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Technical note

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A Procedure for Determining Parameters of a Simplified Ligament Model

TECHNICAL NOTE

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ABSTRACT

A previous mathematical model of ligament force-generation treated their behavior as a population of collagen fibres arranged in parallel. When damage was ignored in this model, an expression for ligament force in terms of the deflection, x, effective stiffness, k, mean collagen slack length, μ, and the standard deviation of slack lengths, σ, was obtained. We present a simple three-step method for determining the three model parameters (k, μ, and σ) from force-deflection data: (1) determine the equation of the line in the linear region of this curve, its slope is k and its x-intercept is $-\mu$; (2) interpolate the force-deflection data when x is $-\mu$ to obtain F_0; (3) calculate σ with the equation $\sigma = \sqrt{2\pi} F_0 / k$.

Results from this method were in good agreement to those obtained from a least-squares procedure on experimental data – all falling within 6%. Therefore, parameters obtained using the proposed method provide a systematic way of reporting ligament parameters, or for obtaining an initial guess for nonlinear least-squares.

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INTRODUCTION

Some ligaments, on a histological level, are composed of a population of collagen fibres arranged parallel to one-another (Chazal et al., 1985; Kumar, 2001). The primary function of ligaments is to maintain the structural integrity of joints by transmitting tensile forces between bones. A secondary, but equally important, role is sensory in nature, which provides proprioceptive information (Johansson, 1991; Solomonow, 2004). Damage to ligaments alters the stability of joints, may cause pain, and may be a catalyst for chronic disorders like osteoarthritis (Kumar, 2001). Because of their pivotal role in healthy joint function, accurate models of their force-production behavior have far-reaching applications from improving larger scale biomechanical models to aiding foundational research that examines the function of ligaments.

Ligaments respond to tensile loading with a characteristic force-deflection curve: featuring a prominent toe region immediately followed by a linear region (Chazal et al., 1985; Frisén et al., 1969a, 1969b; Rigby et al., 1959). The toe region is attributed to the progressive recruitment of collagen fibres as they uncrimp in resisting the applied load (Franchi et al., 2007). As more fibres are gradually involved in providing tension, there is a corresponding gradual increase in the stiffness of the ligament. As there are only a finite number of collagen fibres in a ligament, this process saturates as the stiffness reaches a constant value. With continued stretching the fibres progressively break as their individual tolerance is exceeded. Eventually this can cumulate into complete ligament rupture. This mechanism has now been represented in a model (Barrett and Callaghan, 2017), which, when failure is ignored, encapsulates the toe and linear region behavior with Equation 1.

$$F(x;k,\sigma,\mu)=\frac{k\sigma}{\sqrt{2\pi}}\exp\left(-\frac{(\mu+x)^2}{2\sigma^2}\right)+\frac{k(\mu+x)}{2}\left[\operatorname{erf}\left(\frac{\mu+x}{\sqrt{2}\sigma}\right)+1\right] \quad (1)$$

Here, F is the force produced by a ligament and x is its elongation. There are three parameters: k, the ligaments effective stiffness; σ, which describes the standard deviation of collagen slack lengths; μ is the average collagen slack length; and $\operatorname{erf}(\cdot)$ is the error-function. Here we present a straightforward method for determining these parameters from experimental data. In addition, we attempt to disseminate the implications each model parameter in Equation 1 has on the resulting shape of the force-deflection curve.

METHODS

2.1 A Stepwise Parameter Finding Technique

With an increase in x, Equation 1 is asymptotically equivalent to the equation of a line with slope k and intercept μk (Equation 2). This is because the first term tends to zero, while the term in the square brackets tends to two. This coincides with the linear region from the model, and thus, measuring the slope of the ligament's linear region is equivalent to k.

$$\ell(x)=k(\mu+x) \quad (2)$$

This equation has an x-intercept at $x=-\mu$, thus, extending this line to the x-axis gives the value for μ. Denoting the x-intercept as x_0, with corresponding force-value of F_0. Substituting $x=x_0=-\mu$ into Equation 1, the second term becomes zero and the exponential in the first term becomes unity. This yields a relationship between σ, k and F_0 which can be rearranged for σ:

$$\sigma = \frac{\sqrt{2\pi}\, F_0}{k} \tag{3}$$

Where F_0, in this investigation, was obtained using third-order spline interpolation on the original force-deflection curve. This process is graphically illustrated in Figure 1.

