

# 1 Including Earth-structure uncertainties in nonlinear 2 moment-tensor estimations

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## 5 **SUMMARY**

6

7 Earthquake-source parameters can be estimated from seismic waveforms. Since these  
8 data indirectly observe the deformation process, parameters of a physical model that  
9 quantifies the deformation process are inferred through the inverse problem; which  
10 is under-determined. This requires several assumptions to be made about Earth  
11 structure and other aspects that affect the source parameter estimation. These as-  
12 sumptions primarily include a simplified seismic velocity model of the Earth wave-  
13 form and noise models. The specific model choices affect data residuals and can  
14 lead to biased source parameter estimations and unrealistic assessment of the as-  
15 sociated source-parameter uncertainties. While data errors are routinely included  
16 in parameter estimation for full centroid moment tensors, less attention has been  
17 paid to theory errors related to velocity model uncertainties and how these affect

18 the resulting moment-tensor uncertainties. Here, we study non-linear full moment  
19 tensors with several simulated data sets and demonstrate that subsurface structure  
20 uncertainties can profoundly affect parameter estimation and that their inclusion  
21 leads to more realistic parameter uncertainty quantification. We present a solution  
22 to include model errors by estimating non-stationary (non-Toeplitz) error covariance  
23 matrices that lead to appropriate source-parameter estimates and uncertainties. Fi-  
24 nally, we demonstrate the influence of these noise parameterisations on real regional  
25 seismic data of the  $M_l$  4.4, 13 June 2015 Fox Creek event, Canada. Including un-  
26 certainties in Earth-structure resulted in robust source parameter estimates in case  
27 the structure was poorly known.

28 **Key words:** Bayesian inference, seismic data, velocity model uncertainties, mo-  
29 ment tensor estimation

## 30 1 INTRODUCTION

31 Seismic crustal deformation processes are routinely monitored by broadband seismic networks.  
32 Initial source analysis is often based on seismic moment-tensor parameters that assume a point  
33 source with fixed location, source-time-function (STF) and simple velocity structure (e.g.,  
34 Sipkin 1982; Koch 1991; Tocheport et al. 2007). These assumptions can result in erroneous  
35 estimates of the parameters of the moment tensor (MT) (Šílen et al. 1992; Kravanja et al.  
36 1999, e.g.). Thus, a more comprehensive approach is to determine the location, the STF  
37 and the parameters of the moment tensor simultaneously (e.g., Kravanja et al. 1999; Wéber  
38 2006; Sigloch & Nolet 2006; Ekström 2006; Ekström et al. 2012; Stähler & Sigloch 2014).  
39 In addition, these source parameters should be quantified not only in terms of their optimal  
40 parameter values, but also in terms of their uncertainties. Uncertainty quantification can be  
41 accomplished by formulating the problem via Bayes' Theorem (e.g., Tarantola 2005; Wéber  
42 2006; Dbski 2008; Stähler & Sigloch 2014; Vackář et al. 2017).

43 The physical processes of earthquake deformation have significant non-linearities in source

44 parameters (Cesca et al. 2016), especially for the origin in space and time, which causes numer-  
45 ical challenges in determining source location and mechanism. In addition, seismic data are  
46 contaminated by various noise sources of natural (e.g., meteorological and oceanic) and human  
47 origins (Bonnetfoy-Claudet et al. 2006). The estimation of noise characteristics is important  
48 to obtain appropriate weights for the data in the parameter inference. A simple approach is  
49 to estimate the pre-event noise variance and to derive a diagonal weight matrix (e.g., Duputel  
50 et al. 2012). To account for data correlations, off-diagonal components of the covariance ma-  
51 trix have been estimated by assuming an exponential decay dependent on the shortest period  
52 of the contained frequency-band (e.g., Holland et al. 2005; Duputel et al. 2012). In addition,  
53 the covariances between seismogram components can be estimated, these can account for the  
54 directionality of seismic noise (Tarantola 2005; Vackář et al. 2017). Accounting for such de-  
55 pendence in noise leads to better estimation of the deformation source parameters and their  
56 uncertainties due to a more rigorous quantification of noise.

57 For inverse problems, it has been shown that both data errors and errors due to as-  
58 sumptions in the model formulation affect parameter uncertainty (Tarantola & Valette 1982).  
59 In source parameter estimation, two significant assumptions are made about the Earth struc-  
60 ture (e.g., Tarantola & Valette 1982; Duputel et al. 2014) and the parameterisation of the  
61 deformation source (e.g., Dettmer et al. 2014; Pugh et al. 2016). However, errors due to these  
62 assumptions have mostly been ignored in source studies (e.g., Hofstetter et al. 2003; Fukuda  
63 & Johnson 2008; Baer et al. 2008; Bathke et al. 2013). Recently, there were improvements  
64 in incorporating uncertainties in the assumed Earth structure into distributed slip-estimates  
65 of extended sources through a prediction covariance matrix. For instance, Yagi & Fukahata  
66 (2011) included an additional Gaussian noise term for teleseismic Green’s functions and it-  
67 eratively estimated a prediction covariance matrix in an optimization scheme employing an  
68 Akaike’s Bayesian information criterion (ABIC). Similarly, Minson et al. (2013) estimated a  
69 scale factor for an identity matrix that treats the variance in Green’s Functions to account  
70 for uncertainty in the subsurface structure in Bayesian inference. With linear perturbations  
71 of the original Green’s functions, a prediction covariance matrix including off-diagonal terms  
72 can be formulated (Duputel et al. 2014). This approach thus includes physical constraints to  
73 improve the robustness of finite-fault inversion (Yagi & Fukahata 2008, 2011; Minson et al.

2013; Duputel et al. 2014). Incorporating a prediction covariance matrix to resolve distributed kinematic rupture parameters for data computed from a synthetic dynamic rupture model, Razafindrakoto & Mai (2014) reported loss in resolution on the kinematic rupture parameters through Bayesian inference by using near-field seismic data. However, they investigated only the effect of the variance in the prediction covariance matrix. In moment tensor estimations the components of the moment tensor can be more robustly estimated by including the location uncertainty of the point source in the inference (Duputel et al. 2012). Hallo & Gallovic (2016) showed that including uncertainties in Earth structure in Bayesian linear moment tensor estimation yields more reliable MT estimates and uncertainties. These developments mostly focused on improving the robustness of determining linearly related source parameters under the premise that the source geometry and location was known (and fixed) *a-priori*. However, it remains unclear if improvements can be achieved when estimating other source parameters that are non-linearly related to the observed waveforms (e. g. source location and geometry) by including uncertainties in Earth structure in the inference.

In this work, we propose a strategy to estimate covariance matrices with respect to uncertainties in Earth velocity models and we show how to include these in Bayesian inference. For simplicity, we approximate the source time function (STF) as a delta function, which is a valid assumption if the source duration is shorter than the shortest periods in the waveforms (Aki & Richards 2002). In synthetic tests we demonstrate the influence of various parameterisations of the covariance matrix on parameter estimates of a full non-linear moment tensor and a non-linear double-couple moment tensor. Finally, we apply the approach to regional seismic data to estimate the source parameters of a full moment tensor for the 13th June 2015, Fox Creek (Canada) event.

## 2 METHODS

This section provides background information on source parameter estimation with Bayesian inference. In particular, we consider how uncertainties in Earth structure (i.e., layer depths and elastic parameters) are propagated to source parameter uncertainties by estimating theory errors in terms of covariance matrices.

## 102 2.1 Bayesian Inference

103 Bayes' theorem (Bayes 1763) has been widely applied to study earthquake-source processes  
 104 (e.g., Tarantola & Valette 1982; Wéber 2006; Monelli & Mai 2008; Fukuda & Johnson 2008;  
 105 Duputel et al. 2012; Minson et al. 2013; Dettmer et al. 2014; Razafindrakoto & Mai 2014;  
 106 Vackář et al. 2017). Recently, we introduced a flexible software for source estimations in  
 107 layered elastic halfspaces with Bayesian inference (Vasyura-Bathke et al. 2019, 2020). Using  
 108 this software, we estimate parameters  $\mathbf{m}$  of nonlinear moment tensor parametrizations using  
 109 seismic data  $\mathbf{d}^{obs}$ , i.e., seismic displacement waveforms at regional distances.

110 Assuming Gaussian-distributed noise on the data, a likelihood function is straightforward  
 111 to formulate. However, since data noise can generally not be determined independently, resid-  
 112 ual errors  $\mathbf{r}(\mathbf{m}) = \mathbf{d}^{obs} - \mathbf{d}(\mathbf{m})$  serve as a proxy. The posterior probability density (PPD) for  
 113 residual errors of  $K$  datasets is given by (Tarantola & Valette 1982)

$$p(\mathbf{m}|\mathbf{d}_{obs}) = c \times p(\mathbf{m}) \times \prod_{k=1}^K \frac{1}{(2\pi)^{N/2} |\mathbf{C}_k|^{1/2}} \exp \left[ -\frac{1}{2} [\mathbf{d}_k^{obs} - \mathbf{d}_k(\mathbf{m})]^T \mathbf{C}_k^{-1} [\mathbf{d}_k^{obs} - \mathbf{d}_k(\mathbf{m})] \right], \quad (1)$$

114 where  $\mathbf{d}_k(\mathbf{m})$  represent predicted seismic data at seismic station  $k$  with  $N$  samples that depend  
 115 on the moment-tensor parameters  $\mathbf{m}$ , and  $c$  is a normalizing constant that is not required here.  
 116 The covariance matrices  $\mathbf{C}_k$  represent the noise statistics, and play an important role in the  
 117 parameter estimation as well as in the uncertainty quantification.

## 118 2.2 Residual error covariance matrix

119 The residual covariance matrices include variances and covariances of the data residuals  $\mathbf{r}_k$ .  
 120 Under the assumption that noise between stations is not correlated, one matrix is required for  
 121 each station. The total covariance matrix  $\mathbf{C}_k$  at station  $k$  is the sum of the data covariance  
 122 matrix  $\mathbf{C}_k^d$  that quantifies measurement errors and the model prediction covariance matrix  $\mathbf{C}_k^t$   
 123 caused by physical and mathematical approximations in the forward model (theory errors),

$$\mathbf{C}_k = \mathbf{C}_k^d + \mathbf{C}_k^t. \quad (2)$$

124 Many moment-tensor studies ignore off-diagonal terms in  $\mathbf{C}_k^d$  as well as the component  
 125  $\mathbf{C}_k^t$  (e.g., Cesca et al. 2017; Ekström 2006; Ekström et al. 2012; Vackář et al. 2017). Then,  
 126 only measurement errors are considered and assumed to be from a stationary, uncorrelated  
 127 random Gaussian process (Fig. 1a). For long-period data, it can be useful to estimate diagonal  
 128 (Toeplitz) covariance matrices (Fig. 1b) with exponential decay depending on the shortest  
 129 period  $t_0$  of the data (Duputel et al. 2012, see Tab. 1). For both types of covariance matrices,  
 130 variances  $\sigma^2$  can be estimated from the recorded signal prior to the first arriving wave of the  
 131 seismic event of interest at any given station. However, it must be ensured that there is no  
 132 source of seismic signal other than background noise present in the estimation data; otherwise  
 133 the variance estimation could be biased.

134 Theory errors due to physical model assumptions made when formulating the geophysical  
 135 inverse problem can also result in source parameter uncertainties that are substantially larger  
 136 than those due to measurement errors (Tarantola & Valette 1982). A significant source of  
 137 theory error is from the source parameterisation. One example of theory error could be a pre-  
 138 defined earthquake hypocentre location for focal-mechanism estimation, but this location is  
 139 inconsistent with the centroid moment-tensor location (Duputel et al. 2012; Ragon et al. 2018).  
 140 Another example is if the STF is assumed to be of particular shape (e.g., triangular) that is  
 141 not sufficiently general to describe the moment release of the source (Stähler & Sigloch 2014).  
 142 Often it is possible to account for such issues by formulating model prediction covariance  
 143 matrices, but this is beyond the scope of this study.

144 Yet another important source of theory error is the representation of Earth structure (Min-  
 145 son et al. 2013). While actual subsurface structure is 3D, anisotropic and heterogeneous, Earth  
 146 structure is most often approximated by an isotropic, horizontally stratified half-space. Here,  
 147 we build on a previously proposed strategy (Tarantola & Valette 1982; Yagi & Fukahata  
 148 2011; Duputel et al. 2014) to include theory error due to Earth-structure assumptions via the  
 149 model prediction covariance matrix  $\mathbf{C}_k^t$ . We assume a horizontally stratified, elastic, isotropic  
 150 half-space with uncertainties in the velocity-depth profile. One approach to estimate  $\mathbf{C}_k^t$  in  
 151 this case is to perturb the Green's Functions that relate changes in velocity profile linearly  
 152 to the displacements at the Earth's surface (Du et al. 1994; Duputel et al. 2014). Therefore,  
 153 we calculate the Green's functions for various velocity models, based on the global reference

154 model AK135 (Kennett et al. 1995) in combination with CRUST2.0 (Bassin et al. 2000) for  
 155 the crustal structure. Layer velocities and depths are varied in the crust by Gaussian pertur-  
 156 bations with 10% standard deviation around the reference model (Mooney 1989) to generate  
 157 an ensemble of Earth structures. From this ensemble,  $N_e$  sets of Green’s functions are com-  
 158 puted and efficiently stored (Heimann et al. 2019). Let  $i$  and  $j$  be indices for the rows and  
 159 columns of the covariance matrix. Then, term  $\bar{\mathbf{d}}_{k,i} = \frac{1}{N_e} \sum_{n=1}^{N_e} \mathbf{d}_{k,i}^n(\mathbf{m})$  is the sample mean over  
 160  $N_e$  predicted data vectors at station  $k$  (a similar term is defined for  $j$ ) and a covariance matrix  
 161  $\mathbf{C}_k^t$  is computed according to (Duputel et al. 2012)

$$\mathbf{C}_{k,ij}^t(\mathbf{m}) = \frac{1}{N_e} \sum_{n=1}^{N_e} (\mathbf{d}_{k,i}^n(\mathbf{m}) - \bar{\mathbf{d}}_{k,i})(\mathbf{d}_{k,j}^n(\mathbf{m}) - \bar{\mathbf{d}}_{k,j}). \quad (3)$$

162 This model-prediction covariance matrix needs to be computed with respect to source pa-  
 163 rameters  $\mathbf{m}$  while predicted data  $\mathbf{d}_k^n$  are computed for each realization of Earth structure  
 164  $n$  (sets of Green’s functions) and for each seismic station  $k$ . This covariance matrix  $\mathbf{C}_k^t$  can  
 165 be included in the likelihood function for inference following eqns. 1 and 2. Such formulation  
 166 implies computing the synthetic seismic waveforms for each variation in the Earth structure  
 167 (Fig. 2). As it is prohibitively expensive to calculate a realization of  $\mathbf{C}_k^t$  in each iteration of a  
 168 Monte Carlo algorithm, we assume that  $\mathbf{C}_k^t$  changes less rapidly than the source parameters  $\mathbf{m}$   
 169 in the sampling algorithm and we update it only periodically (Duputel et al. 2014). This ap-  
 170 proach accounts for errors in subsurface structure in addition to data errors in the estimation  
 171 of source-parameters and their uncertainties. Figure 1 (c & d) demonstrates that theory errors  
 172 due to Earth structure result in non-stationary covariance matrices with time-dependent error  
 173 statistics.

174 Such calculation of  $\mathbf{C}_k^t$  is computationally very expensive and depends on the assumed  
 175 variability of the Earth structure. If this variability is poorly known, the approach may result in  
 176 over- or underestimated parameter uncertainties. An alternative approach is to estimate non-  
 177 stationary/non-Toeplitz covariance matrices  $\mathbf{C}$  (Fig, 1e)) based on data residuals (Dettmer  
 178 et al. 2007). This approach naturally includes both data and theory errors, is fast and non-  
 179 parametric, but has the limitation of depending on an initial assumption of uncorrelated  
 180 errors. The non-stationary/non-Toeplitz matrix depends on the forward model and can be

181 computed from parameters estimated initially assuming uncorrelated stationary errors. Here,  
 182 we do not rely on that initial assumption. However, some problems may exhibit convergence  
 183 issues when this assumption is not relied on.

184 In the following we use the terms: *variance*, *exponential*, *variance\_cov*, *exponential\_cov*  
 185 and *non-Toeplitz* to distinguish between the different covariance parameterisations described  
 186 above and listed in Tab. 1.

### 187 3 SIMULATION RESULTS

#### 188 3.1 Simulated Data

189 To demonstrate the effect of the covariance matrix parameterisation and the influence of  
 190 including velocity model uncertainties in earthquake source-parameter estimations, we present  
 191 two simulated test cases. We generate two sets of simulated seismic displacement waveforms  
 192 based on two different Earth structures (Tab. 2, Fig. 2a, blue and red lines) for a double-couple  
 193 moment-tensor source (Tab. 3). We refer to these Earth structures as *reference structures* in  
 194 the following. For each test case we estimate the source parameters of a full moment tensor  
 195 using the simulated data with the five different covariance matrix parametrizations (Tab. 1,  
 196 Sec. 2.2).

197 In these test cases, we simulate theory errors due to unknown Earth structure by assuming  
 198 a different Earth structure for the source estimations than that of the reference model. We  
 199 refer to this modified structure as the *estimation structure*. If no local Earth model is available  
 200 in the study region, one would typically use some global model for the estimation. Here, we  
 201 employ the global AK135 velocity model (Kennett et al. 1995) in combination with CRUST2  
 202 (Bassin et al. 2000) (Fig. 2a)) as the estimation structure for each test case. In the first test  
 203 case, case 1, the reference structure has the same number of layers as the estimation structure,  
 204 but layer velocities and depths differ  $< 10\%$  (Tab. 2, Fig. 2a). In the second case, case 2, the  
 205 reference structure (Hofstetter et al. 2003) differs significantly from the estimation structure  
 206 with a different number of layers, layer velocities and depths (Fig. 2a).

