the correct bending, it does violence to the substance of the beam itself:



As for uniform transformations, real materials can't actually be forced into such configurations by mere stress. Where GMM has patterns like

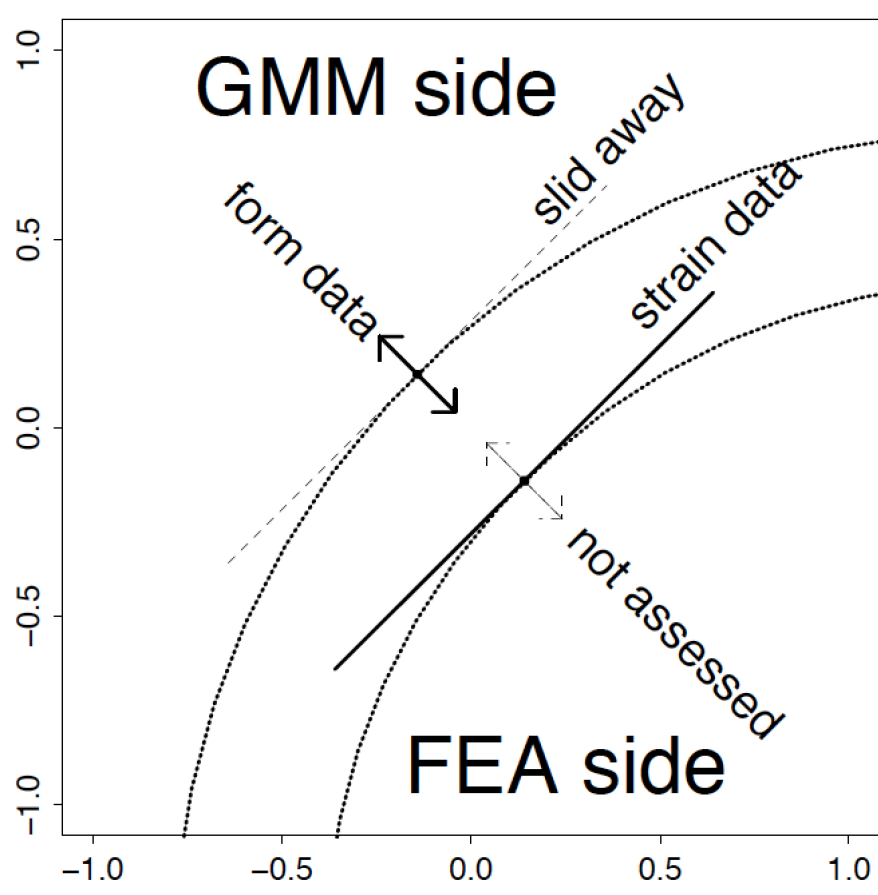


... real material shows patterns like this one instead.