[Please Insert Figure 1 Here]

This method was applied to the force-deflection data from Mattucci (2011) for the anterior longitudinal ligament of the middle cervical spine (C4-C6) of males loaded at a low strain-rate (0.5 /s). Results using this stepwise procedure were compared to a nonlinear least-squares method fitted to the data provided by the scipy python package. The initial guess for the fitting algorithm were the parameters identified through this stepwise procedure. The linear region was pre-determined by Mattucci (2011) using the methods of Chandrashekar (2008).

2.2 Sensitivity Analysis and Compliance Function from Equation 1

To perform a sensitivity analysis on Equation 1, its partial derivative was taken with respect to each parameter (k, μ, σ), and evaluated at the parameter values obtained using the stepwise method (c.f. Cashaback et al., 2014). We plotted these partial derivatives over a range of displacements to determine which regions were more sensitive to changes in which parameters. Additionally, we increased and decreased each parameter value by 10%, independently, and noted the corresponding change in the resulting force-deflection curve, to provide further analysis on these parameters.

Calculating tendon compliance is a crucial step in solving the differential equations that govern the Hill-type muscle model (Zajac, 1989). As tendons and ligaments are similar histologically, it stands to reason that Equation 1 may also be useful as a model of tendon force. We have included the compliance function calculated from Equation 1 in Appendix B.

RESULTS

The results obtained from this simplified method compare very well to using a non-linear least-squares optimization (Table 1), and the resulting curves from the two methods agree very well with experimental data (Figure 2).

[Please Insert Tables 1]

[Please Insert Figure 2 Here]

Perturbations in each parameter resulted in noted changes to the force-deflection curve (Figure 3). Of note, the effects of σ perturbations are quite small, indicating that it takes a fairly substantial perturbation in σ to induce notable changes. Unaltered partial derivatives are calculated and presented in Appendix A.

[Please Insert Figure 3 Here]

DISCUSSION

The proposed method, along with a rigorous sensitivity analysis clarifies how the parameters in Equation 1 interact with one-another in relation to the force-elongation curve. For instance, the effective collagen stiffness, k, is the slope of the linear region of the force-deflection curve (Figure 4): exactly what has been reported in several previous ligament studies (Chandrashekar et al., 2008; Chazal et al., 1985; Trajkovski et al., 2014; Yoganandan et al., 1989). The parameter μ acts as a translation of the force-deflection curve along the x-axis, and essentially quantifies the overall slack length of the ligament. This result is not surprising, as μ represents the average slack length of collagen fibres in the underlying mechanistic model. Finally, σ quantifies the “sharpness” of the toe-region, that is, how quickly the curve transitions from zero-force to the linear region. In particular, a smaller σ is indicative of a more rapid transition from the toe region to the linear region. Together these parameters give future investigators new measures that can be used to compare ligament mechanics between experimental conditions.

The least-squares method provides parameter estimates that are averaged across the entire force-deflection curve, which is appealing since it does not entirely depend on the accuracy of two points on the force-deflection curve. To this end, the proposed method, at the very least, provides a good starting point for a non-linear least-squares optimization approach, seeing as these values are similar to those obtained by least-squares. Using the values obtained here may provide a suitable initial guess for a nonlinear optimization routine to ensure that it falls in a successful local minimum.

