Fitting correlated data in AFM force distance curves

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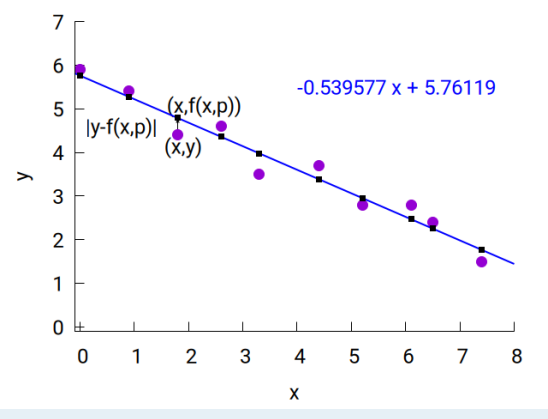
Multimodal Microscopy Workshop 2025

Different approaches on what to optimize (with different names in different context)

Least Squares

$$\min \sum_{i=1}^{N} (y_i - f(x_i))^2$$

sum of squared vertical distances between data and curve



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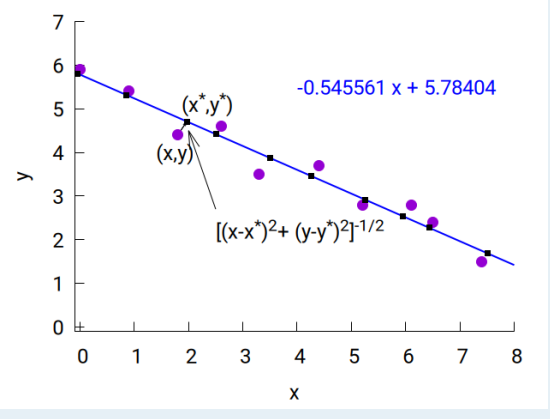
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Orthogonal Least Squares

$$\min \sum_{i=1}^{N} (x_i - x_i^*)^2 + (y_i - f(x_i^*)))^2$$

sum of squared perpendicular distances between data and curve



Curve fitting

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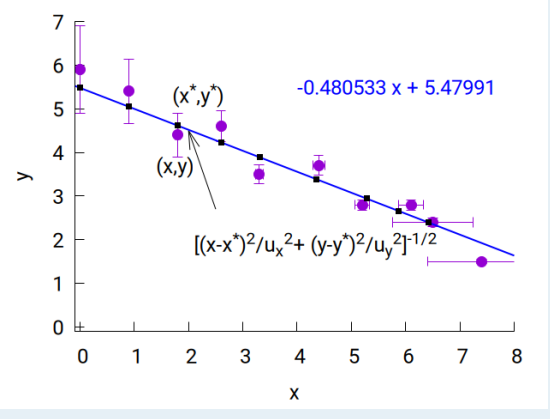
$$\min \sum_{i=1}^{N} (x_i - x_i^*)^2 + (y_i - f(x_i^*)))^2$$

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Weighted orthogonal Least Squares

$$\min \sum_{i=1}^{N} \frac{(x_i - x_i^*)^2}{u_{x,i}^2} + \frac{(y_i - f(x_i^*)))^2}{u_{y,i}^2}$$

sum of squared perpendicular distances between data and curve, weighted by uncertainties



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Errors in Variables

$$\min \left((\mathbf{x} - \mathbf{x}^*)^\mathbf{T} (\mathbf{y} - \mathbf{f}(\mathbf{y}^*))^\mathbf{T}\right) \begin{pmatrix} U_{xx} & U_{xy} \\ U_{xy} & U_{yy} \end{pmatrix}^{-1} \begin{pmatrix} (\mathbf{x} - \mathbf{x}^*) \\ (\mathbf{y} - \mathbf{y}^*) \end{pmatrix}$$

sum of squared distances between data and curve, inverse co-variance matrix as metric

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We get different estimates (and uncertainties) for each approach !

