Supplementary material to:

Comparison of Methods for Estimation of the Intravoxel Incoherent Motion (IVIM) Diffusion Coefficient (D) and Perfusion Fraction (f)

Magnetic Resonance Materials in Physics, Biology and Medicine

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Supplementary information

Segmented model fitting

A MATLAB function was specifically implemented for segmented IVIM model fitting. It was fully vectorized and exploited the fact that the optimization can be reduced to a one-dimensional problem (where D is the only unknown) and therefore reduces the computational time substantially. The function used an iterative procedure to find the value of D for which the partial derivatives of the sum of squared error with respect to D and A (found in Eq. 2) was zero. The problem was reduced to one dimension by calculating the partial derivatives analytically, setting them to zero and rearranging such that the final expression only depended on D.

Least-squares fitting

The model supplied to the *fit* function was given by the function call:

```
sIVIMmodel = fittype( 'S0*((1-f)*exp(-b*D)+f*(b==0))', 'independent', 'b');
```

Bayesian model fitting

The specific settings of the Bayesian model fitting were:

Start values: f = 0.1, D = 1 µm^2/ms and $S_0 = S(0)$, i.e. the measured signal at b = 0

Iterations (after burn-in): 40,000

Burn-in steps: 2000 (with updates of step-length parameters every 100th iteration) + 2000 (without updates of step-length parameters)

The step-length parameters were initialized as one tenth of the corresponding parameter value. At each update the step-lengths were adjusted with the aim of an acceptance rate in the Metropolis-Hastings sampling of approximately 50 % as described previously by Orton et al in ”Improved Intravoxel Incoherent Motion Analysis of Diffusion Weighted Imaging by Data Driven Bayesian Modeling. Magn. Reson. Med. 2014;71:411–420.”

Supplementary figures

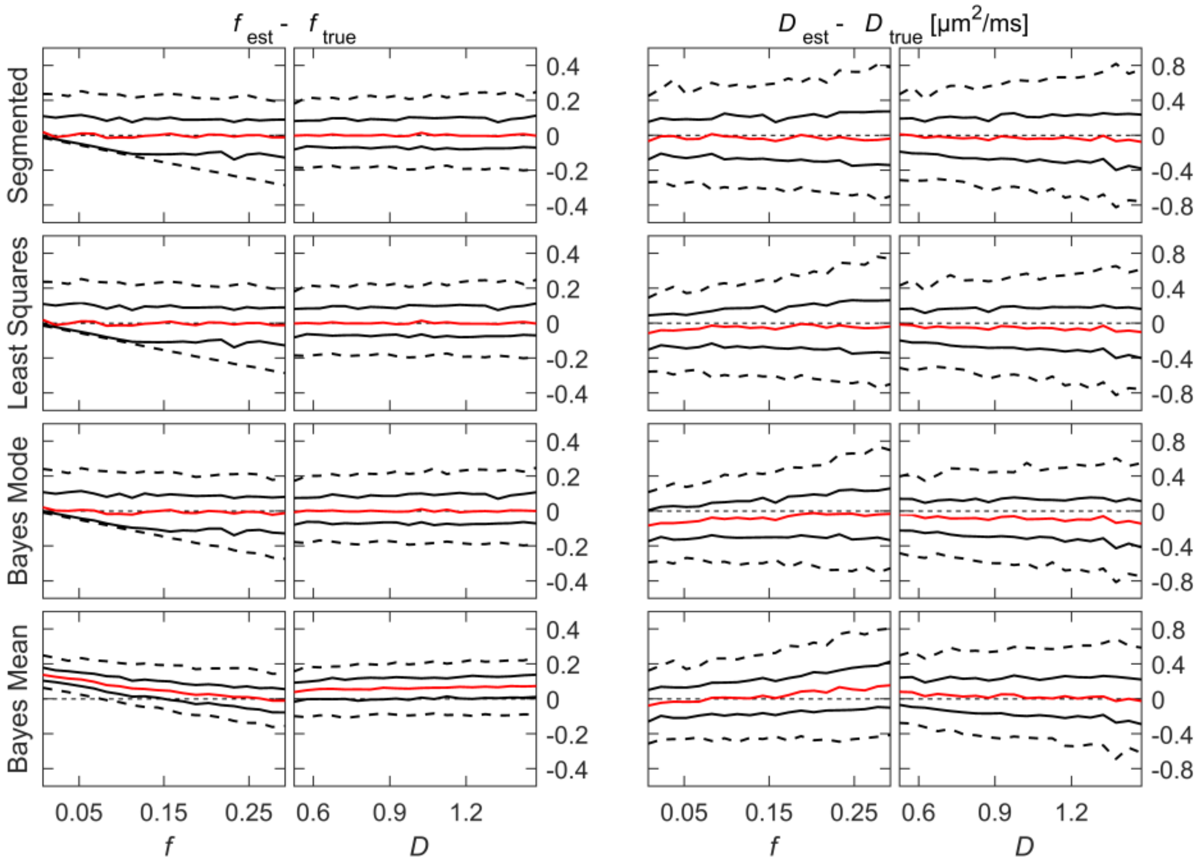

Fig. S1 Parameter estimation error for simulated data (SNR = 10) plotted as a function of simulated parameter value. The plotted lines in a single plot show the 1st, 25th, 50th, 75th and 99th percentiles. The horizontal dotted black line show zero error