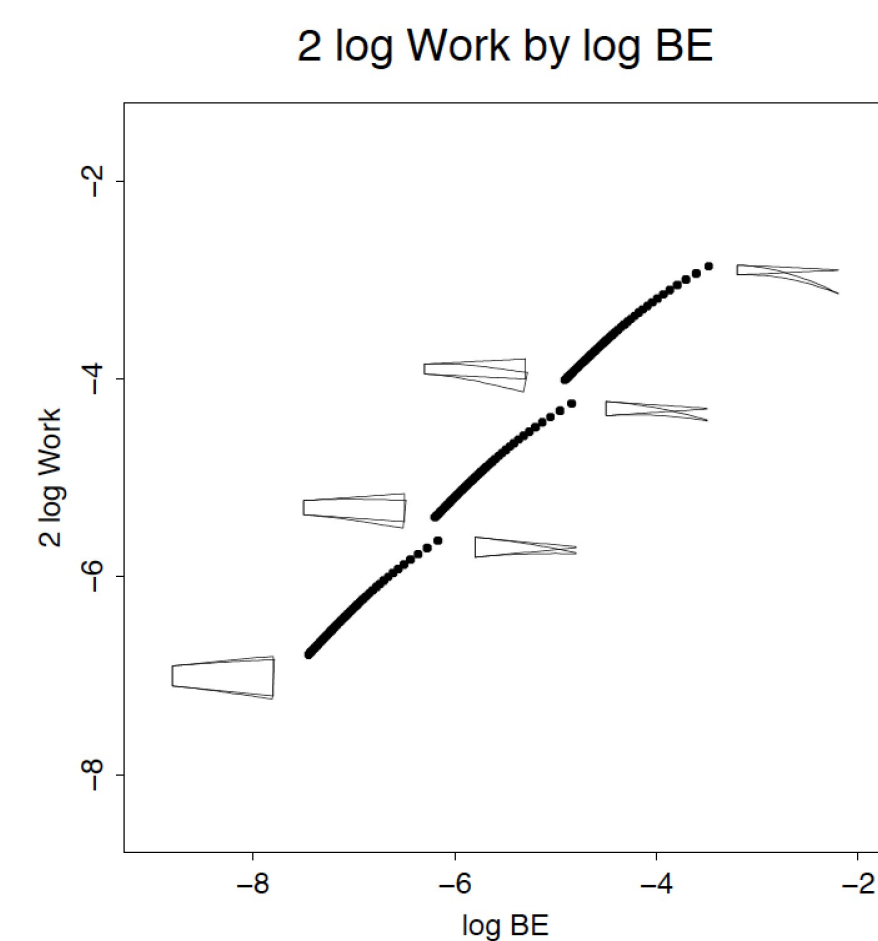


But there is an even more serious problem:

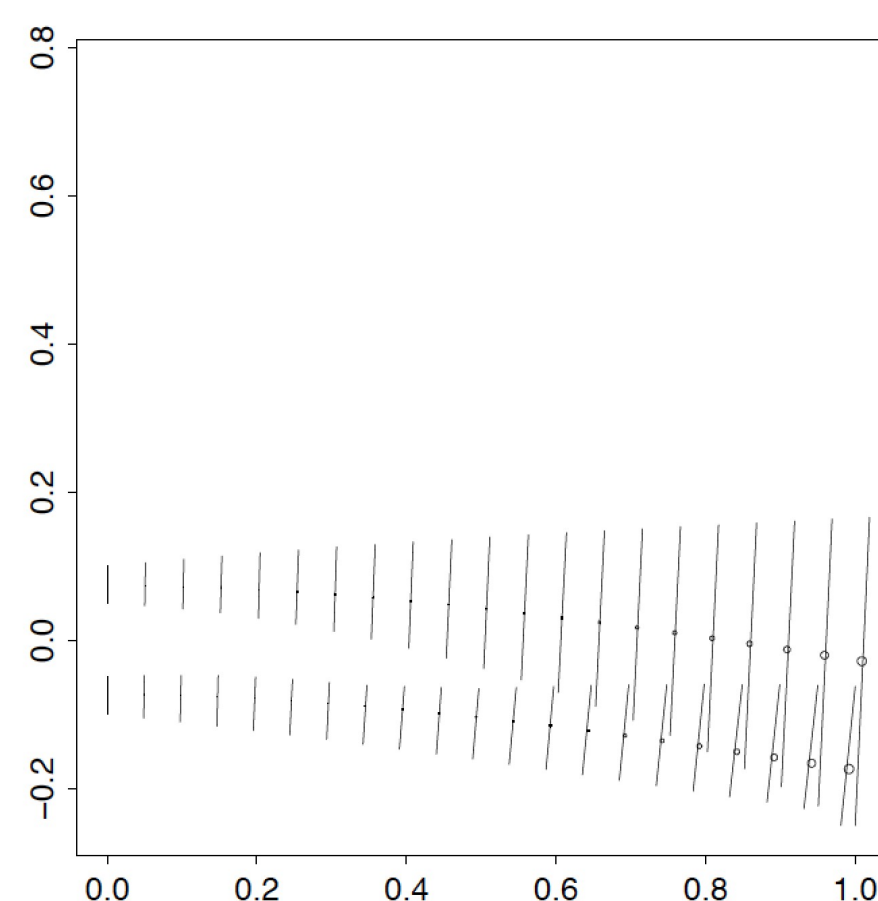
When the topic is the analysis of thin shells or surfaces, such as is usually the case where vertebrate skeletal material is concerned, GMM does not have access to the information it needs to report sensibly on actual material deformations. It is relaxing the coordinates it should be measuring and measuring the coordinates it should be relaxing.