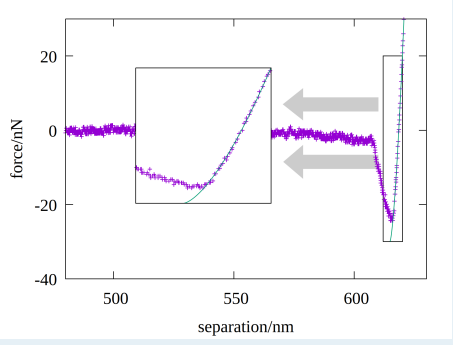
(-0.540, 5.761) vs. (-0.546, 5.784) vs. (-0.481, 5.480)

AFM FD curves

Measure position of cantilever z, deflection of cantilever d
Calculate separation $s = z - d$
Calculate force $F = kd$

Fit with Derjaguin-Muller-Toporov model

$$F = as^{3/2} + F_{\mathrm{adh}}$$

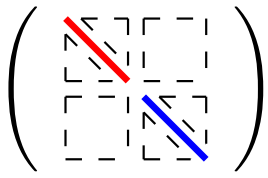


where a depends on material properties E and ν and tip radius R

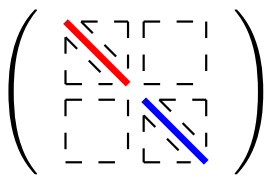
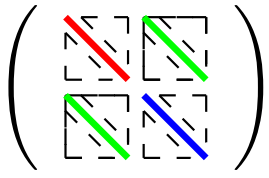
$$a = \frac{4}{3}\frac{E}{1-\nu^2}R^{1/2}$$

Examples of correlation

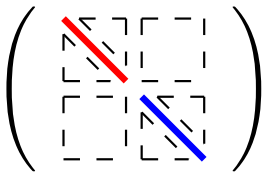
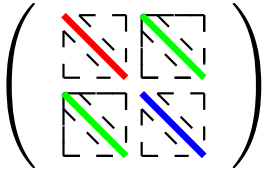
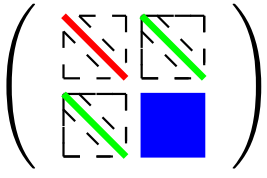
No correlation covariance matrix is diagonal



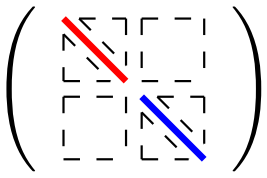
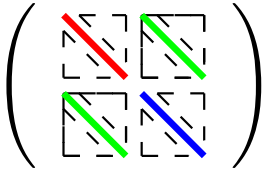
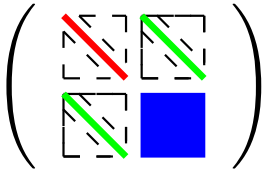
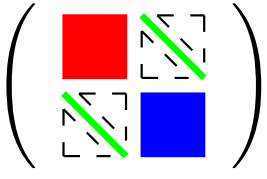
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Deflection used in both force and separation	non zero covariance between force and separation, block diagonal covariance matrix	

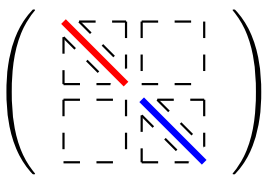
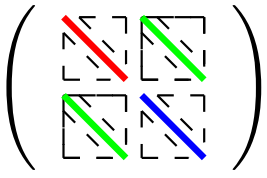
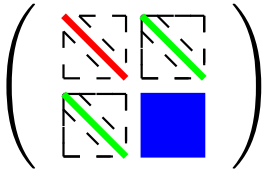
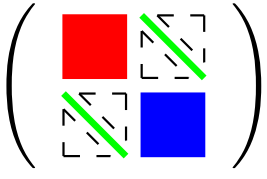
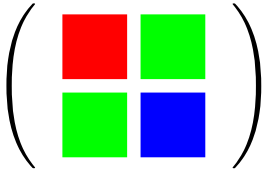
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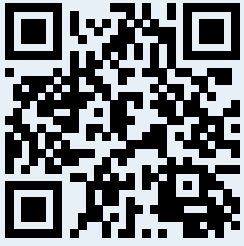
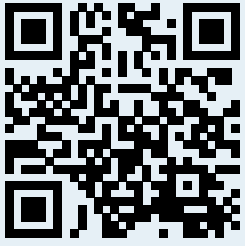
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Contact point	non zero covariance between individual separation data, full separation-separation covariance matrix	
Deflection sensitivity	non zero covariance between any pair of separation and force data, full covariance matrix	

Code available:

- uncertainty in x and y (e.g. ODRPACK, onls)
- uncertainty in x, y, correlation between x_i, y_i (e.g. ODRPACK)
- full uncertainty matrix U_{xx}, U_{yy} for selected functions (e.g. CCC)
- full uncertainty matrix U for explicit and implicit function (e.g. OEFPIL)


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Thank you for your attention.

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