207 We created the reference synthetic kinematic displacements for both test cases with fre-  
 208 quencies up to 2 Hz for ten seismic stations at regional epicentral distances (up to 1000 km)



209 (Tab. 3, Fig. 3). We added uncorrelated, Gaussian-distributed noise with a variance of 5% of  
 210 the maximum waveform amplitude for each station. We filtered the data between 0.01 and  
 211 0.1 Hz and rotated waveform components to transverse and vertical directions to estimate  
 212 the moment-tensor parameters and its centroid location. For each test case, we estimated  
 213 marginal distributions of source parameters while only changing the noise parameterisation  
 214 (Fig. 1, Tab. 1), to demonstrate the influence of  $\mathbf{C}$  on the results. Following the procedure  
 215 in Sec. 2.2, the estimation structure was randomly perturbed 20 times to estimate  $\mathbf{C}_k^t$  in the  
 216 course of the sampling.

### 217 3.2 Results

218 For case 1 (small theory errors), estimation results are summarized in Fig. 4 in terms of  
 219 posterior marginal probability densities. A notable observation is that when only applying  $\mathbf{C}_k^d$   
 220 (i.e., ignoring theory error), the ranges of values obtained by the estimation do not include  
 221 true parameter values. This result shows a significant limitation of applying only measurement  
 222 errors in the estimation. In particular, the *exponential* noise parameterisation performs poorly  
 223 and only the centroid location shows reasonable estimates. The variance parameterisation  
 224 performs better, but marginals of the location parameters exhibit significant bias, while some  
 225 moment-tensor components are resolved (e.g.,  $m_{ee}$ ,  $m_{ne}$ ).

226 Including the  $\mathbf{C}_k^t$  term leads to increased width of the posterior marginals, but more  
 227 importantly, both noise parameterisation types (*variance\_cov* and *exponential\_cov*) resolve all  
 228 moment-tensor parameters (Fig. ,4). However, the location marginals are significantly wider  
 229 than observed for other noise parameterisations. In addition, the true value of north-shift  
 230 is not recovered when using *variance\_cov*. The *non-Toeplitz* parameterisation also resolves  
 231 the parameters, although in some instances, true parameter values are in the tail of the  
 232 marginals (e.g., north-shift,  $m_{nd}$ ,  $m_{ed}$ ). The centroid time is poorly recovered by all other  
 233 noise parameterisations.

234 The results for case 2 (large theory errors) are summarized in Fig. 5. Here, it is clear  
 235 that only using  $\mathbf{C}_k^d$  causes significant errors and true parameter values are rarely recovered  
 236 (*variance* and *exponential* results in Fig. 5). The marginals exhibit even stronger biases with  
 237 respect to the true values. While the location parameters (east-shift, north-shift and depth)

238 are recovered by the *exponential* parameterisation in case 1, these are biased here. The moment  
 239 tensor components are not recovered in either case.

240 Including  $\mathbf{C}_k^t$  has the noticeable effect of substantially widening marginals (*exponential\_cov*  
 241 and *variance\_cov* results in Fig. 5), like for case 1. Only some of the marginals include the  
 242 true value for these parameterisations (e.g.,  $m_{nn}$ ,  $m_{ee}$ ), while many marginals are biased and  
 243 the true values are not recovered. In contrast, the *non-Toeplitz* parameterisation recovers true  
 244 values appropriately and with low uncertainty for most parameters. The centroid time is poorly  
 245 recovered for all parametrizations, but magnitude is well recovered with all parameterisations,  
 246 except for the *variance*, which underestimates.

### 247 3.3 Residual Analysis

248 To increase confidence in the estimation results, we analyze the statistics of the data residuals.  
 249 Since we assume Gaussian-distributed residuals with some covariance matrix (eq. 1), both  
 250 Gaussianity and randomness of standardized residuals should be tested. Standardized residuals  
 251 are obtained by scaling raw residuals with their covariance matrix. That is to say,  $\hat{\mathbf{r}}_k =$   
 252  $\mathbf{L}_k^{-1} \mathbf{r}_k$ , where  $\mathbf{L}_k$  is the lower triangle of the Cholesky decomposition of the total covariance  
 253 matrix  $\mathbf{C}_k = \mathbf{L}_k \mathbf{L}_k^T$ . If the covariance matrix applied in the estimation agrees well with the  
 254 actual correlations, the standardized residuals are uncorrelated Gaussian distributed with  
 255 unit variance. That is to say, standardized residuals should be from an uncorrelated random  
 256 process, which can be assessed by considering their auto-correlations and histograms. Ideally,  
 257 the auto-correlation functions should exhibit a sharp central peak and no or small sidelobes.  
 258 Histograms should agree closely with a Gaussian PDF with unit variance (Dettmer et al.  
 259 2008).

260 Histograms of standardized residuals for cases 1 and 2 (Fig 6, station-individual histograms  
 261 Supplemental Figs. S6-S10) show that for the parameterisations of *variance* and *exponential*  
 262 the assumption of Gaussianity of residuals is not met in the estimation. These distributions  
 263 are more heavily tailed and peaked than Gaussian distributions. Including,  $\mathbf{C}_k^t$  vastly improves  
 264 this issue and the standardized residuals are more Gaussian. In particular, peak height is re-  
 265 duced (i.e., reduced overfitting of data). However, the distributions exhibit extensive tails with  
 266 large standard deviations. The *variance\_cov* performed better than the *exponential\_cov* in this

267 case, while the *non-Toeplitz* parameterisation shows standardized residuals with satisfactory  
 268 Gaussianity.

269 The station-individual autocorrelations show that parametrizations *variance* and *expo-*  
 270 *ponential* have long-wavelength sidelobes (Supplemental Figs. S1, S3). This means that residuals  
 271 contain significant residual correlations that the covariance model in the estimation could not  
 272 capture. Including  $\mathbf{C}_k^t$  reduces the residual correlation for both parametrizations (Supplemen-  
 273 tal Figs. S2, S4). The *non-Toeplitz* covariance accounts for most correlations and standardized  
 274 residuals appear close to random white noise (Supplemental Fig. S5). This result suggests that  
 275 *non-Toeplitz* covariance matrices produce results that are most consistent with the assump-  
 276 tions made in the estimation and can successfully address problems with significant theory  
 277 error.

### 278 3.4 Moment tensor decompositions

279 To evaluate the focal-mechanism representation of the sampled moment-tensor components,  
 280 moment-tensors can be decomposed into isotropic and deviatoric components (Jost & Her-  
 281 rmann 1989). The deviatoric component can be split further into the compensated linear  
 282 vector dipole (CLVD) and double-couple (DC) components. We applied such a decomposition  
 283 to the moment tensor components of the PPDs of both setup cases for each noise parame-  
 284 terisation. In general, the different percentages of the MT components vary between different  
 285 noise parameterisations.

286 For case 1, the differences are noticeable, e.g., *variance* and *exponential* show isotropic  
 287 components between  $\sim 5$  and  $\sim 10$  percent, respectively. Significant CLVD components of up  
 288 to  $\sim 20$  and  $\sim 25$  percent were estimated by using the *exponential* and *exponential\_cov* noise  
 289 parameterisations, respectively (Fig. 7a). For case 2, *exponential* and *exponential\_cov* show  
 290 noticeable isotropic components, while the CLVD component of the *variance\_cov*, *exponential*  
 291 and *exponential\_cov* noise parameterisations is significant (Fig. 7b).

292 Since the target source was a pure double-couple moment tensor, it is obvious that theory  
 293 errors cause significant, erroneous CLVD and isotropic MT components if the noise param-  
 294 eterisation of the covariance matrix is inappropriate. In this regard, the *non-Toeplitz* noise  
 295 parameterisation outperformed all the other parameterisations with overall the smallest errors

296 in estimating isotropic and CLVD components for both cases. However, it is worth noting that  
 297 the *variance* noise parameterisation is the second best.

### 298 **3.5 Double-Couple Moment Tensors**

299 Sometimes, moment tensors are estimated under the assumption of a pure double-couple model  
 300 for the earthquake. This assumption removes the possibility estimating erroneous isotropic or  
 301 the CLVD components. Consequently, the estimation may be more successful as long as this  
 302 assumption is consistent with the actual rupture mechanism. Figure 8 presents results (Tab. 2)  
 303 for assuming a pure double-couple moment tensor model. For case 1, *variance* and *exponential*  
 304 parameterisations cannot recover the true values (Fig. 8). Including  $\mathbf{C}_k^t$  allows to recover true  
 305 parameters, but neither location nor time parameters are estimated well. While parameters are  
 306 not fully recovered by the *exponential* parameterisation, there is a vast improvement when  
 307 including  $\mathbf{C}_k^t$  (e.g., rake, time, depth, magnitude). Only the *non-Toeplitz* parameterisation  
 308 recovered the true source mechanism, magnitude and centroid location. The centroid time  
 309 was recovered only by the *exponential\_cov* noise parameterisation.

310 For large theory errors the source mechanism and location could only be recovered by  
 311 the *non-Toeplitz* parametrization (Fig. 9). Including  $\mathbf{C}_k^t$  did not help to reliably recover the  
 312 true parameter values. Only the source magnitude was recovered by most parameterisations,  
 313 except for the *variance* parametrization.

314 Our results show that under the assumption of a double-couple moment tensor, source  
 315 parameters can be biased if correlated, non-stationary data errors are ignored in the noise  
 316 parameterisation of the covariance matrix. Similar to the results for the full moment tensor,  
 317 for small theory errors, including  $\mathbf{C}_k^t$  improved source parameter estimates. For large theory  
 318 errors, only the *non-Toeplitz* parameterisation resolved the true source parameters success-  
 319 fully.

## 320 **4 APPLICATION TO FOX CREEK EARTHQUAKE**

321 This section applies the various approaches to theory-error estimation to a regional earth-  
 322 quake. Regional seismic data are considered for the  $M_1=4.4$  earthquake on 13 June 2015 near

323 Fox Creek, Alberta, Canada (Wang et al. 2016) (Fig. 10). The event is related to hydraulic  
 324 fracturing operations in this area, which was previously seismically relatively inactive (Schultz  
 325 et al. 2015). Thus, the possibility of sizable non-couple source components due to fluid effects  
 326 could be expected, and hence it is justified to do a full moment tensor estimation.

327 We use data from stations up to a distance of 300 km wrt. the event location from the  
 328 gCMT catalog at latitude  $54.102^\circ$  and longitude  $-116.95^\circ$ . We convert the data to displacement  
 329 waveforms, downsample them to 1.0 Hz and rotate them to radial (R), transverse (T) and  
 330 vertical (Z) components. We then estimate parameters (location, MT components, centroid  
 331 time) of a full moment tensor using body waves (band-pass filtered to 0.08-0.3Hz) and surface  
 332 waves (band-pass filtered to 0.04-0.1Hz) for each noise parameterisation (Tab. 2).

333 To test our method we use two reference subsurface structures, a regional structure (Wang  
 334 et al. 2016) and the global AK135 earth structure (Kennett et al. 1995) (Supplemental material  
 335 Fig. S11). Following our procedure from Sec. 2.2, we vary these reference structures 20 times  
 336 each with standard deviations of 15% and 35% for velocity and layer depth values for the  
 337 regional structure and 15% and 10% for the global structure (Supplemental material Fig. S11).

#### 338 4.1 Results

339 For the regional subsurface structure, estimation results are summarized in Fig. 11 in terms of  
 340 marginal probability densities. It is most striking that *variance*, *exponential* and *non-Toeplitz*  
 341 parameterisation show similar results all across parameters. This observation implies that it  
 342 is not necessary to account for non-stationary correlated noise and that the theory error is  
 343 small. Including  $\mathbf{C}_k^t$  into estimation significantly widens the marginals and results in shifts of  
 344 the marginals (e.g. magnitude, depth,  $m_{ne}$ ). By artificially introducing theory error through  
 345  $\mathbf{C}_k^t$  the *variance\_cov* and *exponential\_cov* marginals resemble uncertainty, which in reality may  
 346 not be present, correspondingly we likely overestimated the errors in the regional structure  
 347 (supplementary material Fig. S11a). Consequently, the results become worse accounting for  
 348 theory error in this case when the subsurface structure seemed to be well known.

349

350 For the global subsurface structure, estimation results of *variance* and *exponential* param-  
 351 eterisations show higher magnitude estimates and earlier centroid times as well as shallower

352 source depth (Fig. 12). Results become more consistent including  $\mathbf{C}_k^t$  and *variance\_cov* and  
 353 *exponential\_cov* marginals mostly contain the *non-Toeplitz* marginals. The *exponential\_cov*  
 354 and *variance\_cov* parameterisations lose the source depth resolution. This indicates that the  
 355 global structure contains significant theory error for data of the study area and accounting  
 356 for it through  $\mathbf{C}_k^t$  helped in this case.

357 We note that the published solution of Wang et al. (2016) is contained in the marginals  
 358 of *variance*, *exponential* and *non-Toeplitz* by using the regional structure and it is contained  
 359 in the somewhat wider marginals for *variance\_cov*, *exponential\_cov* and *non-Toeplitz* by using  
 360 the global structure.

361 The fit to the data is in this case better for the surface wave arrivals than for the body  
 362 wave arrivals due to the lower frequency content (Fig. 13). Including  $\mathbf{C}_k^t$  mostly leads to larger  
 363 variations in amplitude of predicted waveforms for body wave arrivals (supplemental material  
 364 Fig. S12). Not surprisingly the fit to the data is better when using the regional subsurface  
 365 structure rather than the global subsurface structure (supplemental material Fig. S13).

366 To better visualize and interpret the marginals of the sampled moment tensor components  
 367 we apply moment tensor decomposition (also see Sec. 3.4) for each noise parameterisation and  
 368 subsurface structure (Fig. 14). It is noticeable that in case of a poor choice of noise parameter-  
 369 isation the isotropic component seems to be large, i.e. *variance\_cov* and *exponential\_cov* for  
 370 the regional structure and *variance* and *exponential* for the global structure.

371

372 Wang et al. (2016) report a CLVD component of  $\sim 23 \pm 17\%$  which is lower and more  
 373 uncertain than our estimates obtained using the regional subsurface structure. Using the  
 374 global structure the CLVD component is poorly constrained. If the event was indeed caused  
 375 by hydraulic fracturing a large CLVD component would not be unlikely.

## 376 5 DISCUSSION AND CONCLUSION

377 We investigated the influence of noise parameterisation on the estimated parameters of a  
 378 non-linear full moment-tensor in a layered elastic half-space by means of Bayesian inference  
 379 using synthetic and real seismic data at regional distances. Five different ways of covariance  
 380 estimation were tested in the presence of small and large theory errors caused by assuming a

381 wrong velocity structure of the Earth. Repeated perturbation of the Earth structure model  
 382 and subsequent forward simulation of the seismic waveforms allows to estimate a prediction  
 383 covariance matrix  $\mathbf{C}_k^t$  describing the theory error.

384 Including  $\mathbf{C}_k^t$  in the estimation improves parameter estimates if the velocity-model vari-  
 385 ations that are used for computing  $\mathbf{C}_k^t$  cover the true velocity model (case 1 and Fox Creek  
 386 global). If the true velocity model is not covered by the variations of the velocity models,  
 387 including  $\mathbf{C}_k^t$  into the optimization does not lead to better parameter estimates (case 2).  
 388 Parameter uncertainties also depend on the chosen distribution for velocity and layer depth  
 389 errors employed to compute  $\mathbf{C}_k^t$ . Notably, this likely is a subjective choice with limited infor-  
 390 mation available to aid this process. Depending on the choice of velocity errors, uncertainties  
 391 will likely be larger than for other parameterisations and may be even biased (Fox Creek  
 392 regional).

393 Estimating  $\mathbf{C}_k^t$  with the approach chosen here is computationally expensive as the varia-  
 394 tions in Earth structure require generating the Green's Functions for many velocity profiles.  
 395 To improve the efficiency of computing  $\mathbf{C}_k^t$ , Hallo & Gallovic (2016) developed an approach  
 396 that could allow to update  $\mathbf{C}_k^t$  in every step of the sampling. The method was applied to  
 397 moment tensors assuming known centroid location. However, matrix inversion/decomposition  
 398 is still required and may be computationally costly. Similar to the approach presented here  
 399 their approach also requires calculation of Green's Functions for a distribution of velocity  
 400 profiles which may be difficult to constrain objectively.

401 Errors in Earth structure may lead to correlated data error since data are band limited  
 402 and sampled discretely in space and time (Stähler & Sigloch 2016; Hallo & Gallovic 2016). To  
 403 account for spatially correlated data errors across stations, Stähler & Sigloch (2016) employed  
 404 an empirical likelihood function based on a waveform cross-correlation criterion. Our likelihood  
 405 function is rigorous in that it is formally derived from the assumption of Gaussian-distributed  
 406 residuals but ignores spatial correlations between stations.

407 In conclusion, our results suggest that applying the *non-Toeplitz* covariance matrix param-  
 408 eterisation provides a reliable and, straightforward approach to account for correlated errors  
 409 in source parameter estimation. The results produced with this parametrization performed  
 410 best in the test cases considered in this work. The formulation is non-parametric and therefore

411 fast to compute. Importantly, it intrinsically accounts for all theory errors, including but not  
412 limited to errors due to Earth-structure mismatch and centroid location mismatch.

413 The noise parameterisations presented here are implemented in the open software BEAT (Vasyura-  
414 Bathke et al. 2019, 2020). Users are free to apply BEAT without the need for additional im-  
415 plementation. BEAT also provides the opportunity to apply these noise parametrizations to  
416 rectangular sources and finite fault models.

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425

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**Table 1.** Noise parameterisations used in this study. The data covariance matrix  $\mathbf{C}_k^d$ , can be estimated from waveform data before the arrival time of the event of interest.