Using Equation 1 provides two advantages when compared to its alternatives: an experimental advantage and a modelling advantage. From an experimental point-of-view, deriving parameters using this standardize approach allows for easier comparison between studies. Currently, studies characterizing the mechanical properties of ligaments measure the slope of the linear region (Bass et al., 2007; Chazal et al., 1985; Trajkovski et al., 2014; Yoganandan et al., 1989), there have also been those which report the secant slope (the average rate of change in force with respect to elongation) from onset to failure (Przybylski et al., 1996; Shim et al., 2006). Additionally, little attention has been payed to the toe region, with parameter studies abstracting the force-deflection curve as either a piecewise-linear (Chandrashekar et al., 2008) or piecewise-quadratic (Li et al., 1999) approximation which does not respect its underlying mechanism. The lack of standardization makes it difficult to compare stiffness values across studies, and impossible to appraise potential differences in the toe region. The proposed method is an approach that can address these limitations by offering a systematic means of arriving at parameters, which have physical interpretation that are derived from a mechanistic model of ligament force generation behaviour. Secondly, using Equation 1 in biomechanical models is that it is infinitely differentiable. This means that it is straightforward to evaluate instantaneous stiffness or compliance values (see Appendix B), which may be useful in future biomechanical models. Since tendons and ligaments are similar histologically, and portray similar force-elongation curves (Gutsmann et al., 2004), Equation 1 may also be useful for quantifying the tendon compliance in forward dynamic biomechanical models.

The most substantial limitation of this model is its oversimplification of ligament histology. Indeed, ligaments are inherently more complex than bands of collagen fibres arranged in parallel: some have collagen fibres spanning many directions, while others contain a considerable amount of elastin relative to collagen. Inclusion of these histologies requires a generalization to three dimensions and the inclusion of elastin as part of the mechanistic model.

CONCLUSION

The proposed method for ascertaining ligament force-displacement parameters in the toe and linear regions was successful. This simple analytic method performed similar to a non-linear least-squares routine. It may be useful for future investigators to quantify characteristic parameters of these regions in ligament loading. Furthermore, it highlights how the parameters in Equation 1 interact in relation to the force-elongation curve.

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CONFLICT OF INTEREST STATEMENT

We declare that we have no financial or personal relationships with people or organizations which could alter the integrity of our work.

APPENDIX A

In analyzing the partial derivatives of Equation 1, it became clear that the model is mainly sensitive to k and μ in the linear region, and σ in the toe region (Figures 3 and 4).

[Please insert Figure 4 Here]

APPENDIX B

Equation 1 is not easily invertible. However, the derivative of its inverse (sometimes termed ligament or tendon compliance) can be easily computed by way of the Inverse Function Theorem. To begin with we have the derivative of Equation 1 with respect to displacement:

$$\frac{dF}{dx} = \frac{k}{2}\left(\operatorname{erf}\left(\frac{\mu + x}{\sqrt{2}\sigma}\right) + 1\right) \tag{A.1}$$

From the inverse function theorem we have:

$$\frac{dx}{dF} = \left(\frac{dF}{dx}\right)^{-1} \tag{A.2}$$

And so the compliance is given by:

$$\frac{dx}{dF} = \frac{2}{k\left(\operatorname{erf}\left(\frac{x + \mu}{\sqrt{2}\sigma}\right) + 1\right)} \tag{A.3}$$

And this is a useful function of displacement, which are the variables that the differential equations which it applies to (c.f. Zajac, 1989) are cast in.

NOMENCLATURE

F	Force
x	Displacement from neutral
μ	The average slack length in the population of collagen fibres.
σ	The standard-deviation of slack lengths in the population of collagen fibres.