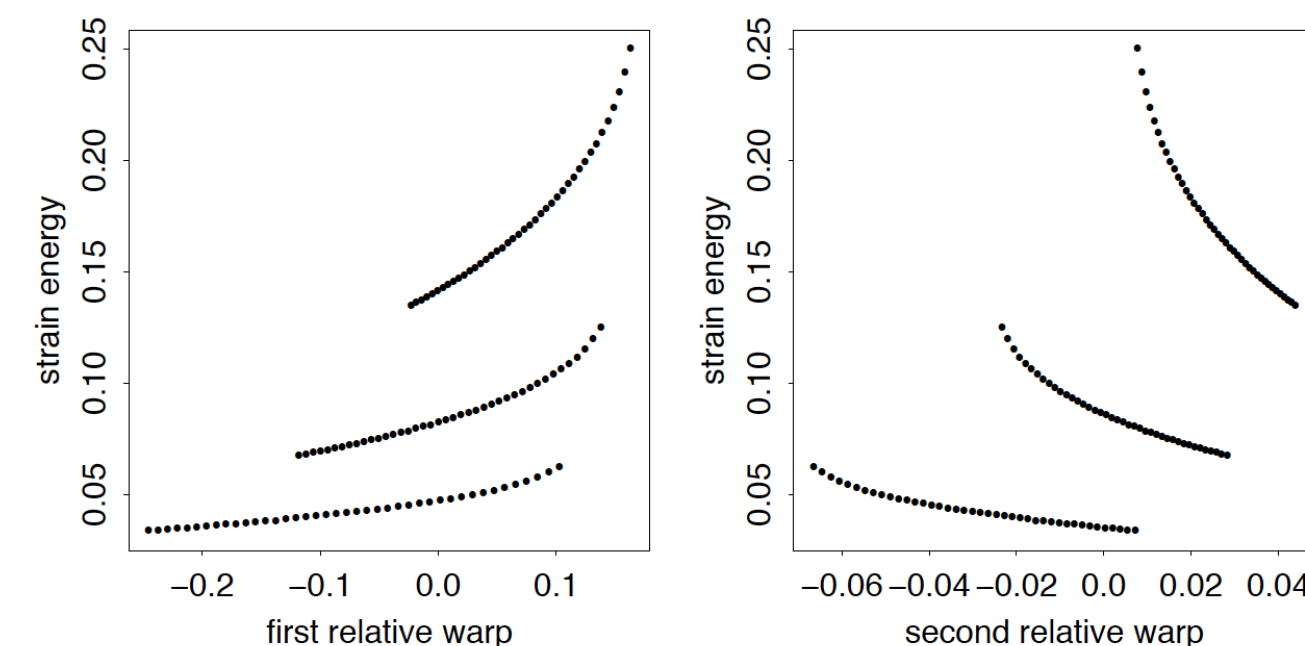
It can easily be shown to follow that GMM's relative warps are of hardly any use for summarizing actual material deformations. Here is the example from Bookstein, 2013: a collection of 123 simulated wedges, varying by thickness and taper, made of uniform material, clamped at one end, and subjected to a uniform load at the other end. GMM and bioengineering certainly have access to the same information, but they use it entirely differently.



Here (drawn as tiny circles) are the prediction errors of the resulting bending --- these look close enough ---