NOISE TERISATION	PARAME- TERISATION	COVARIANCE COMPONENTS	MATRIX	COLOR COD- ING	REFERENCES
variance		$\mathbf{C}^d = \sigma^2 \mathbf{I}$		light yellow	
exponential		$\mathbf{C}_{ij}^d = \sigma^2 \exp - \Delta t^{ij} /t_0$		light blue	Duputel et al. (2012)
variance_cov		$\mathbf{C}^d + \mathbf{C}^t$		dark yellow	Tarantola & Valette (1982); Yagi & Fukahata (2011); Duputel et al. (2014)
exponential_cov		$\mathbf{C}_{ij}^d + \mathbf{C}^t$		dark blue	Tarantola & Valette (1982); Yagi & Fukahata (2011); Duputel et al. (2014)
non-Toeplitz		$\mathbf{C}$		red	Dettmer et al. (2007)

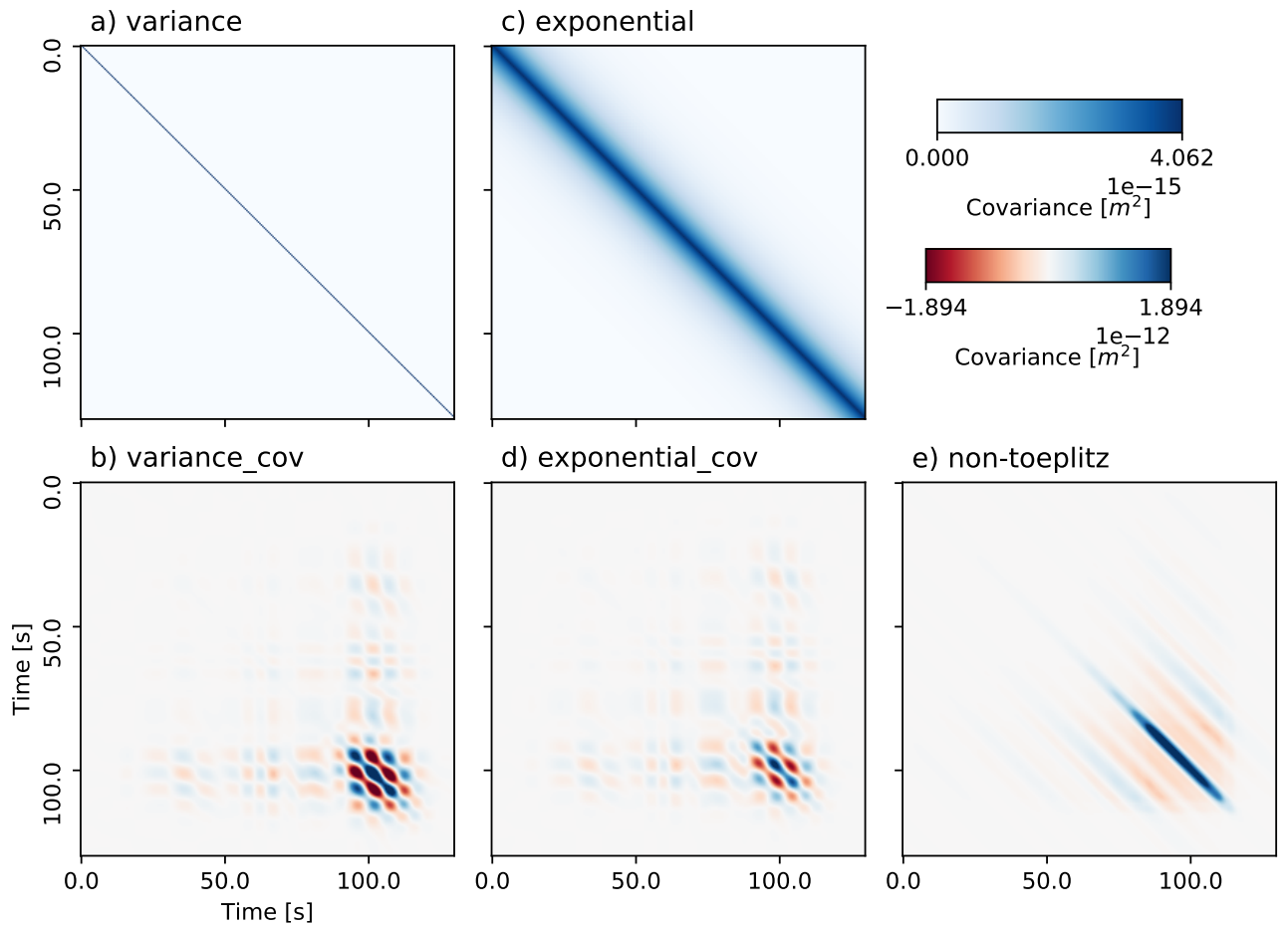
**Table 2.** Synthetic tests setup cases.

SETUP CASE	VELOCITY STRUCTURES	
	REFERENCE	ESTIMATION
1.small theory error	blue	dark gray
2.large theory error	red	dark gray

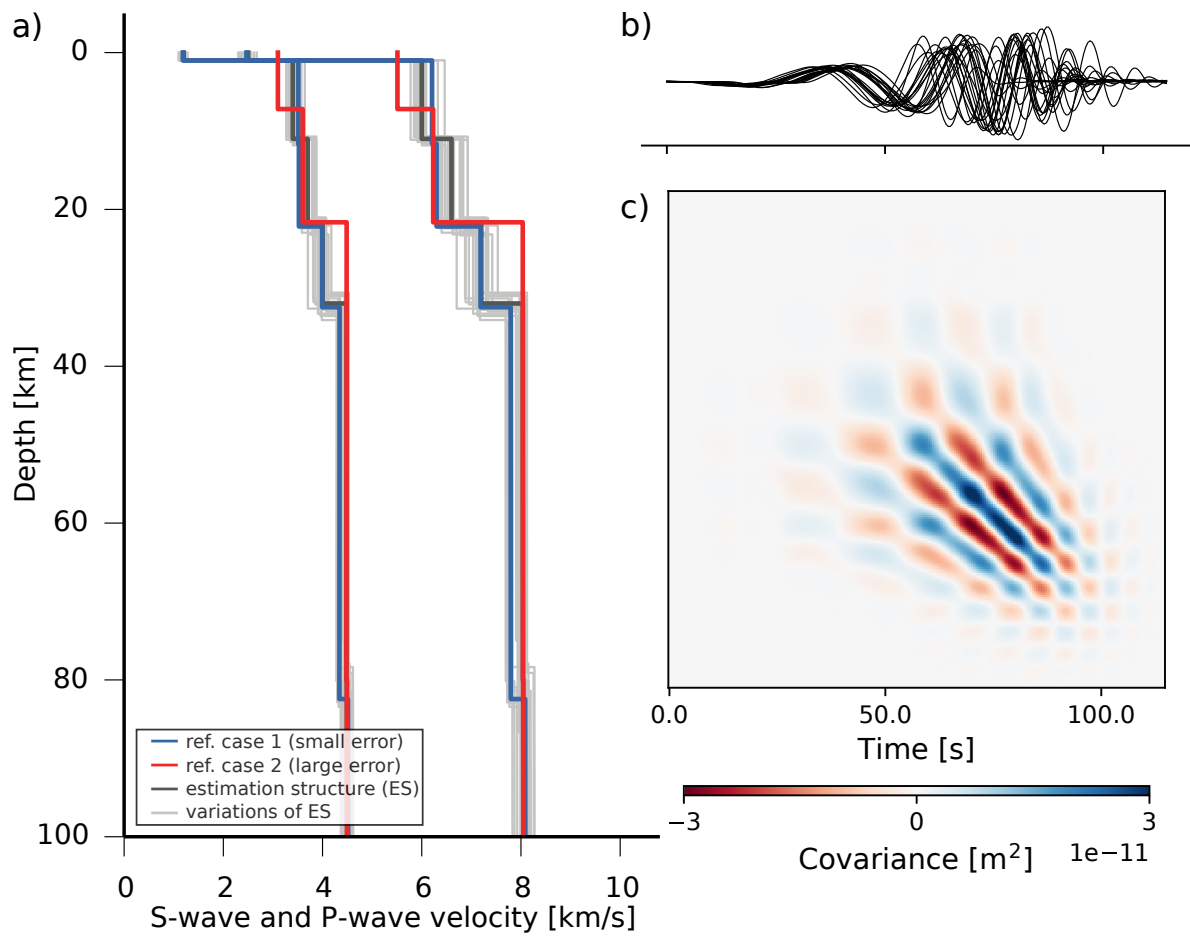
**Table 3.** Target source parameters of the double-couple moment tensor.

SYNTHETIC TESTS				
MOMENT TENSOR				
LOCATION	east-shift [km]	10.0		
	north-shift [km]	20.0		
	depth [km]	8.0		
STRENGTH	magnitude	4.8		
TIMING	source time [s]	-2.7		
MECHANISM	mnn	0.846	strike [deg]	150.0
	mee	-0.759	dip [deg]	75.0
	mdd	-0.087	rake [deg]	-10.0
	mne	0.513		
	mnd	0.146		
	med	-0.257		

541 8 FIGURES

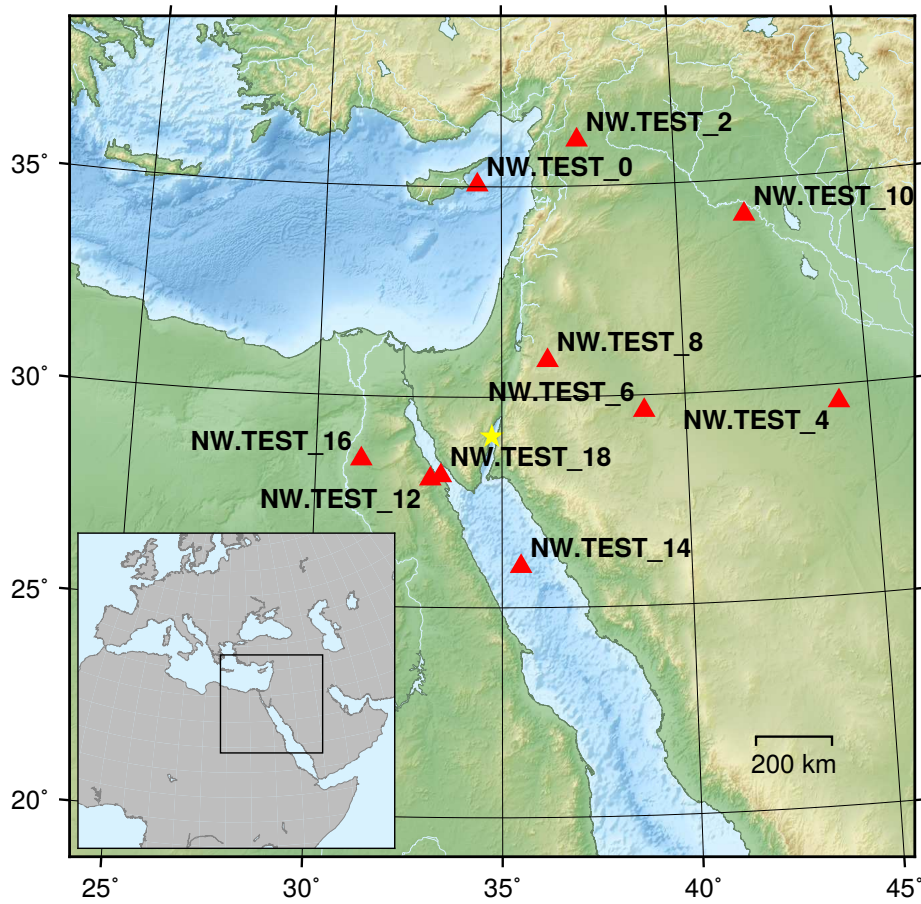


**Figure 1.** Covariance matrixes  $\mathbf{C}$  with different noise parameterisations (Tab.1). The parameterisations in a) and c) comprise only  $\mathbf{C}_k^d$  while b), d) and e) also include  $\mathbf{C}_k^t$ , thus the ranges of covariance matrix values vary significantly.

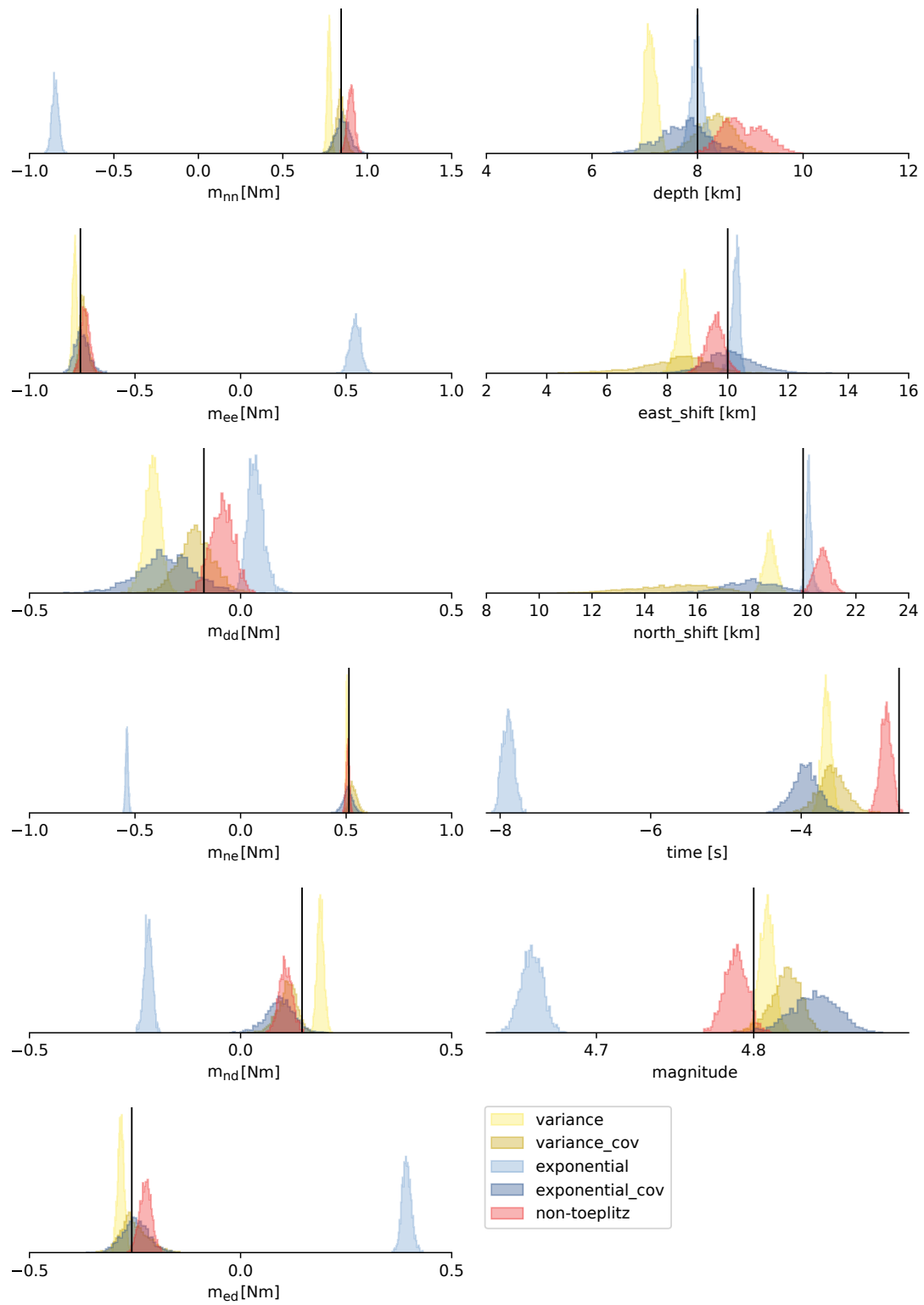


**Figure 2.** Steps to calculate the model prediction covariance; a) velocity model profiles; b) synthetic waveforms (vertical component) for the reference source simulated for each realization of the Earth structures; c) Covariance matrix  $C_k^t$  of seismic traces from b) following eq. 3.

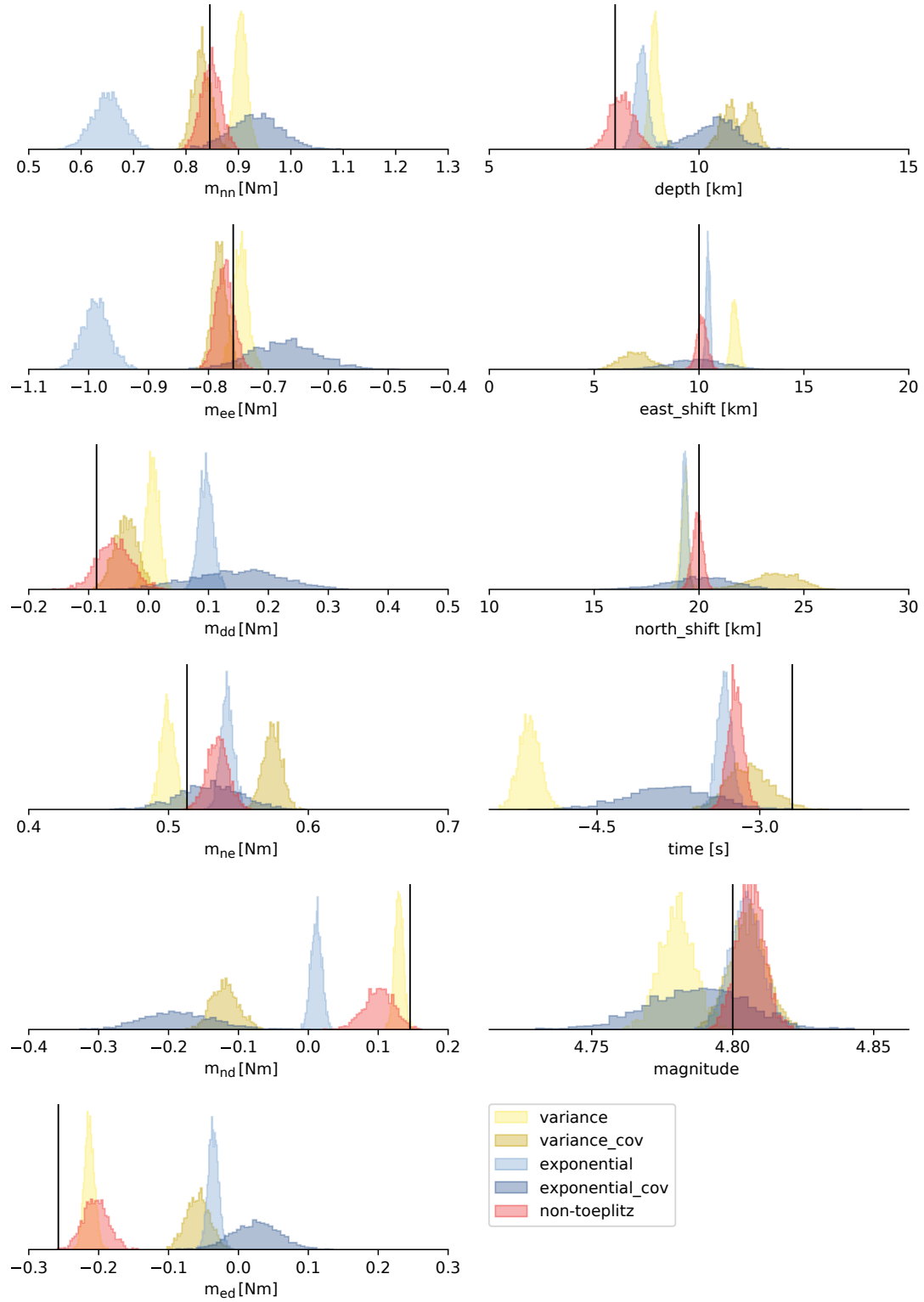




**Figure 3.** Stations (red triangles) used in the synthetic test that simulates a moment tensor optimization at regional distances. Station locations are randomly chosen around the reference event marked by the yellow star. The black box in the inset marks the outline of the station map.