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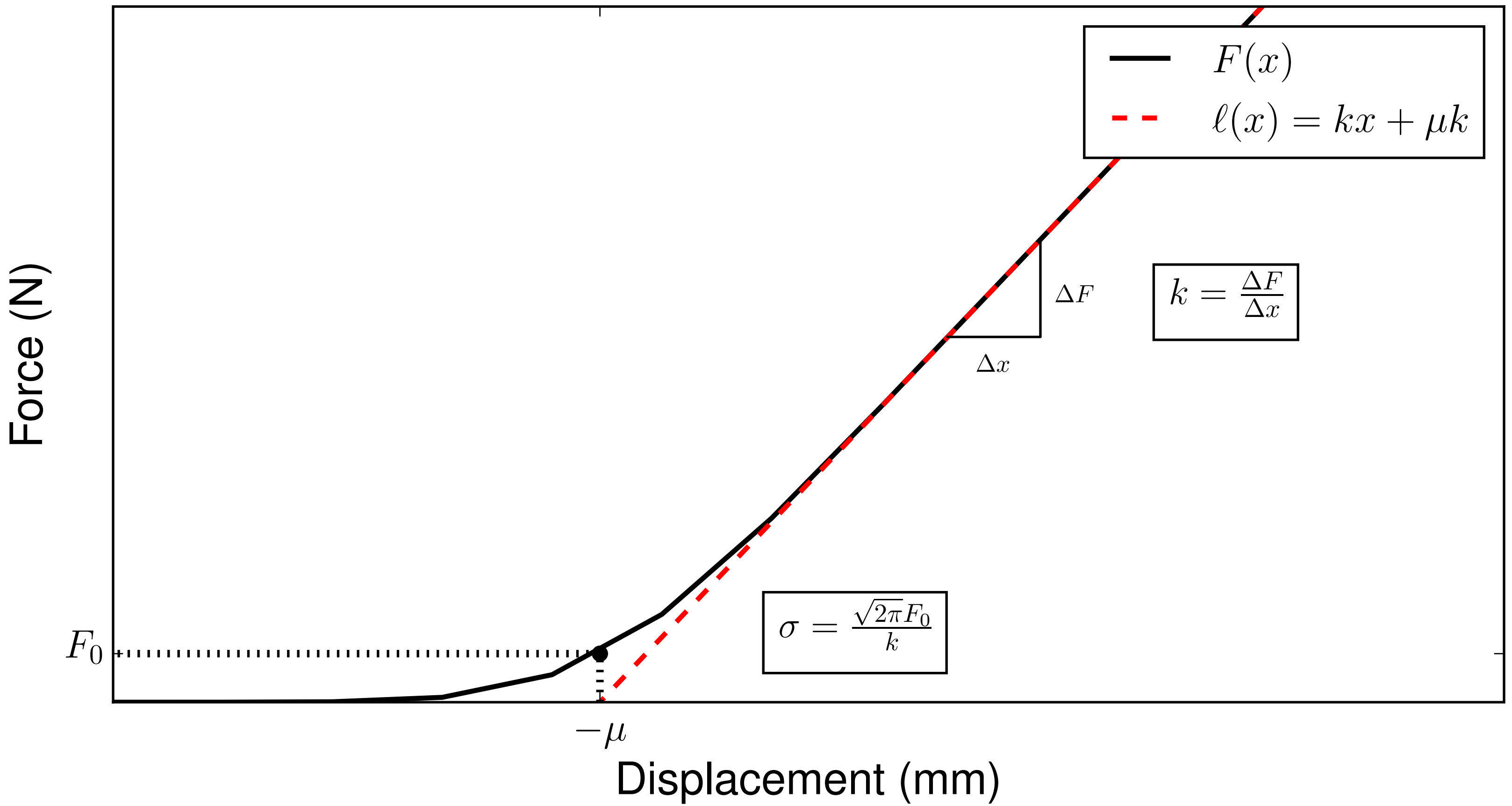
Figure 1: A graphical representation of the procedure for obtaining model parameters. Starting with a Force-Deflection Curve, obtained from experimental data (F(x)), continuing the line from the linear region to the x-axis provides -μ. Taking a vertical line from this point up to the original Force-Deflection curve gives the value F_0, which can be used to calculate σ, with k being the slope of the linear region of the original force displacement data.

Figure 2: Comparison of the fit between the piecewise method, least-squares and the data presented by Mattucci (2011).

Figure 3: Response of the force-deflection curve to 10% changes in parameters. In each case, the black line indicates the force-deflection curve using parameters obtained from the stepwise procedure, and the grey lines what the curve looks like once a given parameter has been perturbed by 10%. On the left, k has been perturbed by 10%; in the middle, the parameter is μ and; on the right, it is σ that has undergone the perturbation. Note that changes in σ yield very small responses on the force-deflection curve (the inset) magnifies part of the toe region where changes in σ impact the curve.

Figure 4: Partial derivatives of $F(x; k, \mu, \sigma)$ with respect to its parameters.