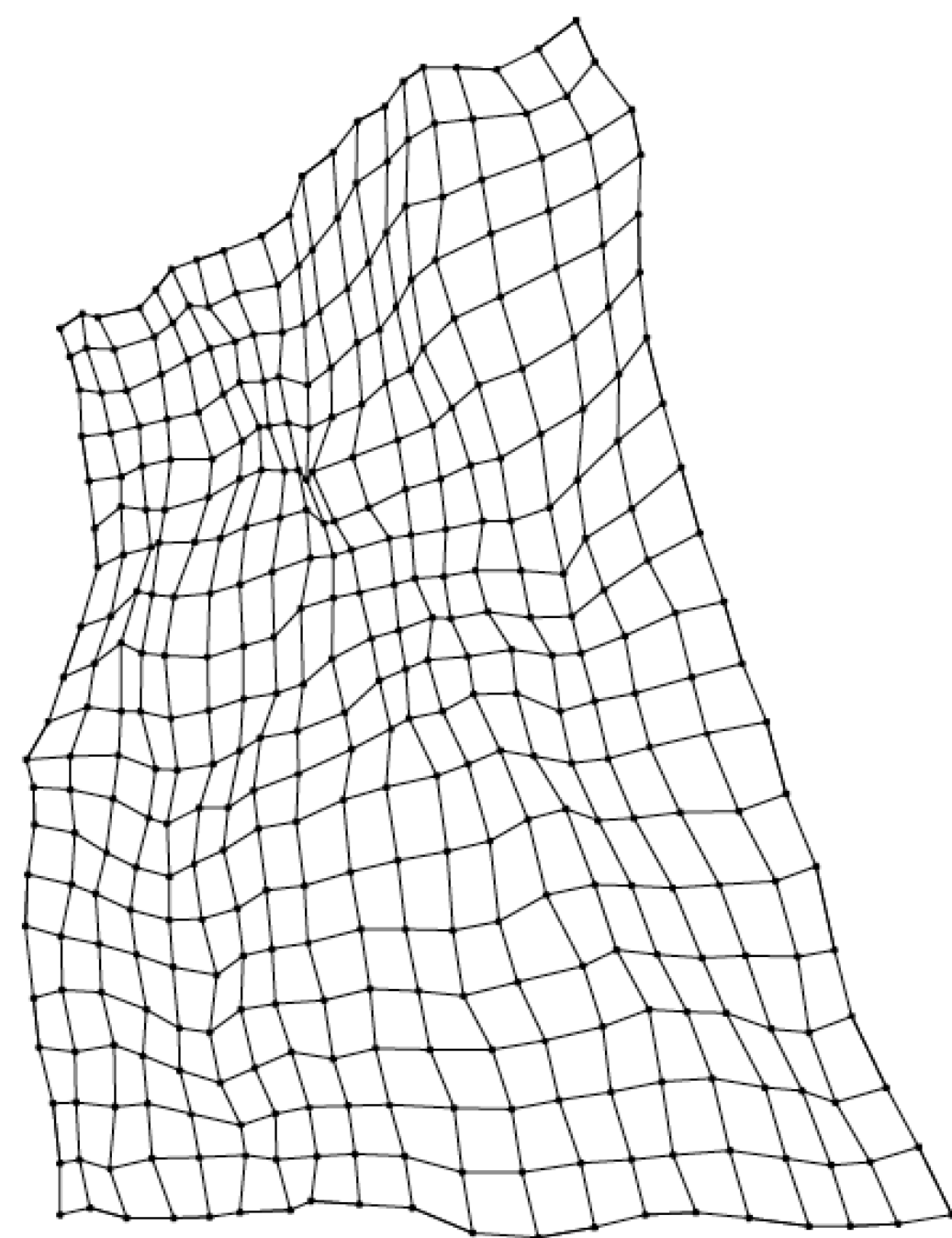
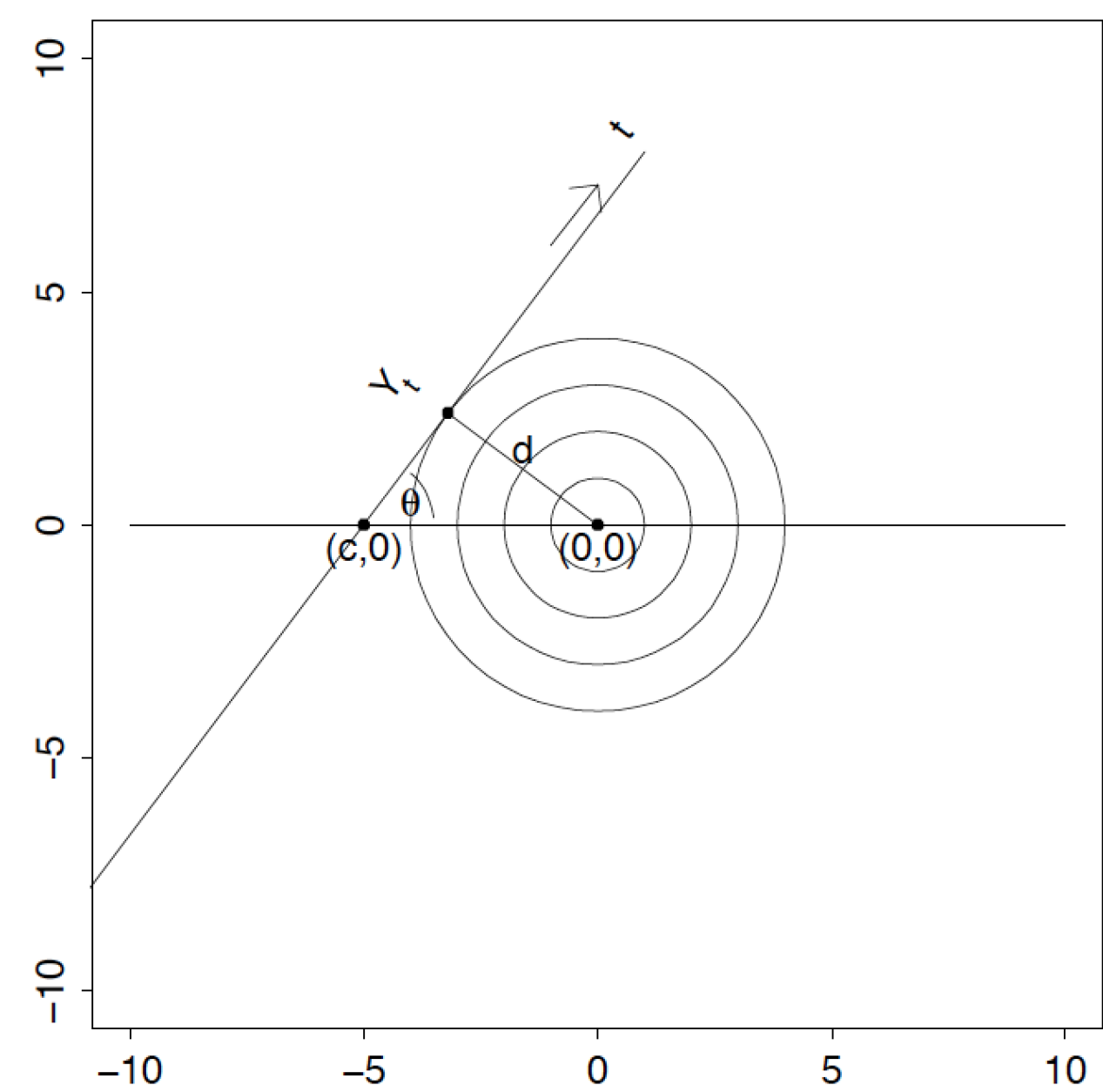
... but the machinery is a prediction entirely oblique to the relative warps themselves, requiring them to be squared and multiplied together --- quite severe algebraic rearrangements are required if we are to arrive back at established bioengineering science.