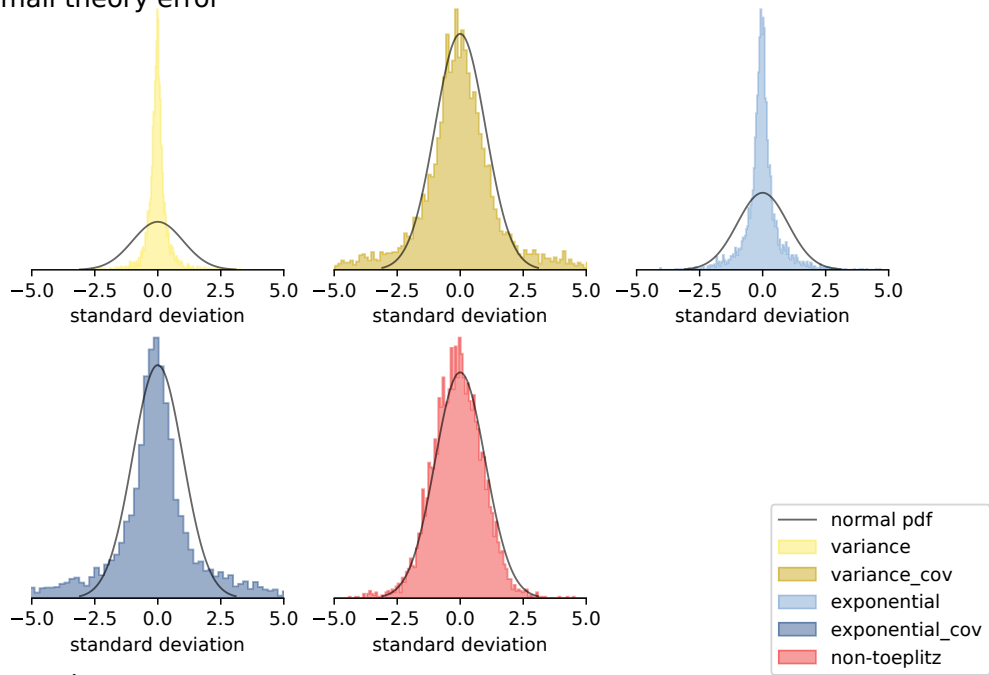


**Figure 4.** Case 1 with small theory error: histograms of the posterior marginal distributions for the parameters of a full moment tensor. The different colors of the histograms mark the results for different noise parameterisations (see legend). (Table 2).

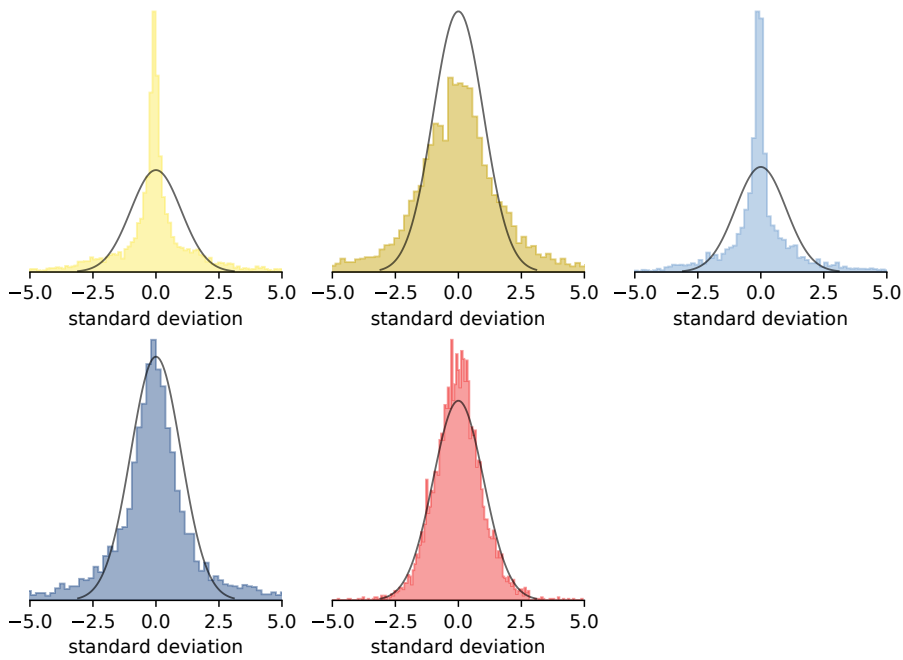


**Figure 5.** Case 2 with large theory error: histograms of the posterior marginal distributions for the parameters of a full moment tensor. The different colors of the histograms mark the results for different noise parameterisations (see legend). (Table 2).

a) small theory error

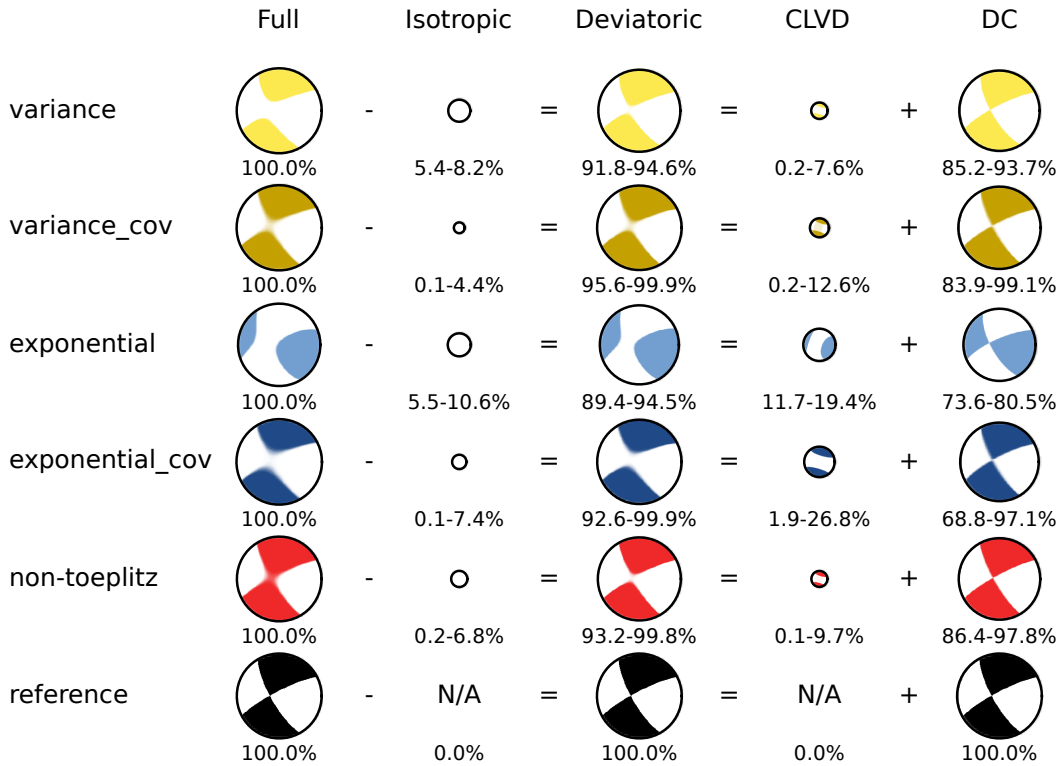


b) large theory error

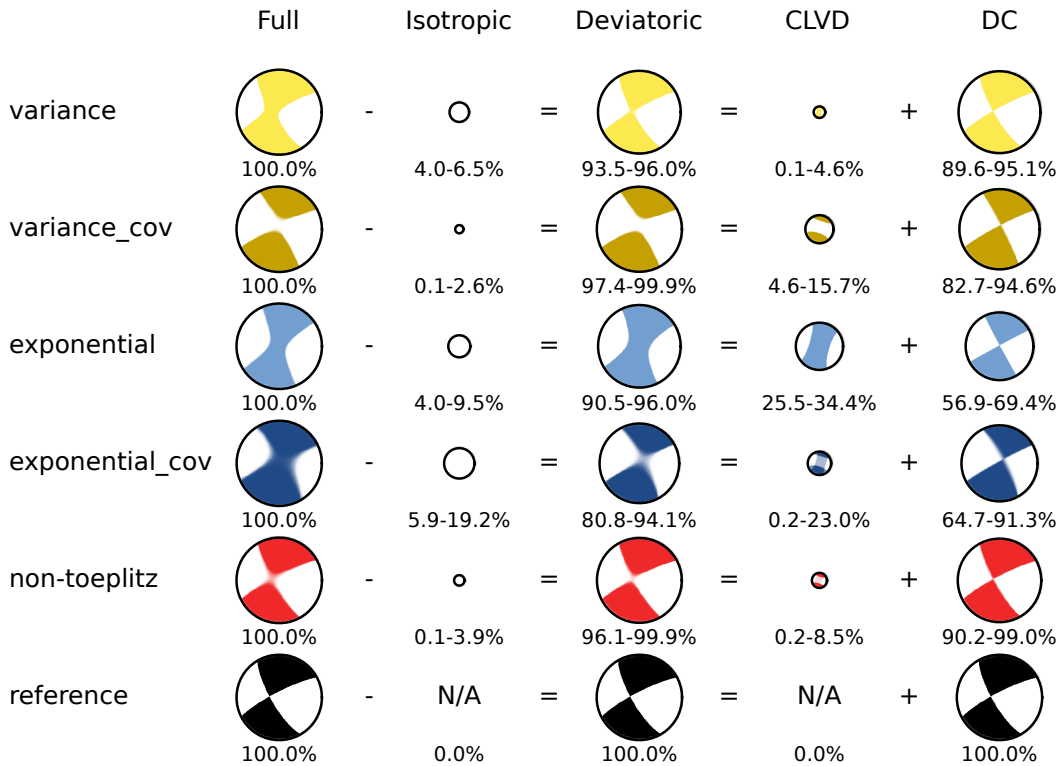


**Figure 6.** Standardized residuals for the different noise parameterisations for a) small theory error and b) large theory error. The black line marks the analytic normal distribution with zero mean and standard deviation of one. All histograms are normalized.