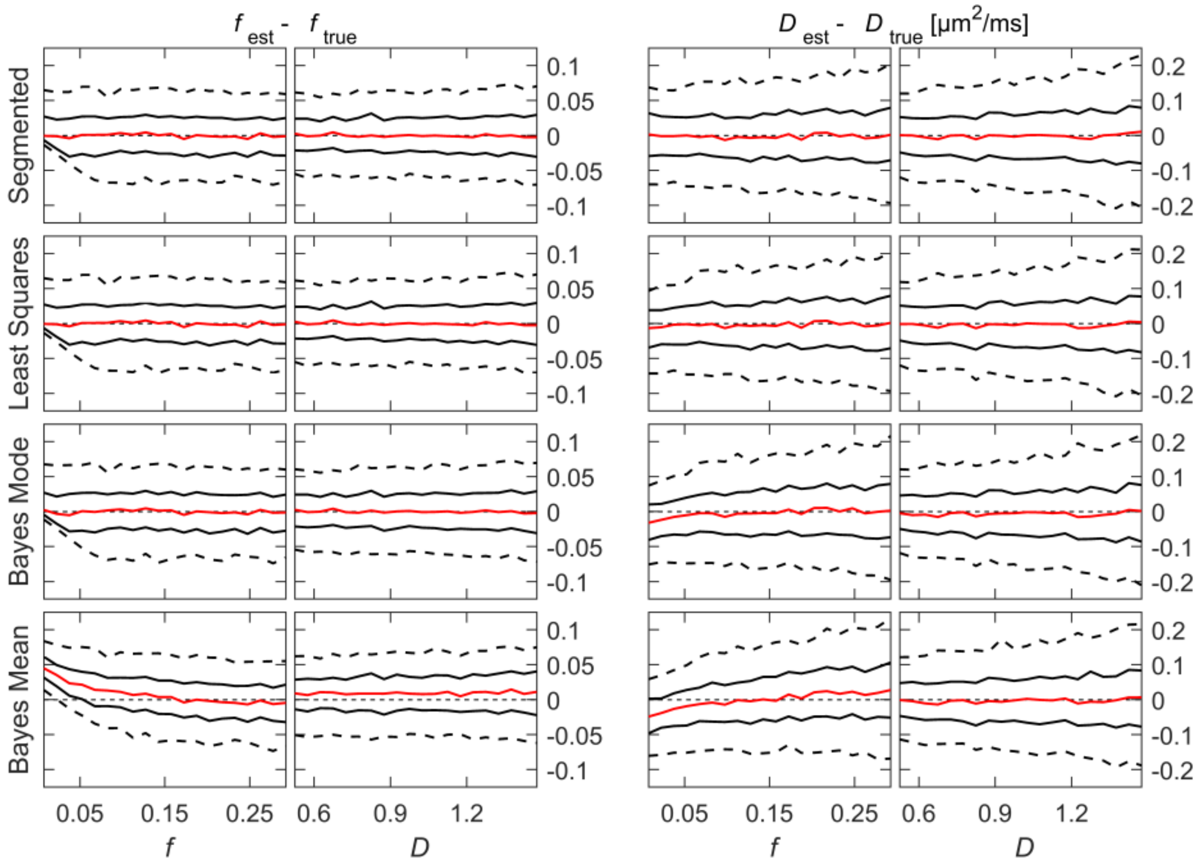

Fig. S2 As S1, but SNR = 40. Note the different scales on the y-axes

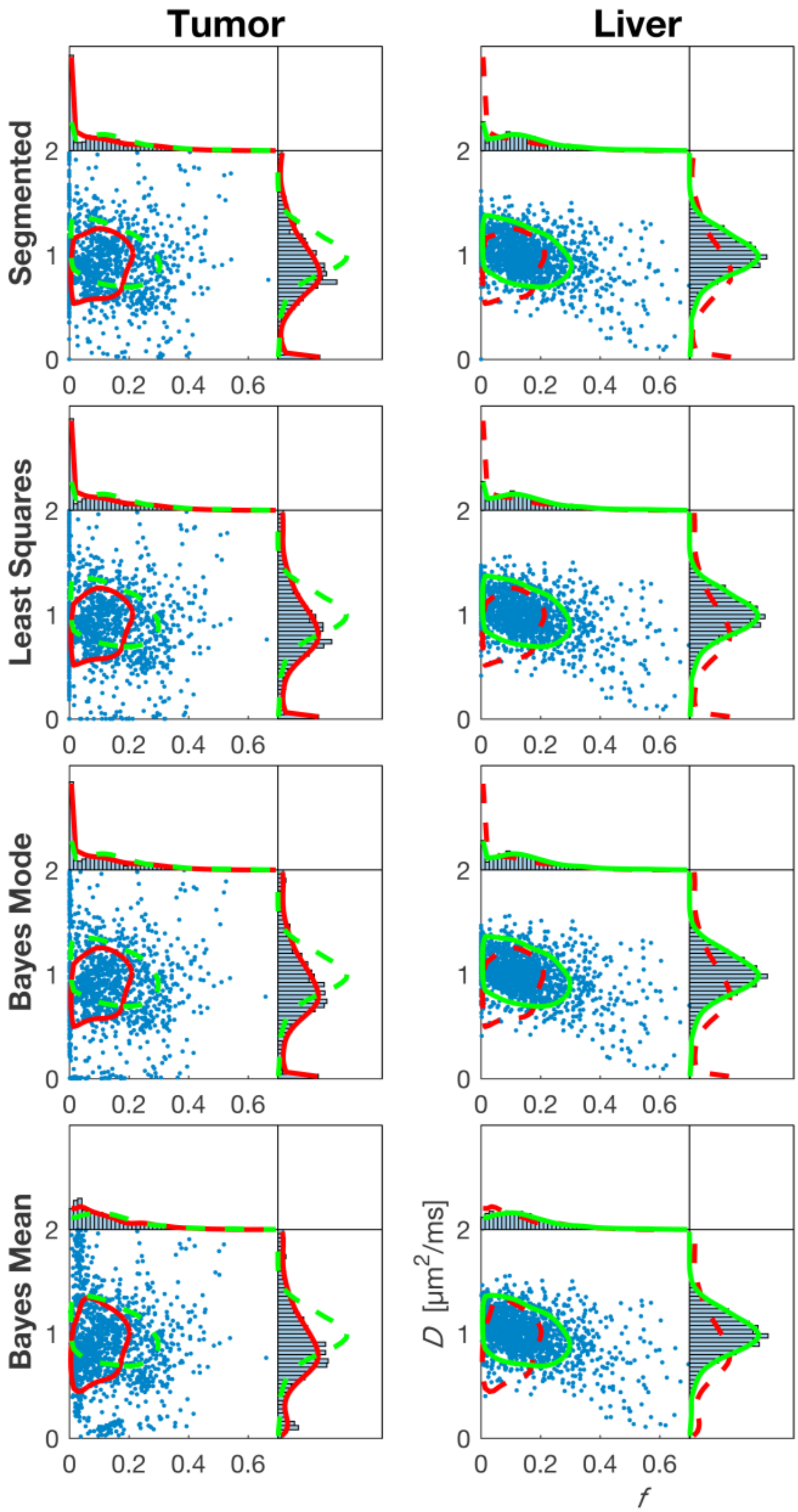

Fig. S3 Scatter plots and histograms showing the distribution of voxel values of *D* and *f* in tumor and healthy liver tissue at three months after treatment for each model fitting approach. Kernel density estimates of tumor (red) and liver (green) are overlaid on the scatterplots and histograms (solid line) and reproduced in the other tissue type (dashed line) for comparison. The two-dimensional kernel density estimate is represented by a contour at an arbitrarily chosen level (same in all plots)