To phrase this mutual ignorance of methodology even more pessimistically:

A formalism of sliding landmarks that minimize bending energy cannot cope with realistic transformations having a substantial large-scale component.

In fact, sliding cannot even cope with affine transformations, the simplest that we ever see. Somebody should have noticed this before, but perhaps we were all distracted by the sheer computational elegance of being able to slide hundreds of surface semilandmarks at the same time. The paradox is easiest to see if we consider sliding just one single semilandmark, the sliding point on the oblique line of the next figure. This is the classical (Ann Arbor, Vienna) construction of the sliding point Y'_t when it is the only one to slide. It is sent to the point on its line that is nearest to the locus (here set to (0,0)) where it would be placed by the spline computed using solely the ordinary point landmarks (Bookstein, 1991).



Now shear the target form by a uniform (affine) transformation while leaving everything else unchanged. We see that the corresponding SL has not slid correspondingly, because the circles we use to measure distance have not altered their form to the ellipses that correspond to them in the sheared figure.

In other words, our standard semilandmarks are suitable only for mainly nonaffine transformations. These are, in general, the transformations of systematics, not the transformations of growth or functional anatomy (Oxnard, bless him, says exactly this somewhere). **Uniform changes change the metric of morphometrics** according to which we are sliding the semilandmarks in the first place. The current formalism treats the metric as invariant regardless of finite strains; this seems inappropriate in any biomaterial science where finite strain is either explanans or explanandum, which is to say, nearly all of the contemporary quantitative biosciences. Tomorrow's semilandmark methods will need to handle material strains as well as the almost purely nonaffine taxonomic rearrangements with reference to which today's methods were evaluated.

Concluding exhortation

The current formalism of semilandmarks is biomathematically incoherent, and cannot be trusted for any study that extends beyond morphometric data to incorporate insights from any other quantitative branch of biology. **You should see this situation as very troublesome**, troublesome enough to engender substantial skepticism about the pattern claims produced by a GMM analysis except in domains like taxonomy and forensics where they are not confronted with any requirement of concision with reductionist forms of explanation.

Thank you for helping me to think through this far deeper biomathematical issue, which goes well beyond any questions of matrix algebra to the root of what we biologists really mean by "morphological explanation" in a world of images communicated at previously unimaginable levels of detail as pixel or voxel counts surge into the millions or billions. My very last figure, from Bookstein (2009), conveys my current best guess about how to handle all these problems (the problems of an enlightened **systems biology**) better. The map here is an **intrinsic random field** for which the deviation away from affine shape variation of every small element, regardless of shape or orientation, is statistically uniform. This model corresponds much better than any Procrustes-derived formalism to the null model against which I believe we should be reporting shape phenomena beginning about ten years from now. In its stochastics, its geometry, and especially its matrix algebra it is entirely unrelated to anything we are currently doing with our morphometric data.

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