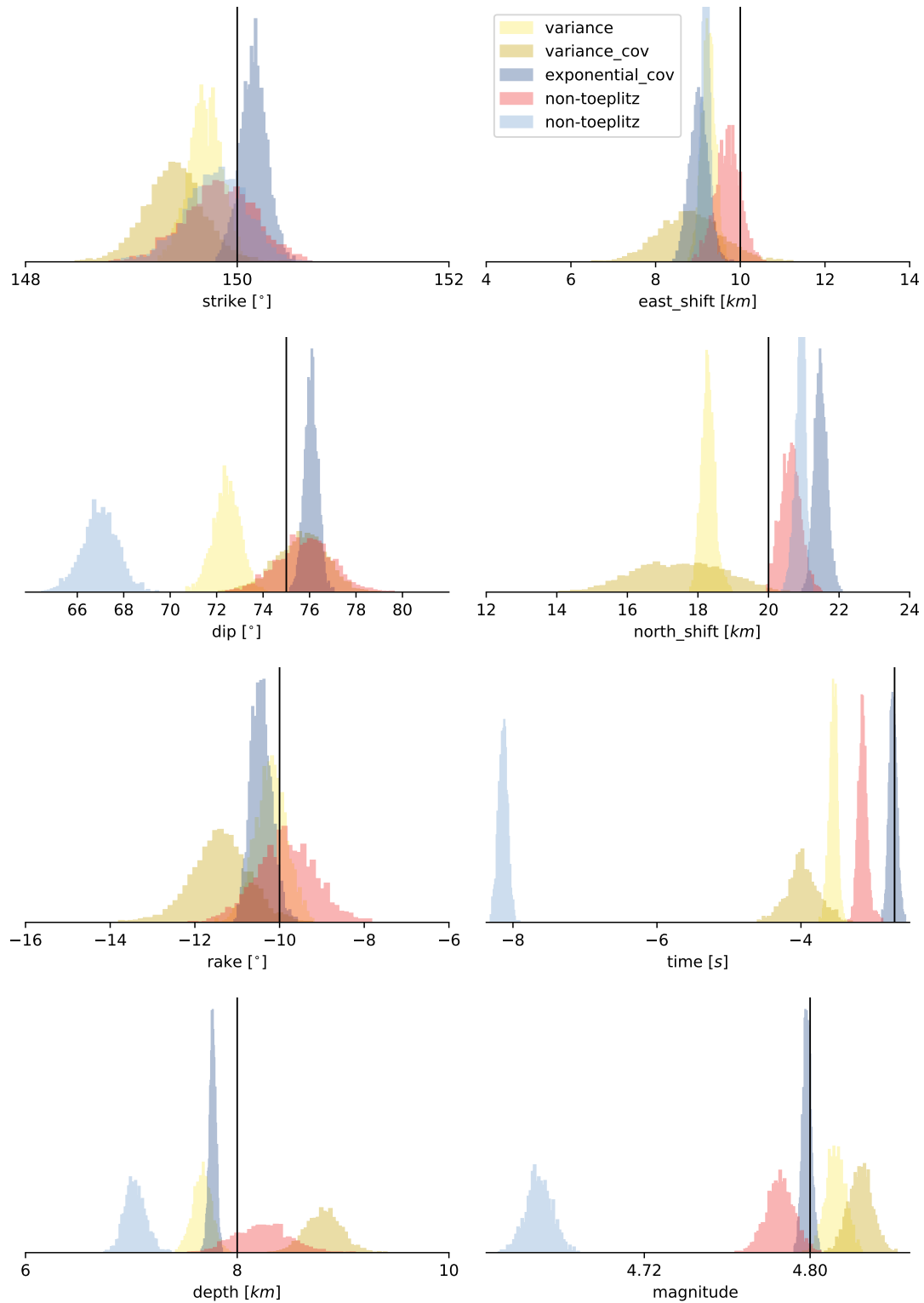
## a) small theory error



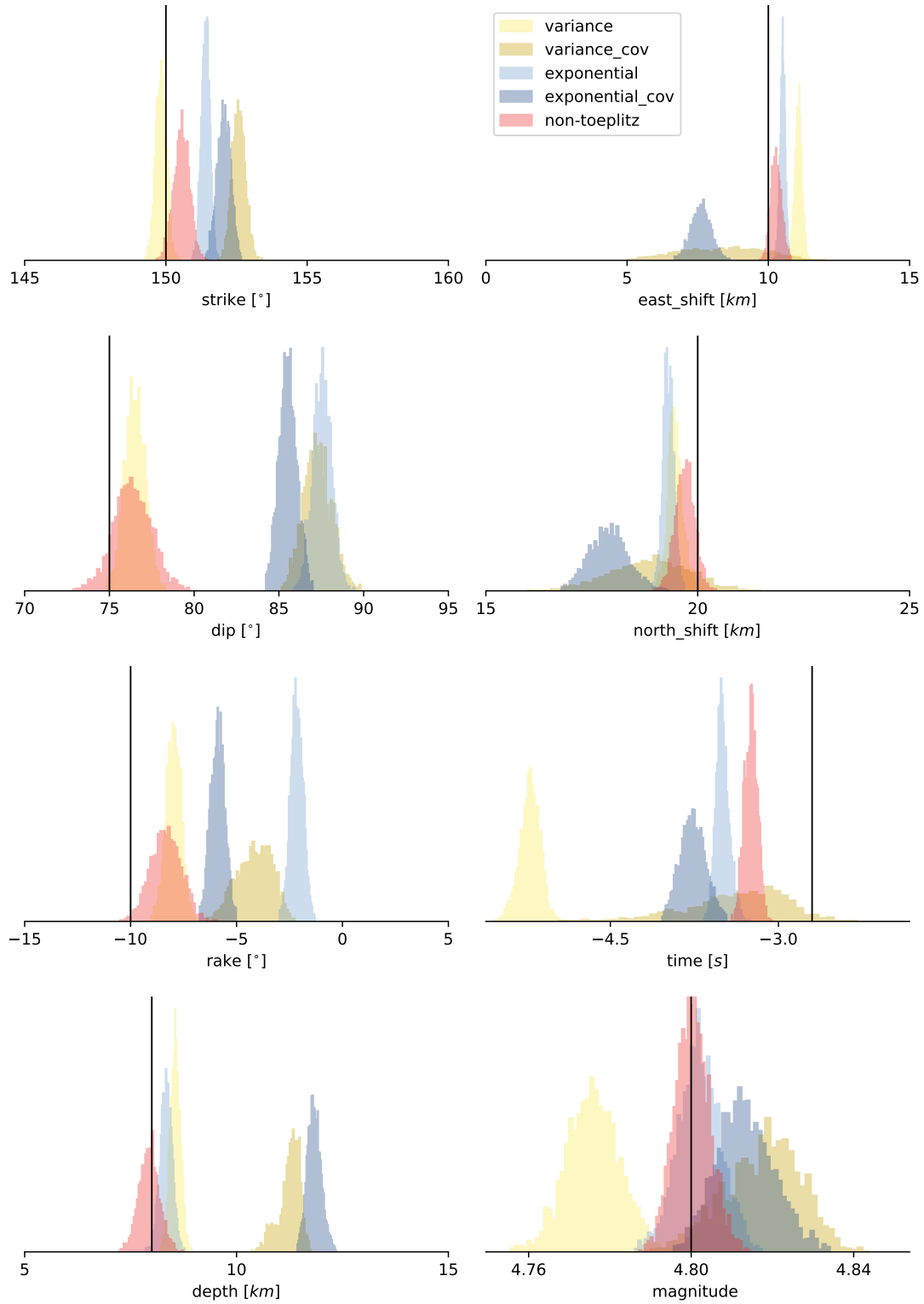
## b) large theory error



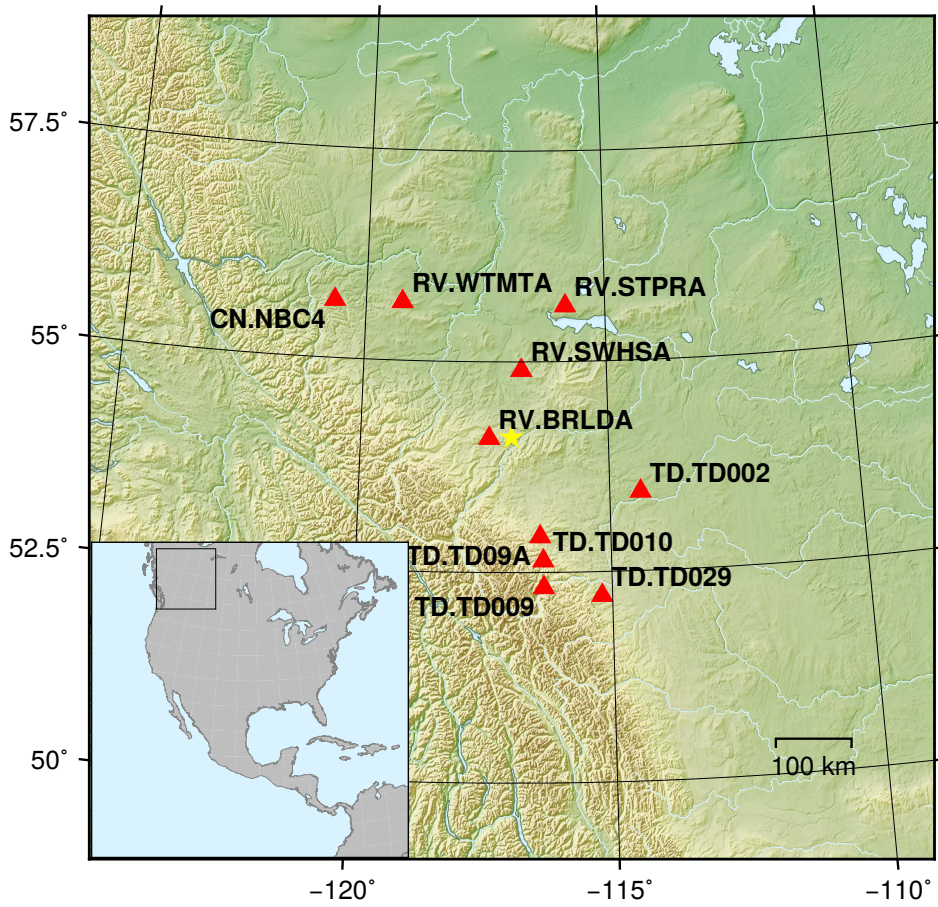
**Figure 7.** Moment tensor decompositions for a) case 1 with small theory error and for b) case 2 with large theory error. Each row shows the decomposition for a different noise parameterisation following the color-coding in Tab. 1 and Fig. 6. The sizes of the focal mechanisms are scaled with respect to MAP magnitudes.



**Figure 8.** Double-couple moment tensor with small theory error: histograms of the posterior marginal distributions for the parameters of a double-couple moment tensor. The marginal for the rake for the *exponential* case is omitted here, as it is far off the displayed interval at a rake of 155-160. Different colors of the histograms mark results for different noise parameterisations (see legend). (Table 2).

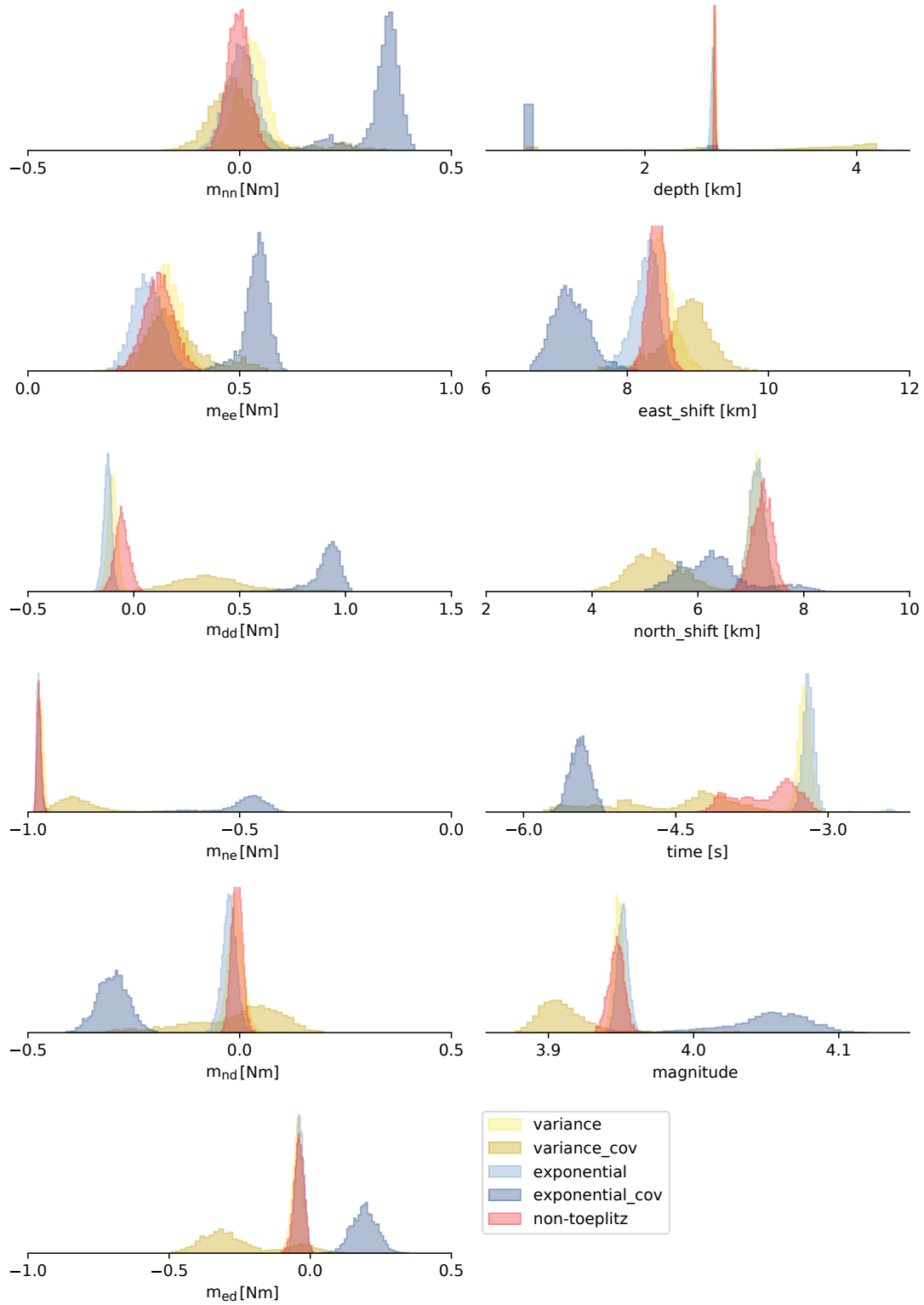


**Figure 9.** Double-couple moment tensor with large theory error: histograms of the posterior marginal distributions for the parameters of a double-couple moment tensor. The different colors of the histograms mark results for different noise parameterisations (see legend). (Table 2).

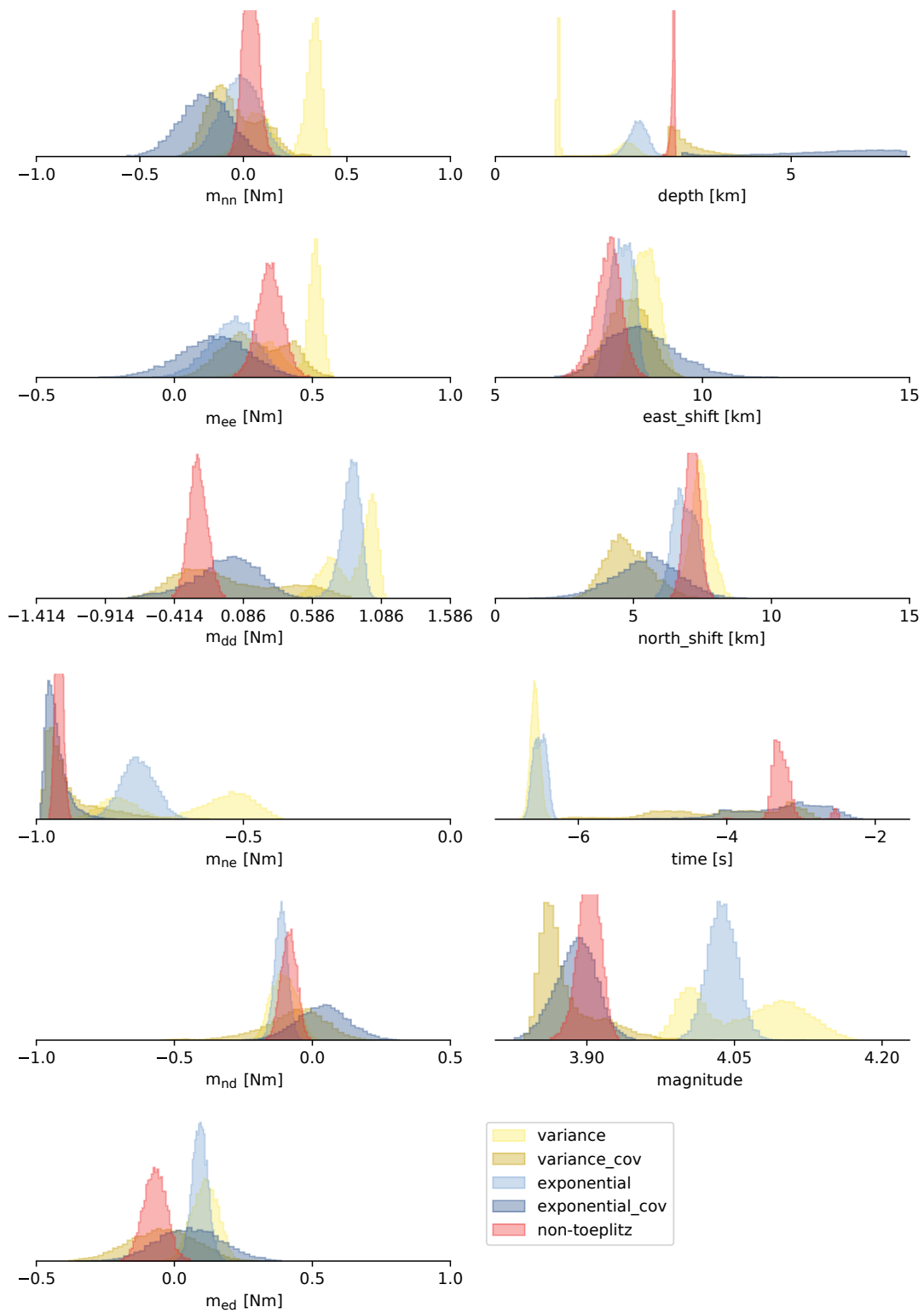


**Figure 10.** Stations (red triangles) used in the full moment tensor estimation at regional distances for the 13th June 2015 Fox Creek event (yellow star at latitude  $54.102^\circ$  and longitude  $-116.95^\circ$ ). The black box in the inset marks the outline of the station map.

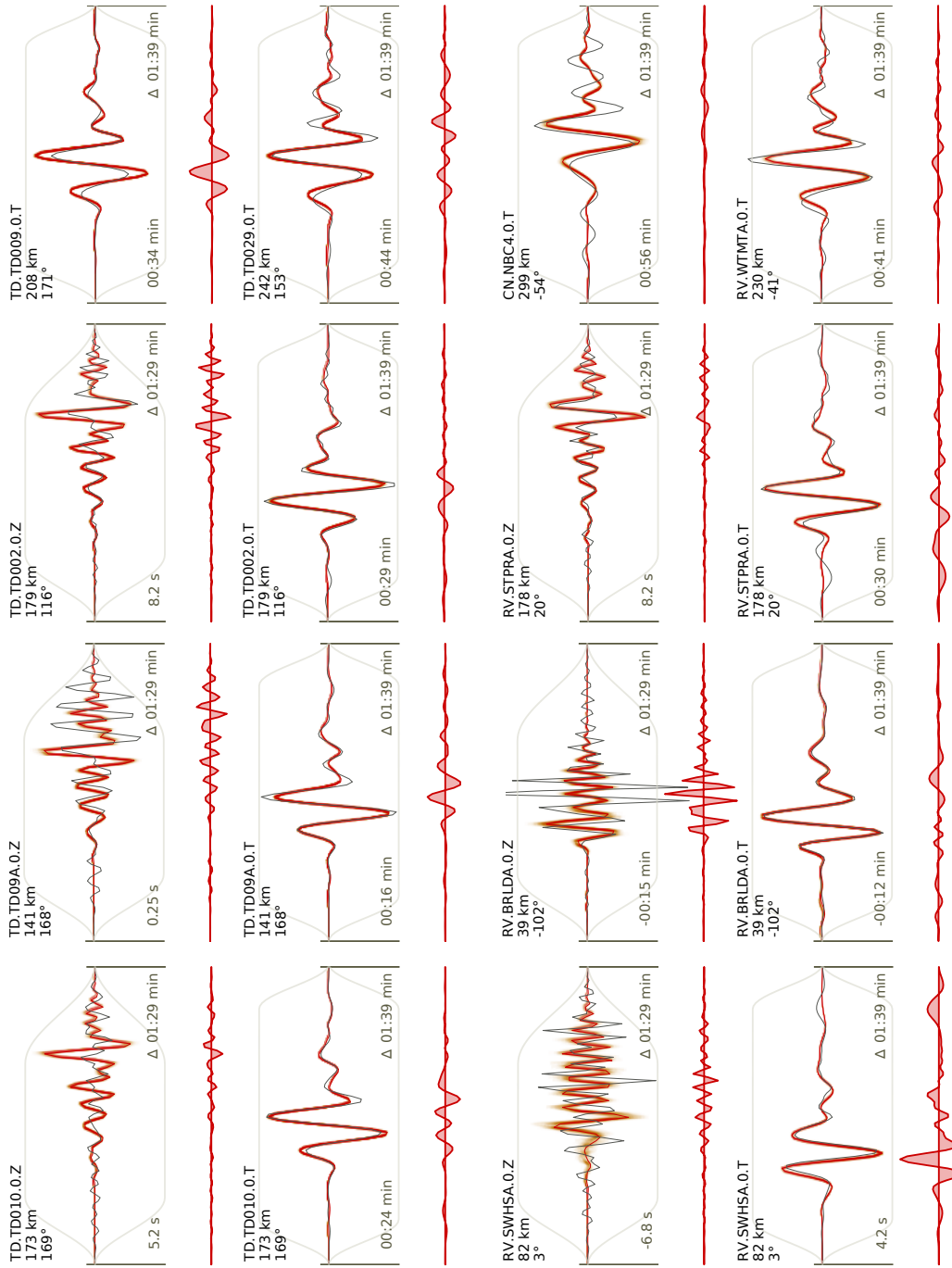




**Figure 11.** Histograms for the study of the Fox Creek 2015 event with regional Earth structure, showing the posterior marginal distributions for the parameters of a full moment tensor. The location estimates are relative to the reference location from the gCMT catalog at latitude  $54.102^\circ$  and longitude  $-116.95^\circ$ . Different colors of the histograms mark results for different noise parameterisations (see legend). (Table 2).

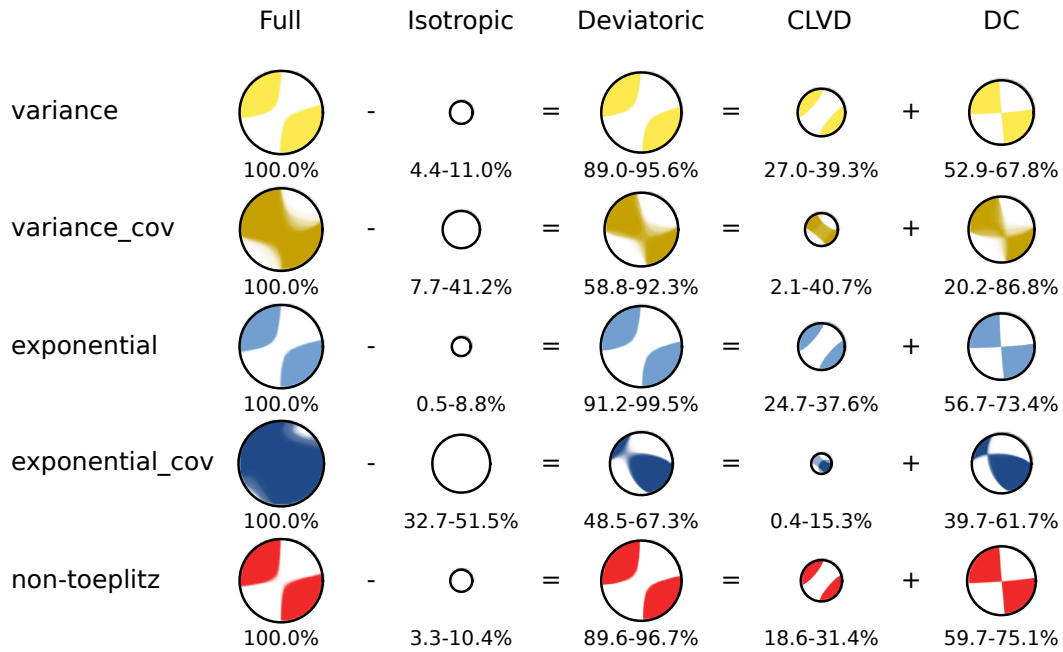


**Figure 12.** Histograms for the study of the Fox Creek 2015 event with global Earth structure. For details see Fig. 11.