Figure 1



Force (N)
Displacement (mm)
F_0
$-\mu$
$F(x)$
$\ell(x) = kx + \mu k$
ΔF
Δx
$k = \frac{\Delta F}{\Delta x}$
$\sigma = \frac{\sqrt{2\pi}F_0}{k}$

Figure 2

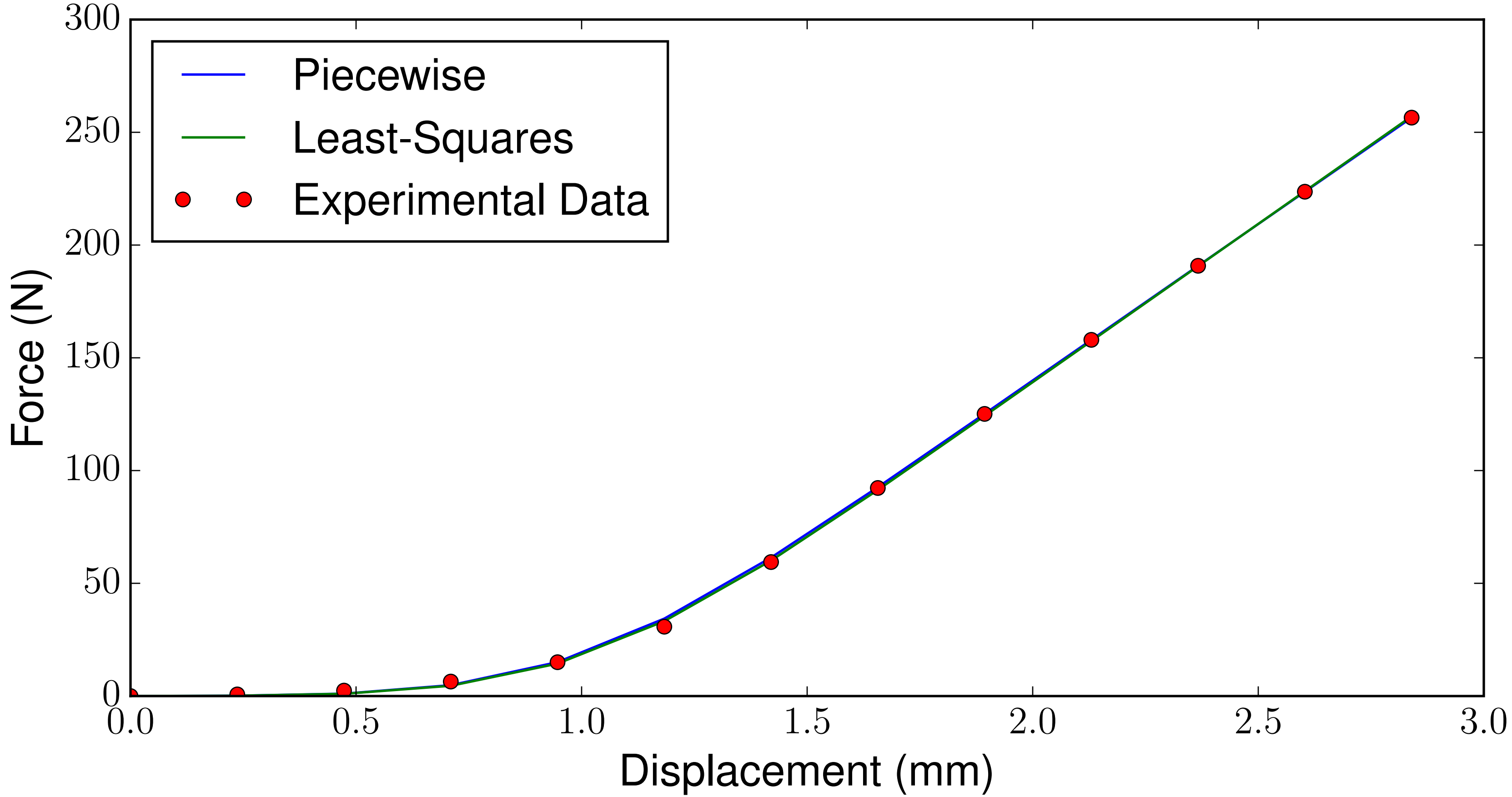
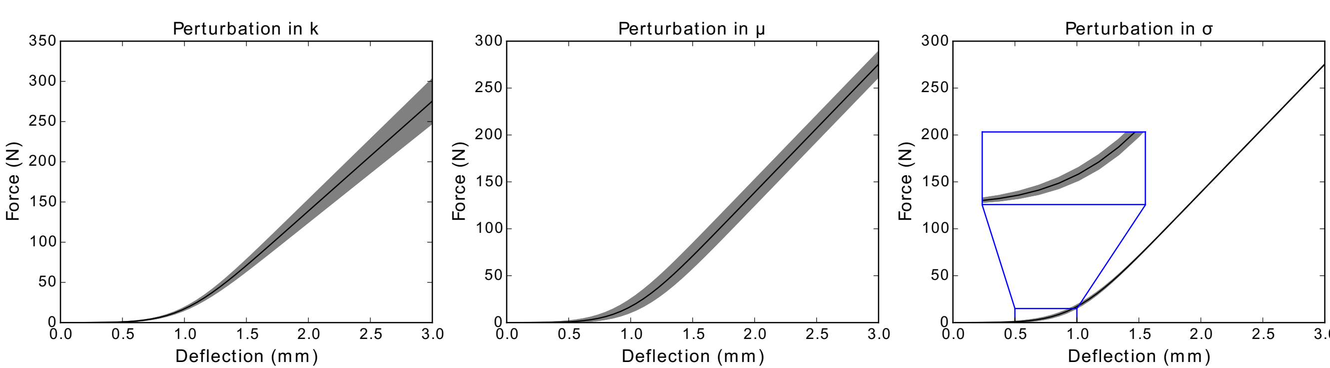