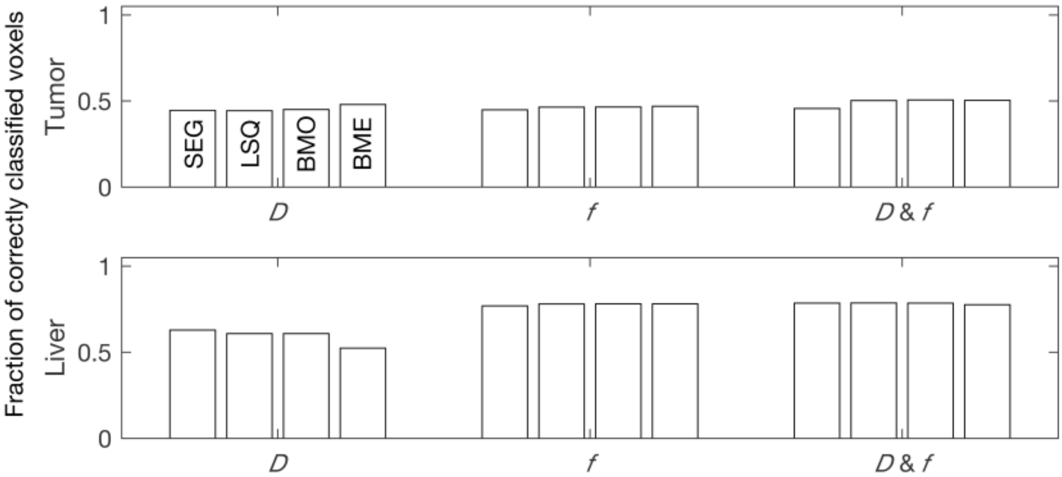

Fig. S4 Classification performance between tumor and healthy liver tissue for all four evaluated approaches: segmented fitting (SEG), least-squares fitting (LSQ), and Bayesian fitting using either the posterior marginal modes (BMO) or the posterior means (BME), based on D and f at three months after treatment. The bars show the average fraction of correctly classified voxels given by the cross validation. The classifier was trained using D, f or both D and f (indicated under each corresponding group of bars in the graph)