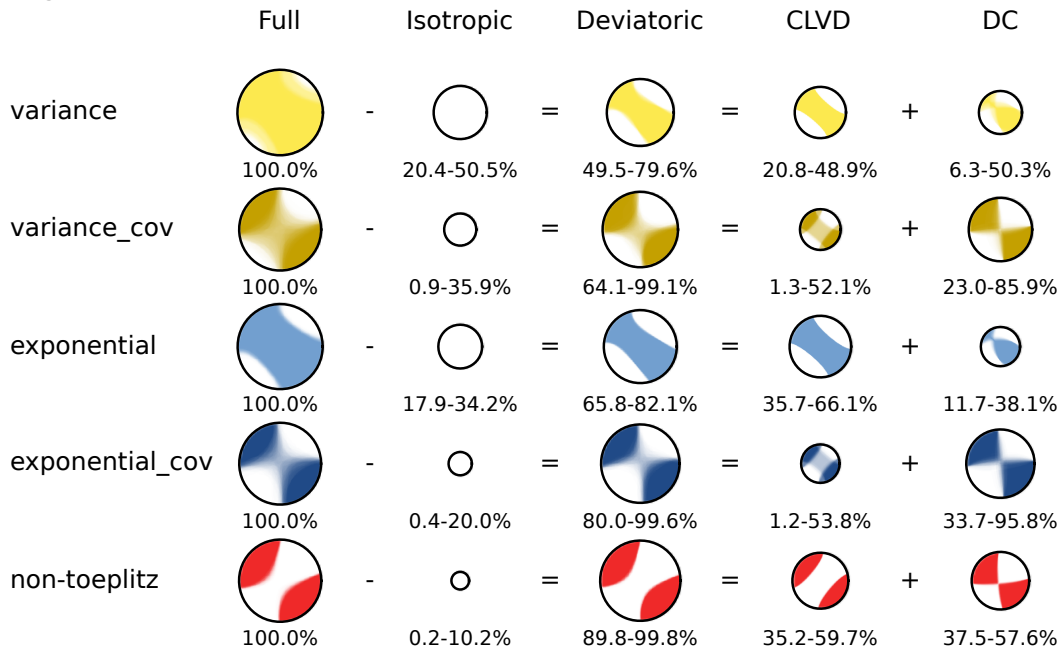


**Figure 13.** Waveform fits for the full moment tensor solution with *variance* noise parameterisation using the regional subsurface structure. The filtered displacement waveform data (dark grey solid line) for body (Z-component 0.08-0.3Hz) or surface wave arrivals (T-component 0.04-0.1Hz) and filtered synthetic displacement waveforms (red solid line) are shown together, with brown shading indicating 100 random draws of the filtered synthetic displacements from the PPD. The residual waveforms are shown below each waveform as filled red-line polygons. Each trace is annotated with the station name and component, as well as the distance and azimuth from the maximum a-posterior solution of the moment tensor location. The arrival time wrt. the centroid time and the duration of each window are shown in the lower left and right, respectively.

a) regional earth structure

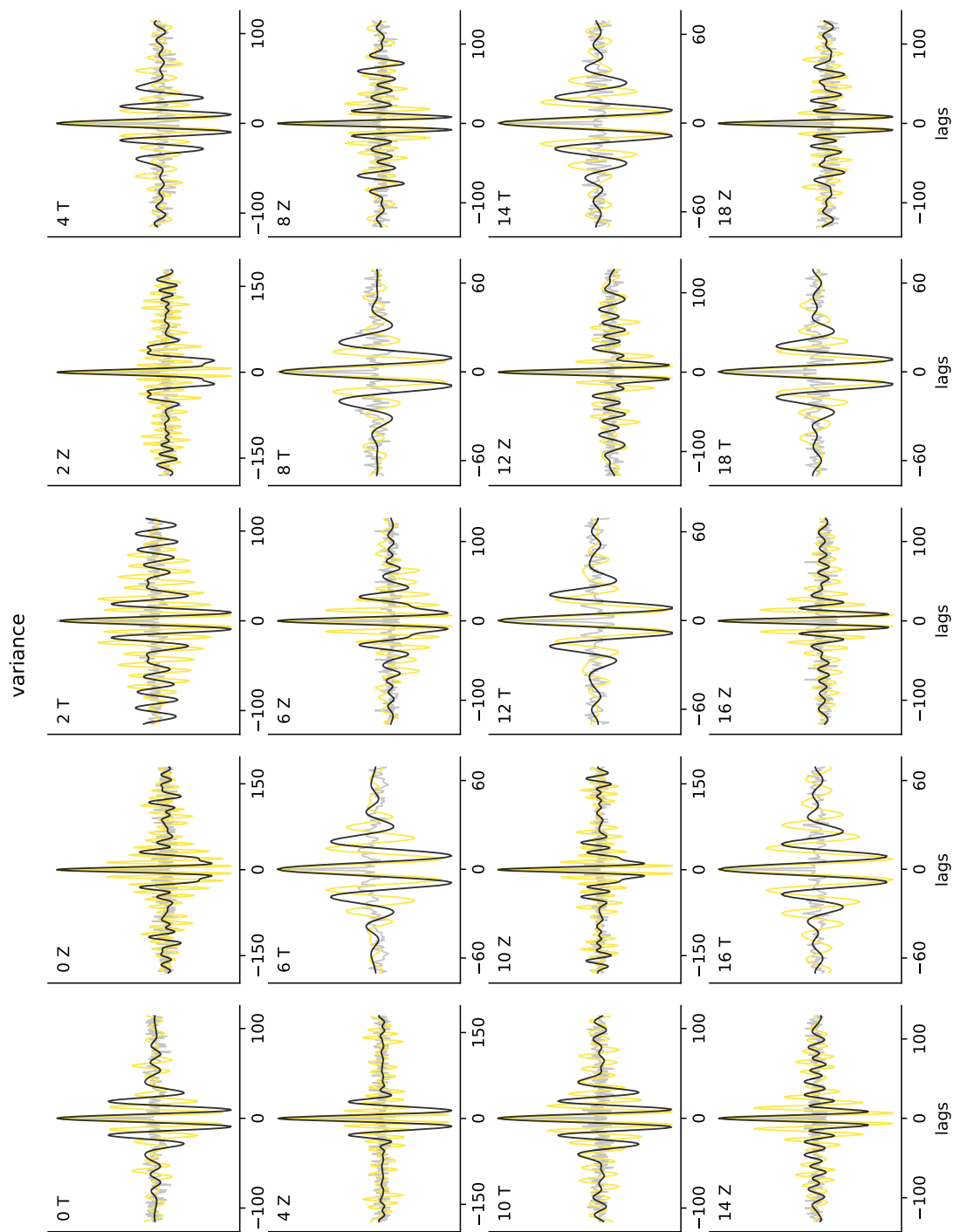


b) global earth structure



**Figure 14.** Fox Creek 2015: Moment tensor decompositions of the estimation results from different noise parameterisations for a) regional Earth structure and b) global Earth structure. See also Fig. 7 for complete caption.

542 **9 SUPPLEMENTAL MATERIAL**



**Figure S1.** *Variance* parameterisation: Autocorrelations of raw residuals(black), random white noise (light gray) and standardized residuals (colored) of each component and station (shown in the upper left of each subplot).

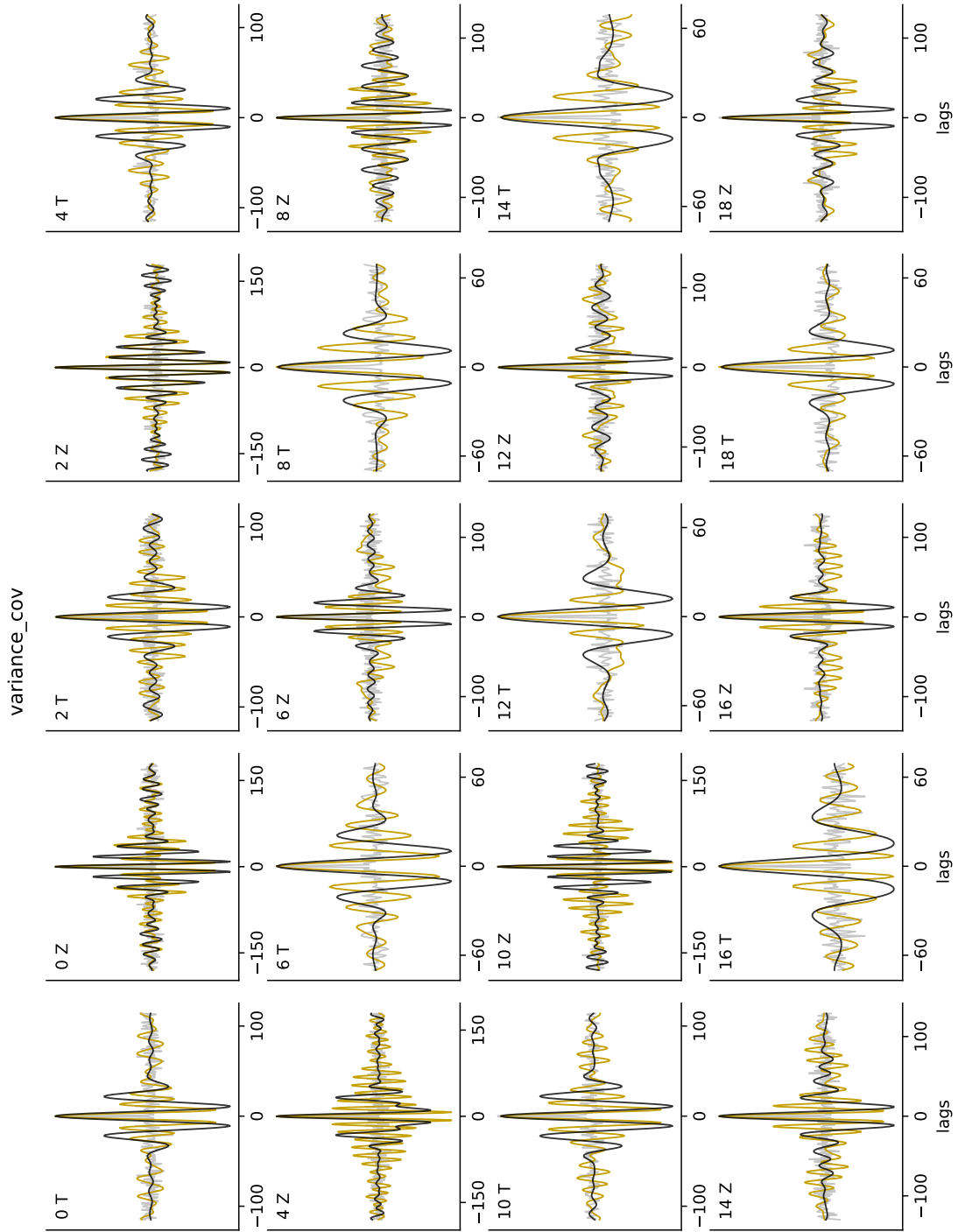
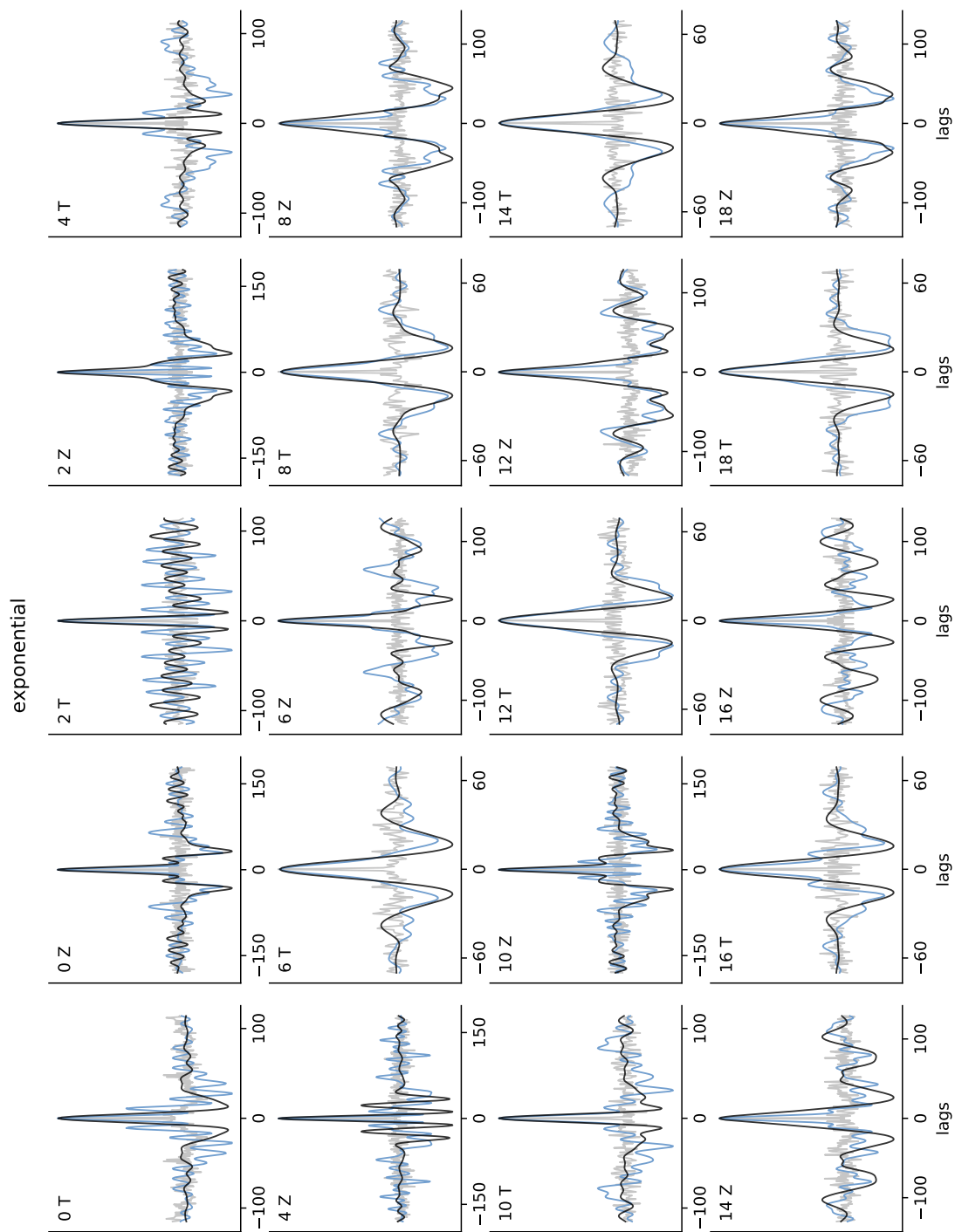


Figure S2. *Variance\_cov* parameterisation: Details are described in Fig. S1.