Piecewise
Least-Squares
Experimental Data
Force (N)
Displacement (mm)
0
50
100
150
200
250
300
0.0
0.5
1.0
1.5
2.0
2.5
3.0

Figure 3


Perturbation in k
Perturbation in μ
Perturbation in σ
Force (N)
Deflection (mm)
0
50
100
150
200
250
300
350
0.0
0.5
1.0
1.5
2.0
2.5
3.0

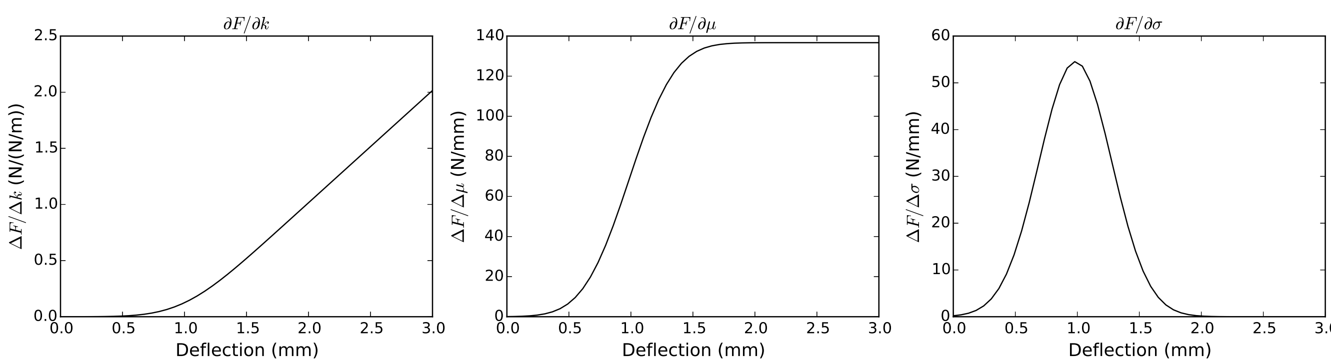

$\partial F/\partial k$
$\Delta F/\Delta k$ (N/(N/m))
Deflection (mm)
$\partial F/\partial \mu$
$\Delta F/\Delta \mu$ (N/mm)
Deflection (mm)
$\partial F/\partial \sigma$
$\Delta F/\Delta \sigma$ (N/mm)
Deflection (mm)

Table 1: Comparison of Parameters obtained from this method versus that of least-squares (k, σ, μ), and the coefficient of determination and the root-mean-squared error between each method and least-squares.

Parameter	Stepwise Method	Least-Squares
$\boldsymbol{k}$ (N/mm)	138.8	140.7
$\boldsymbol{\sigma}$ (mm)	0.3114	0.3302
μ (mm)	-0.992	-1.011
R^2	0.99979	0.99987
RMSD (N)	1.29	1.07