**Figure 1.** Reference invasion pattern at times t = 1,3,5,6,8 and 10. Tumour cell density is shown as a blue curve, ECM density as a red curve and MDE concentration as a green one.

**Figure 2.** Initial (blue) and final (black) densities of the parameters in the PDE model estimated using the ABC related scheme. Sample means are marked with “X” on the x axis, and the reference parameter values are shown with a red vertical dotted line. (See Appendix B (a) for the detailed density evolutions of the parameters in different rounds.)

**Figure 3.** Pairwise heat maps of the final parameter densities in the first run of the ABC-related scheme on the main reference dataset.

**Figure 4.** Average parameter estimates from gradient matching scheme over 200 simulated datasets at each of 5 levels of measurement error. Horizontal red dashed lines: true values of the parameters. Black line: parameter estimates where all parameters are estimated. Other lines show parameter estimates where some parameters are fixed at their true value: blue, and fixed; red, and fixed; green line, , and fixed.

**Figure 5.** Temporal and spatial gradients in the model at different measurement error CVs. Red dashed lines: reference gradients predicted by GAM at CV equals 0. Dark purple solid lines: true gradients calculated by the finite difference scheme. Other solid lines show estimated gradients averaged over time and 200 data sets from the gradient matching scheme at CVs of 0.01 (black), 0.025 (green), 0.05 (blue), 0.075 (cyan) and 0.1 (magenta). A larger-sized version of these plots is provided in the Github repository mentioned in the “Data Accessibility" statement at the end of the manuscript.

**Figure 6.** Average parameter estimates from gradient matching scheme over 200 simulated datasets at each of 5 levels of measurement error. Black line: parameter estimates where all parameters are estimated with the gradients fitted by GAM. Other lines show parameter estimates where some gradients are replaced by the reference ones or truncated: blue, truncated gradients; red, tumour cells temporal gradients, and spatial gradients replaced by the reference ones; green, all tumour cells related gradients replaced by the reference ones; magenta, all tumour cells related gradients and spatial gradients replaced by the reference ones.

**Figure S1.** Evolution of densities after each Tumour cells, MDE and ECM-related round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S2.** Evolution of densities after each Tumour cells, MDE and ECM-related round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S3.** Evolution of densities after each Tumour cells, MDE and ECM-related round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S4.** Evolution of densities after each ECM-related (Upper plot) and MDE & ECM related (lower plot) round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S5.** Evolution of densities after each Tumour cells & MDE & ECM-related round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S6.** Evolution of densities after each MDE & ECM-related (Upper plot) and MDE & ECM & Tumour cells-related (lower plot) round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S7.** Evolution of densities after each MDE & ECM-related (Upper plot) and MDE & ECM & Tumour cells-related (lower plot) round of the ABC optimization scheme applied to the main reference dataset. Sample mean of each round is marked with a cross on the x-axis.

**Figure S8.** Reference invasion pattern (upper 2x3) vs. simulated solution pattern (lower 2x3) for the main reference dataset, ABC-related scheme.

**Figure S9.** Reference invasion pattern (upper 2x3) vs. simulated solution pattern (lower 2x3) for the main reference dataset, gradient matching scheme.

**Figure S10.** Tumour cells temporal gradients ) at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM with no perturbation added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S11.** Second order diffusion gradients () of tumour cells at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S12.** Spatial gradients of haptotaxis () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S13.** Spatial gradients of logistic growth () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S14.** Temporal gradients of ECM () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S15.** Spatial gradients of ECM decay () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S16.** Temporal gradients of MDE () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S17.** Second order diffusion spatial gradients of MDE () at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.

**Figure S18.** Linear growth spatial gradients of MDE ) at different time points under different CV on absolute difference scale, averaged over 200 data sets. Red dashed lines, reference gradients estimated by GAM when no perturbation was added to the data; dark purple, true gradients calculated by the finite difference scheme; black, cv = 0.01; green, cv = 0.025; blue, cv = 0.05; cyan = 0.075; magenta, cv = 0.1.