**Figure S3.** *Exponential* parameterisation: Details are described in Fig. S1.



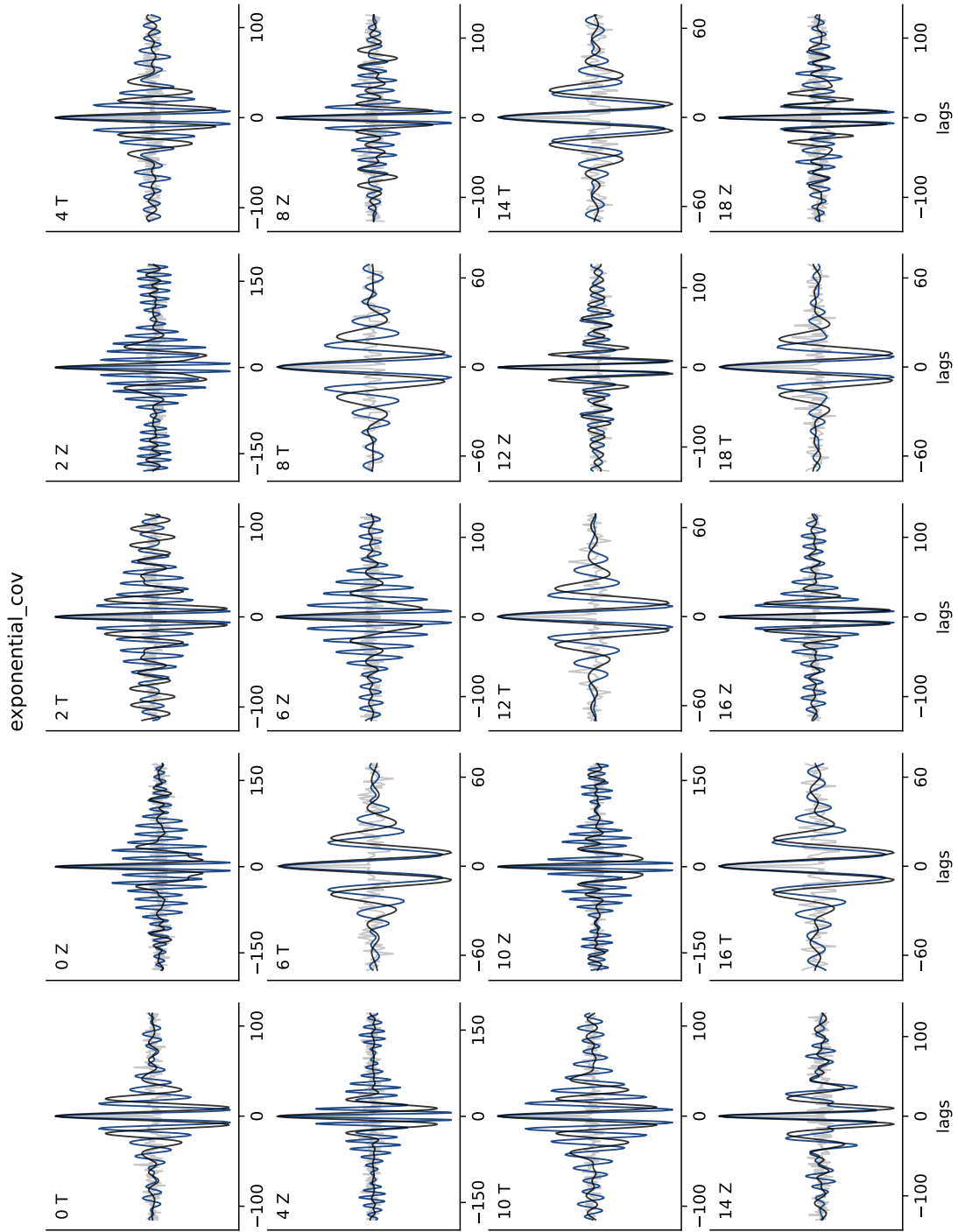
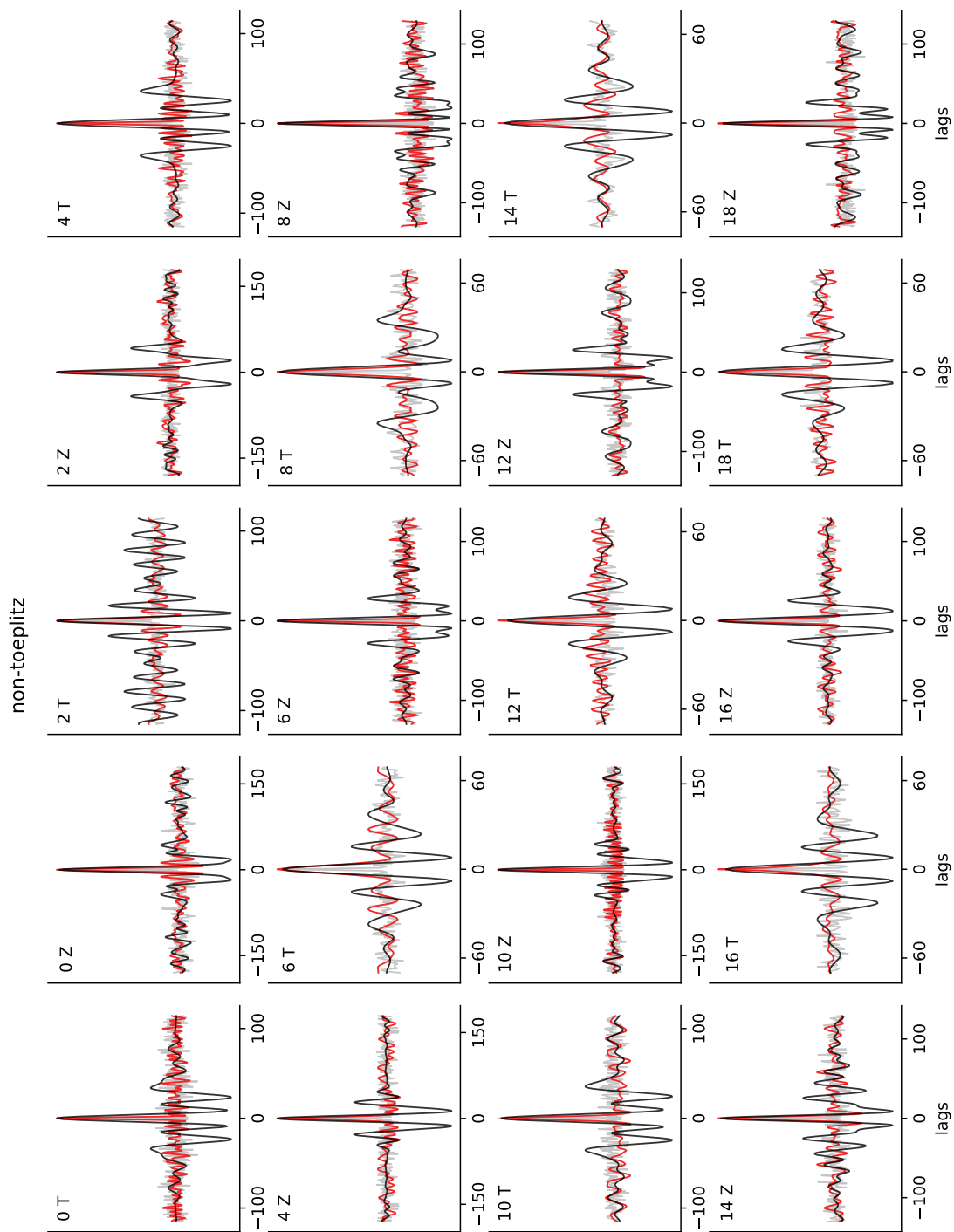
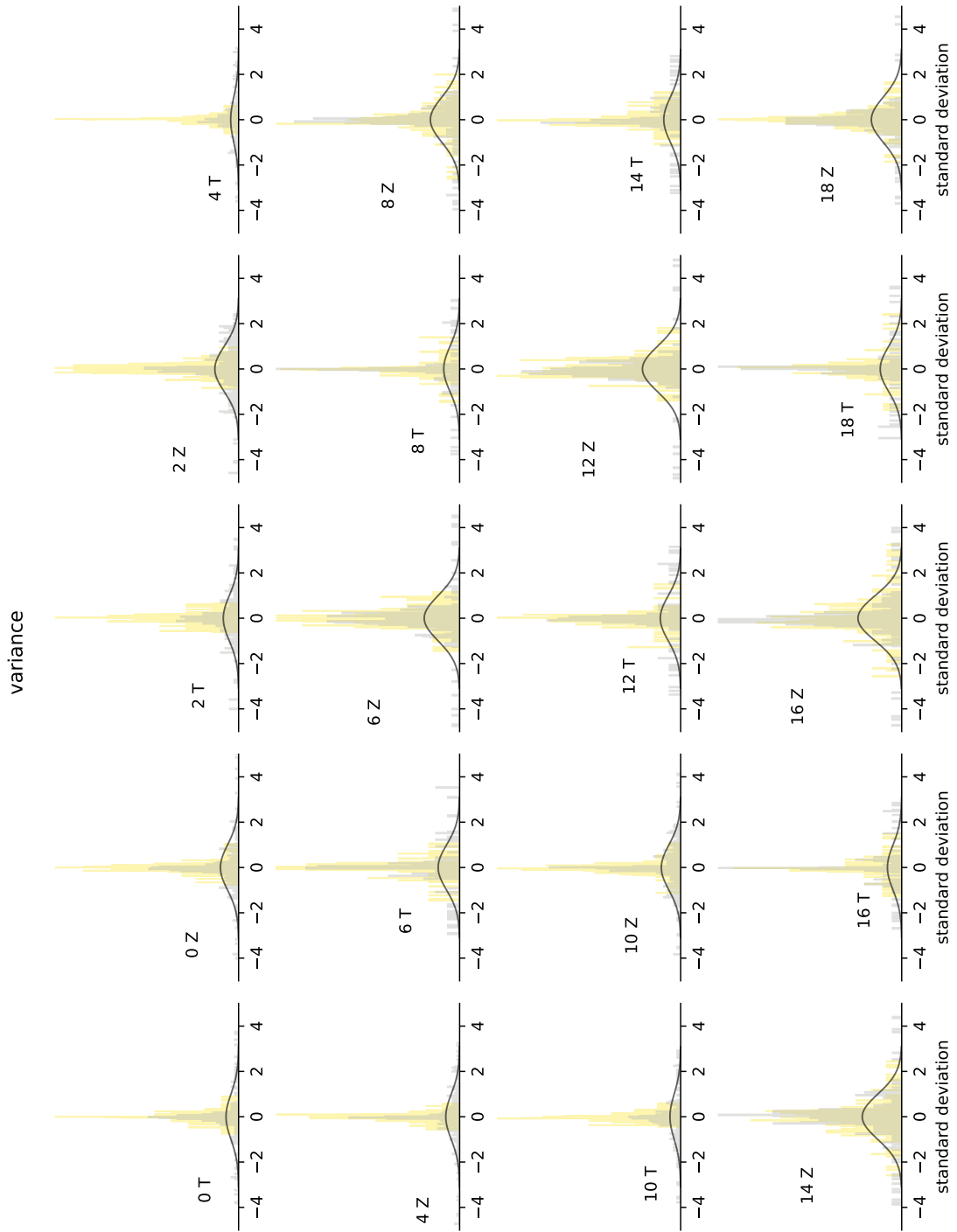


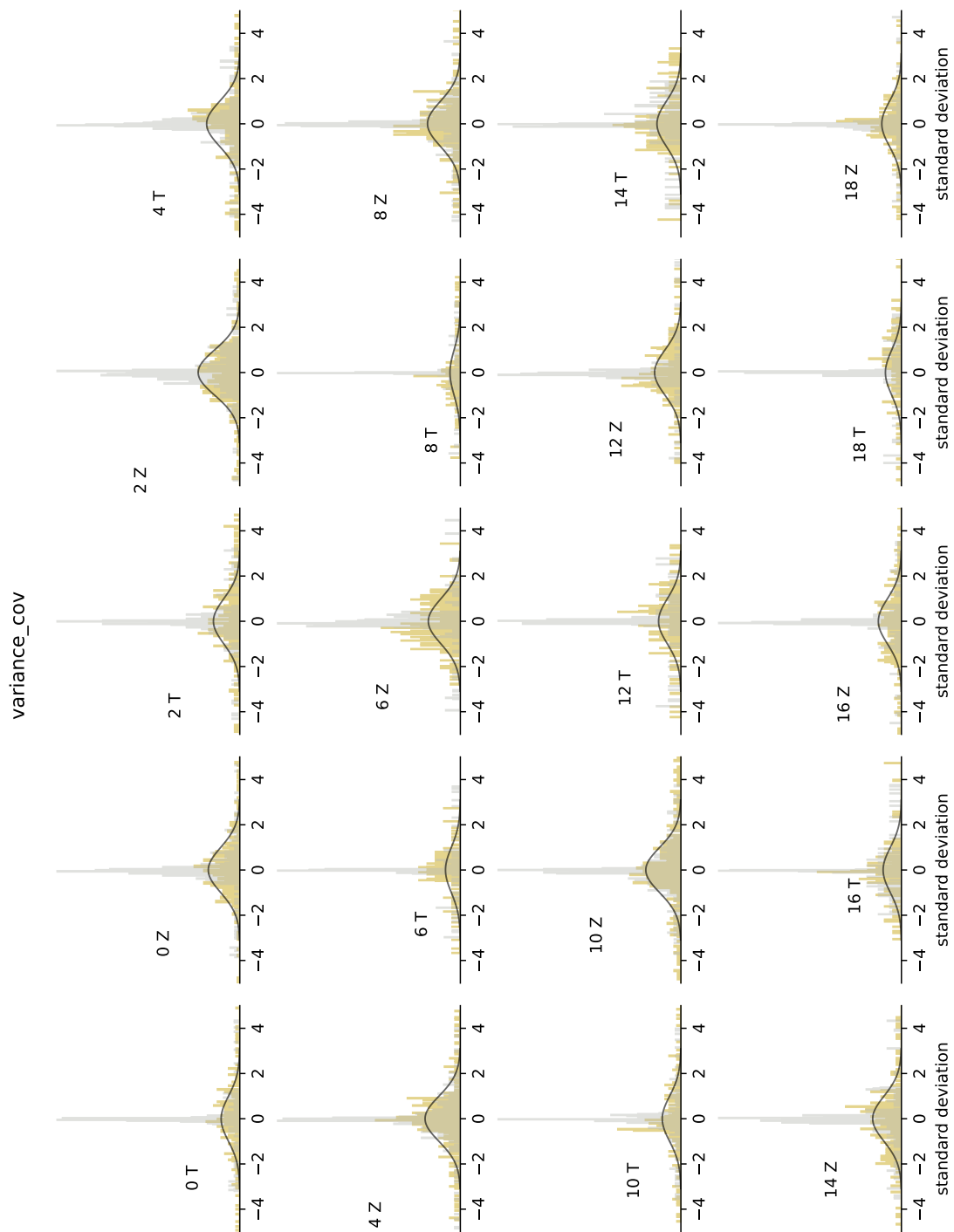
Figure S4. *Exponential\_cov* parameterisation: Details are described in Fig. S1.



**Figure S5.** *non-Toeplitz* parameterisation: Details are described in Fig. S1.



**Figure S6.** Variance parameterisation: Histograms of raw-residuals (light gray), standardized residuals (colored), analytical Gaussian of zero mean and one-sigma standard-deviation (black).



**Figure S7.** *Variance\_cov* parameterisation: Details are described in Fig. S6.

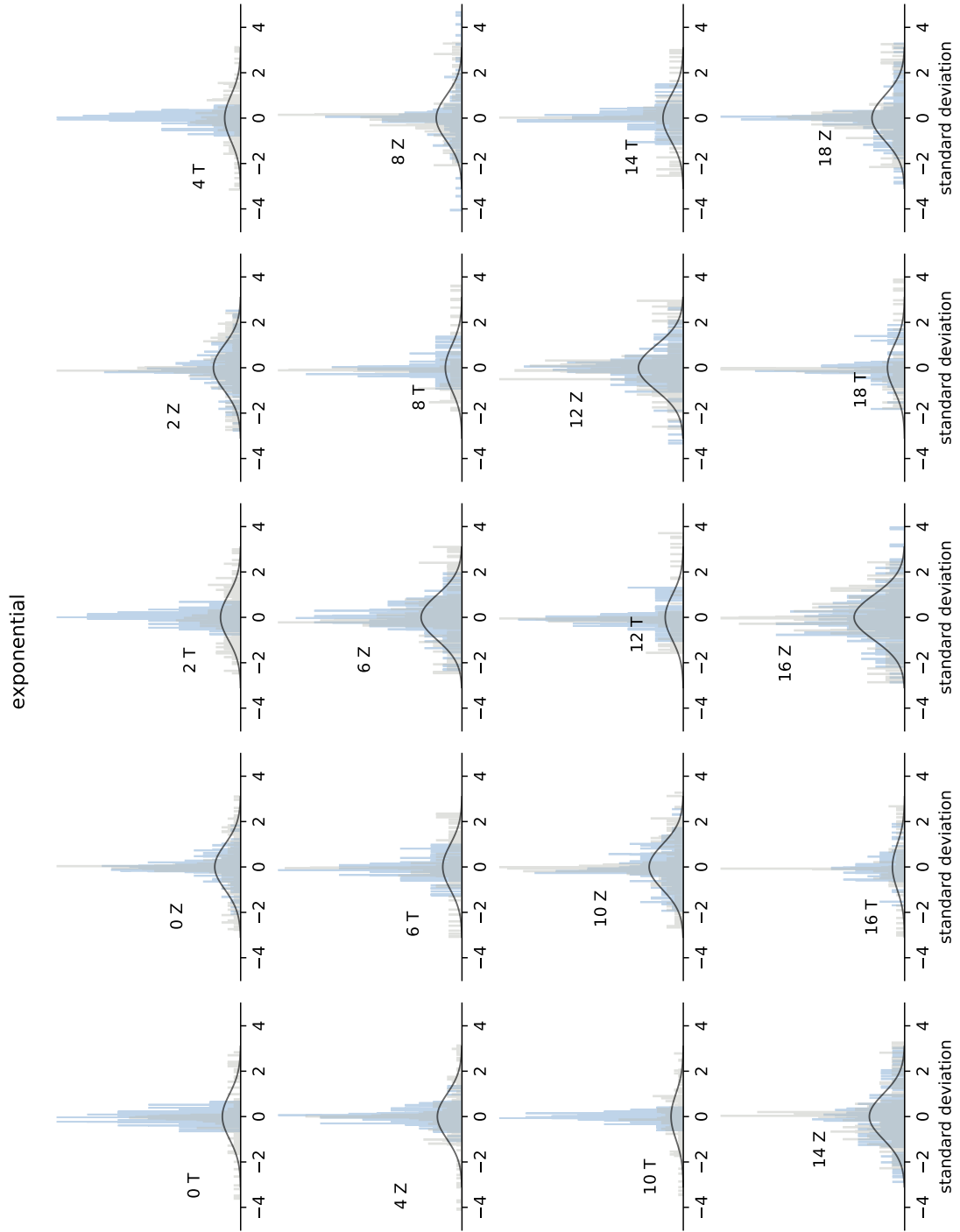
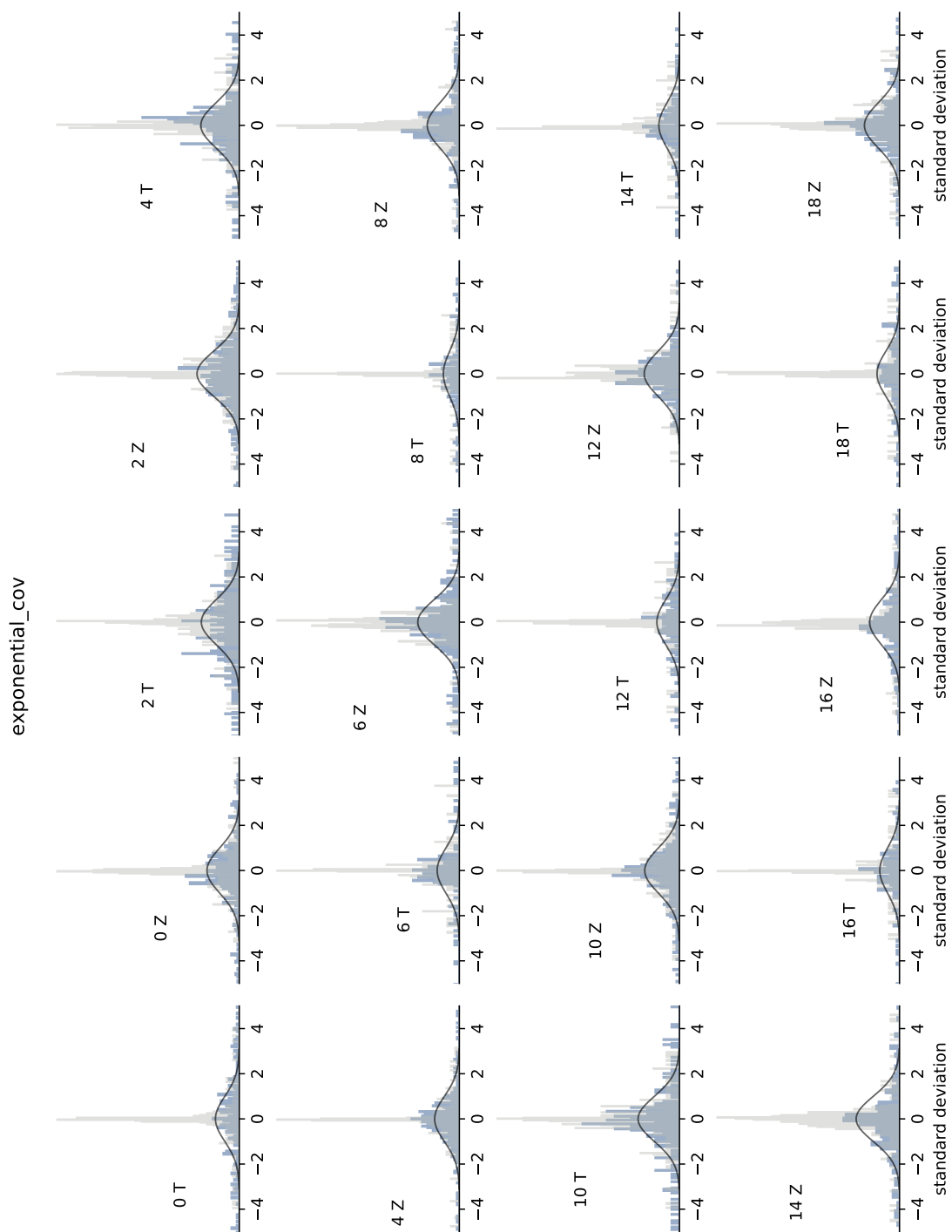


Figure S8. *Exponential* parameterisation: Details are described in Fig. S6.



**Figure S9.** *Exponential\_cov* parameterisation: Details are described in Fig. S6.

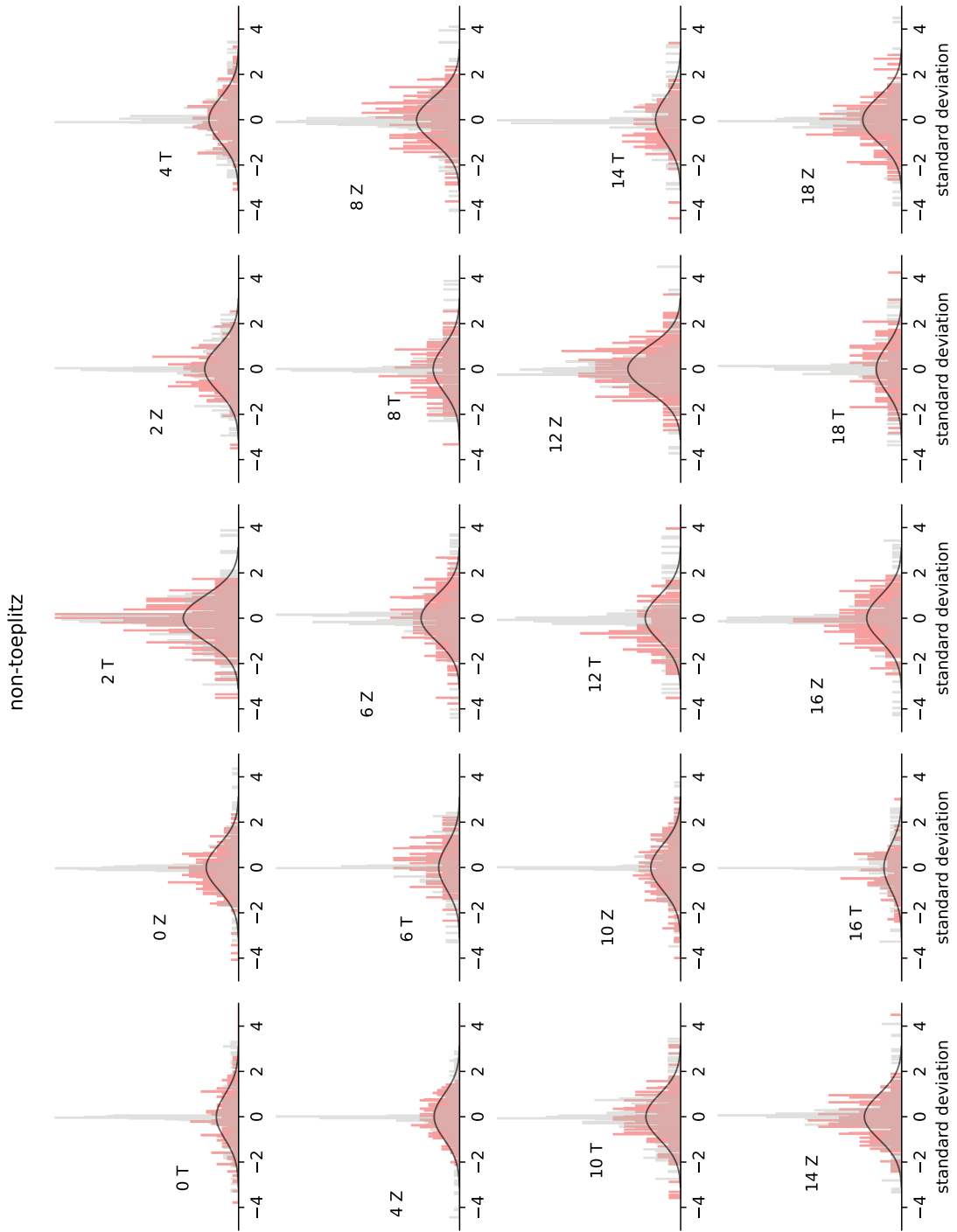
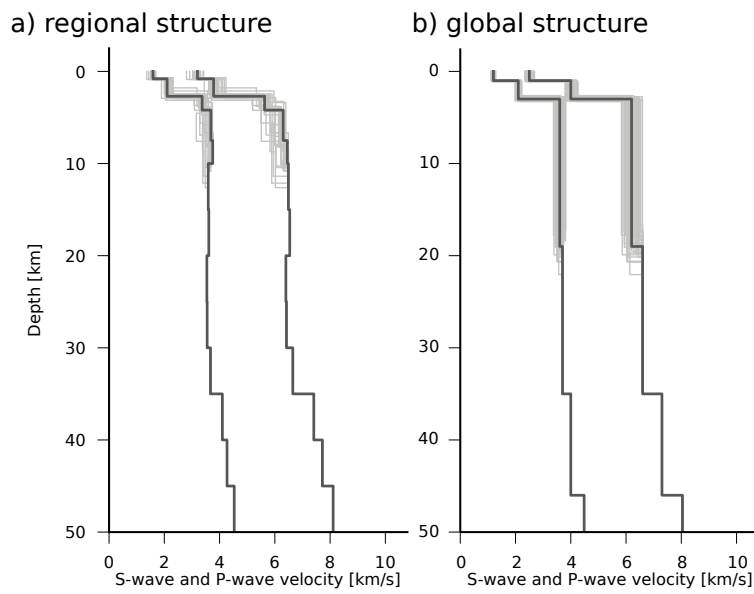
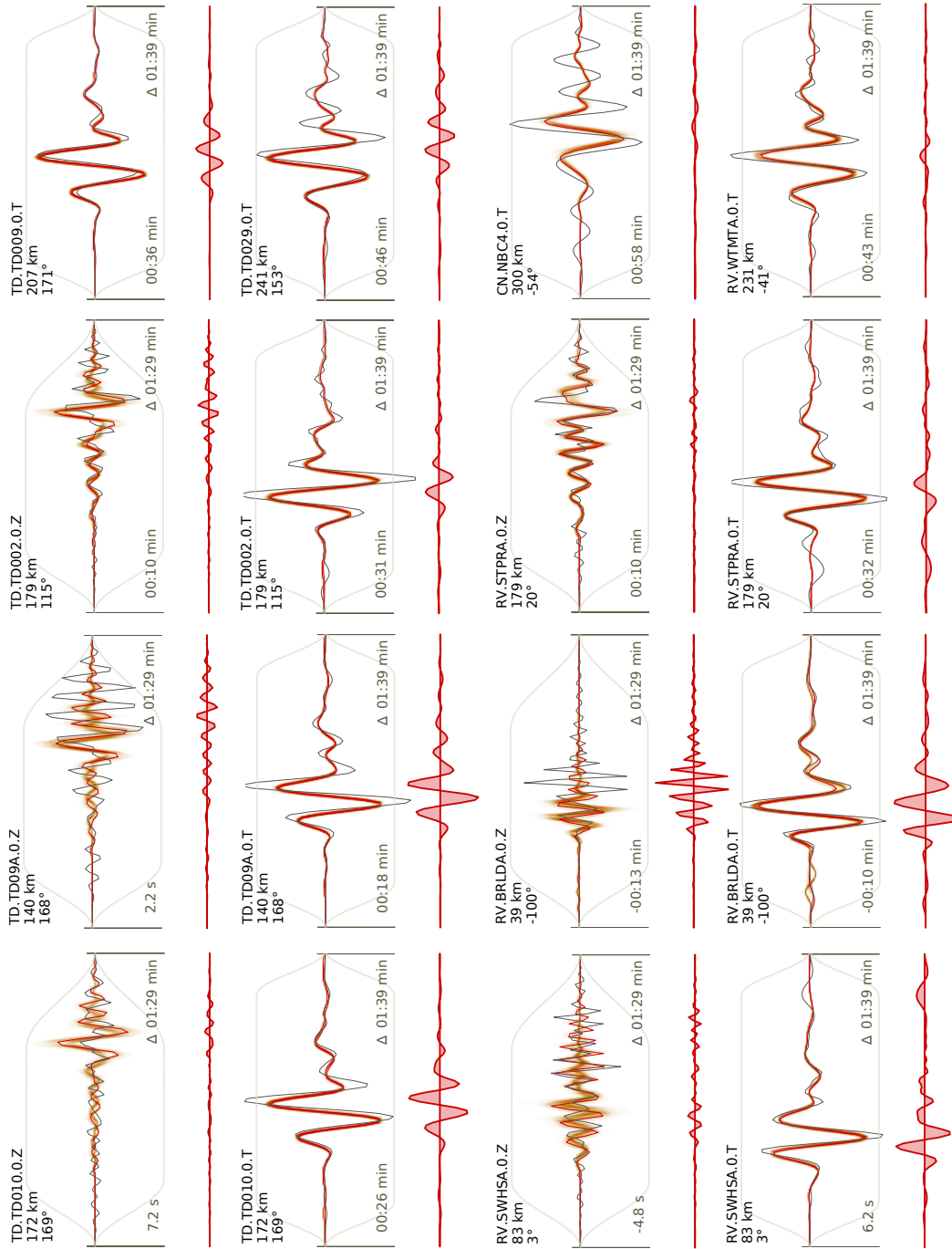


Figure S10. *non-Toeplitz* parameterisation: Details are described in Fig. S6.

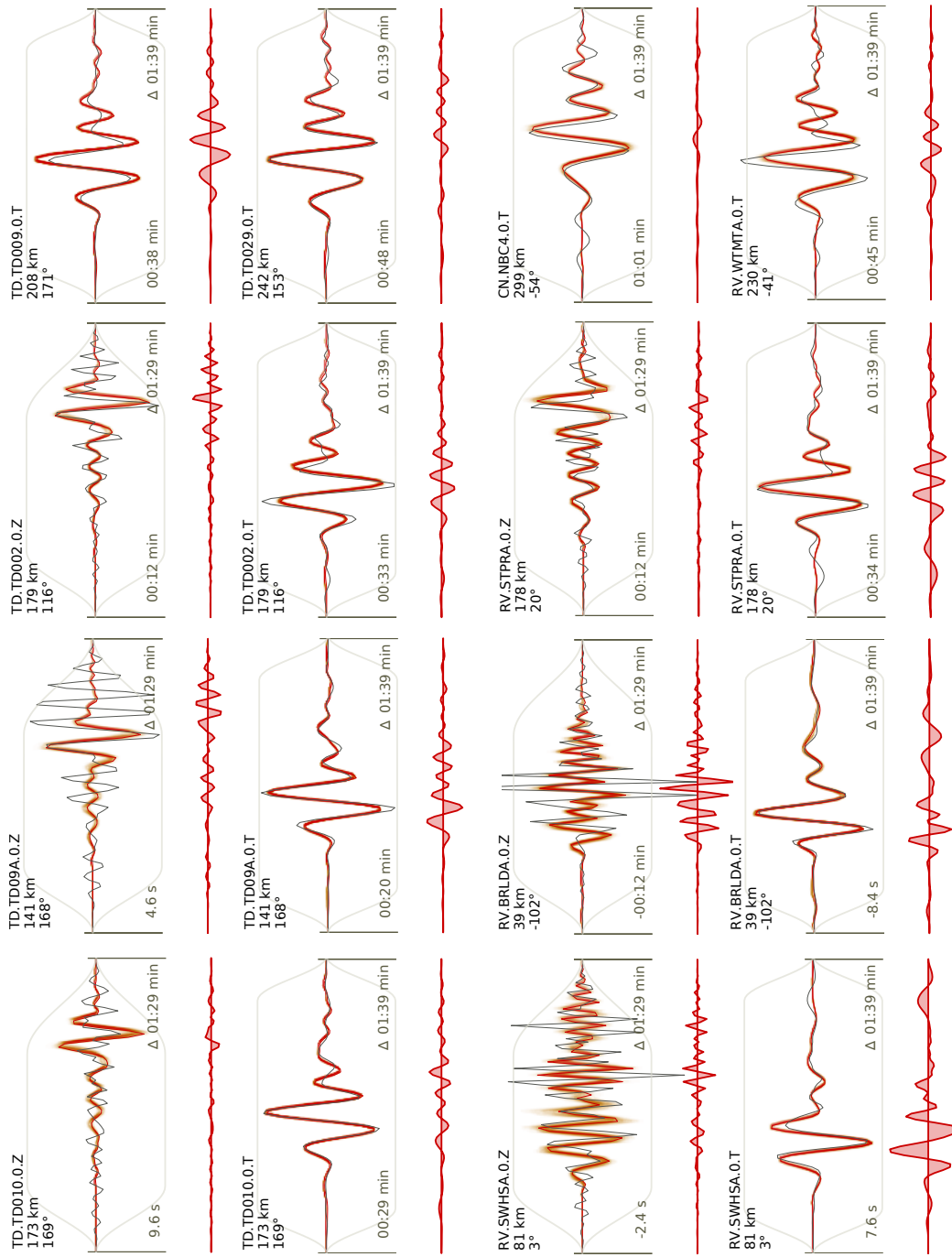


**Figure S11.** Earth structures (dark gray) a) regional (Wang et al. 2016) and b) global ak135 (Kennett et al. 1995) and their variations (light gray) that have been used in the full moment tensor estimation of the Fox Creek event.





**Figure S12.** Waveform fits for the full moment tensor solution with *variance\_cov* noise parameterisation using the regional subsurface structure. The filtered displacement waveform data (dark grey solid line) for body (Z-component 0.08-0.3Hz) or surface wave arrivals (T-component 0.04-0.1Hz) and the filtered synthetic displacement waveforms (red solid line) are shown together, with the brown shading indicating 100 random draws of the filtered synthetic displacements from the PPD. The residual waveforms are shown below each waveform as filled red-line polygons. Each trace box is annotated with the station name and component, as well as the distance and azimuth from the maximum a-posterior solution of the moment tensor location. The arrival time wrt. the centroid time and the duration of each window are shown in the lower left and right, respectively.



**Figure S13.** Waveform fits for the full moment tensor solution with *variance* noise parameterisation using the global subsurface structure. A detailed description of plotted features is given in Fig. S12

543 **APPENDIX A: SAMPLING ALGORITHM**

544 Using a Monte Carlo method allows drawing samples from a posterior PDF (eq. 1); once  
 545 enough samples are drawn the resulting distribution is a valid approximation of the posterior  
 546 probability density (PPD). To sample the posterior PDF we use a Sequential Monte Carlo  
 547 (SMC) sampler (Moral et al. 2006; Ching & Chen 2007), similar to Minson et al. (2013). Here,  
 548 we outline the main features of the algorithm, however, for more details we refer the reader  
 549 to the original references. Obtaining samples from a posterior PDF that has a complex topol-  
 550 ogy (high-dimensional, multimodal, flat, ...) is difficult and inefficient. Therefore, sampling is  
 551 done starting from the prior PDF via several intermediate PDFs that change following a self  
 552 adjusting cooling parameter starting at zero (similar to Simulated Annealing (Sambridge &  
 553 Mosegaard 2002)) (Moral et al. 2006; Minson et al. 2013):

$$f(\mathbf{m}|\mathbf{d}_{obs}, \beta_k) \propto p(\mathbf{d}_{obs}|\mathbf{m})^{\beta_k} p(\mathbf{m})$$

$$k = 0, 1, \dots, K \quad (\text{A.1})$$

$$0 = \beta_0 < \beta_1 < \dots < \beta_K = 1$$

554 Each intermediate PDF  $f(\mathbf{m}|\mathbf{d}_{obs}, \beta_k)$  is sampled in parallel by a pre-defined number of  
 555 Monte Carlo (MC) chains. Each chain samples the solution space with a predefined number  
 556 of steps, where step size and directions are determined according to a proposal distribution.  
 557 When sampling of all chains for the intermediate PDF is completed the algorithm enters a  
 558 transitional stage:

559 (i) The likelihood of each Markov chain end-point is used to form an intermediate likelihood  
 560 distribution.

561 (ii) This likelihood distribution (at  $\beta_k$ ) is compared to the previous intermediate likelihood  
 562 distribution (at  $\beta_{k-1}$ ) by evaluating the coefficient of variation (COV). If they differ signif-  
 563 icantly ( $\text{COV} > 1$ ) the cooling parameter  $\beta_k$  is incremented only by a small amount. On  
 564 the other hand, if the distributions are similar ( $\text{COV} < 1$ ) the tempering parameter  $\beta_k$  is  
 565 increasing faster.

566 (iii) The proposal distribution is updated based on the distribution of model parameters  
 567 in the MC chain end-points.

568 (iv) Optional: update  $\mathbf{C}$  in each transitional stage using the mean of each model parameter  
569 distribution (Dettmer et al. 2007; Minson et al. 2013; Duputel et al. 2014) (see eq. 3).

570 (v) The ensemble of Markov chain end-points at  $\beta_{k-1}$  is resampled according to the inter-  
571 mediate likelihoods. Hence, the next stage of Markov chains at  $\beta_k$  are seeded on the end-points  
572 of the previous chains, which had the highest likelihoods; unlikely chains are discarded.

573 Finally, if the cooling parameter satisfies  $\beta_k \geq 1$ , the posterior distribution is reached  
574  $f(\mathbf{m}|\mathbf{d}_{obs}, \beta_K = 1) \propto p(\mathbf{m}|\mathbf{d}_{obs})$  and one last sampling of all MC chains with the defined  
575 number of steps is executed; then the algorithm stops. For the proposal distribution we use a  
576 multivariate Gaussian distribution similarly to Minson et al. (2013).

577