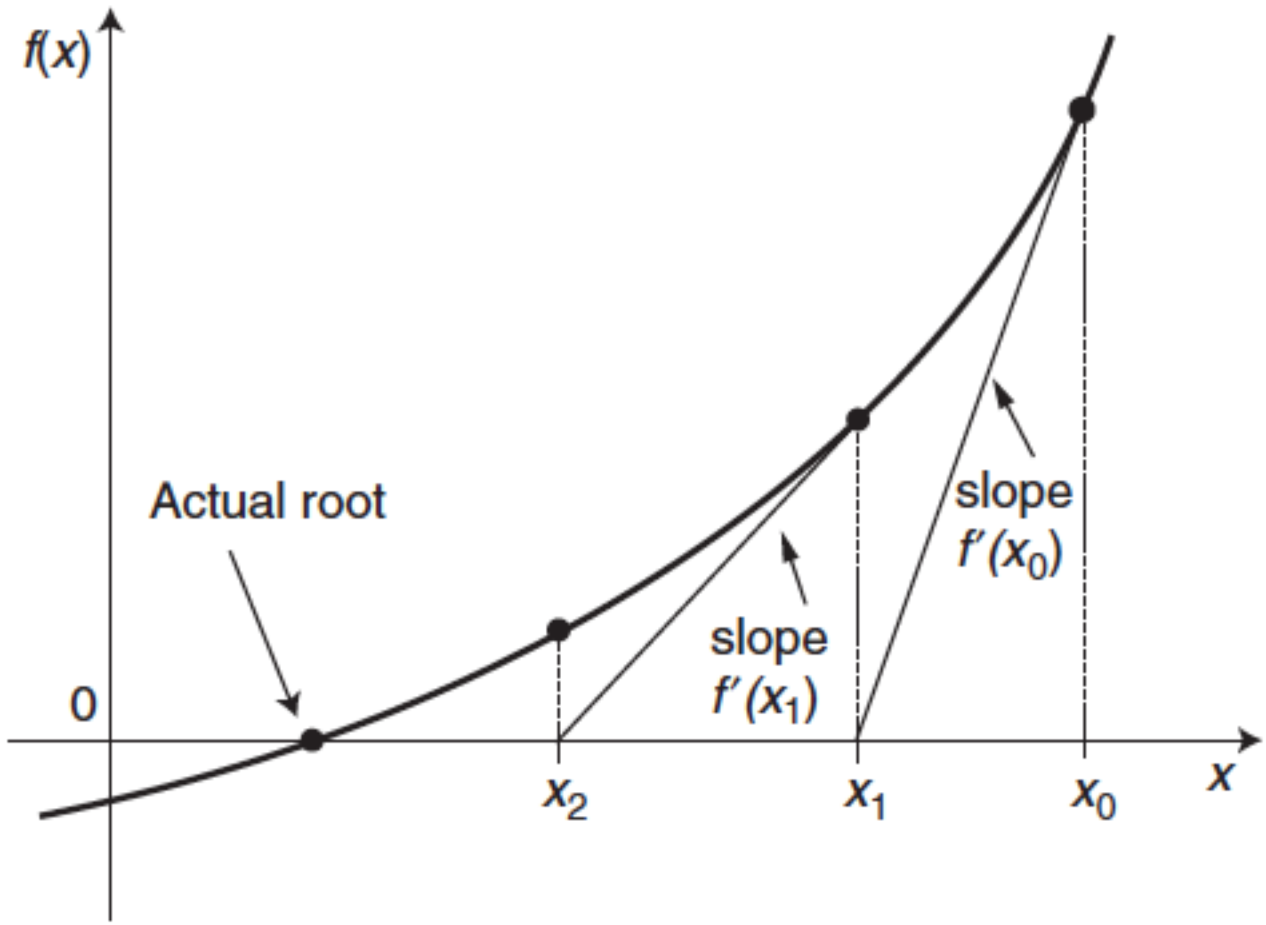
Newton’s Method

- Let’s look at a method with faster convergence: Newton’s Method.
- In this method we compute both $f(x_i)$ and $f'(x_i)$.
- We fit the function with a tangent line (e.g., truncate the Taylor series after the linear term) and find the root.
- This gives us our next guess!

Newton's Method

Illustration of Newton's method.



Newton's Method

- How do we get x_{i+1} ?

  $f(x) = f(x_i) + f'(x_i)(x - x_i) + \ldots$

  truncate here

- So set:

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

$$\boxed{x_{i+1} = x_i - f(x_i)/f'(x_i)}$$

Newton's Method

- Let's use this method to calculate the sqrt(2).
- This is equivalent to the root of:

  $f(x) = x^2 – 2 = 0$
- Thus, $f'(x) = 2x$
- and $f(x)/f'(x) = (x^2 – 2)/(2x)$
- So $x_{i+1} = x_i – (x_i^2 – 2)/(2x_i)$
- We start at $x_0 = 1$

Newton's Method

- Thus, $x_1 = 1 – (1 – 2)/2 = 1.5$

  $x_2 = 1.5 – (1.5^2 – 2)/3 = 1.41666...$

  $x_3 = 1.41666$

  $– (1.41666^2 – 2)/(2*1.41666)$

  $= 1.4142157...$
- Vs. exact solution $x^* = 1.4142136...$
- How fast did this converge?

Newton's Method

- $e_0 = 0.4142136$
  $e_1 = 0.085786$
  $e_2 = 0.002453038$
  $e_3 = 2.138 \times 10^{-6}$
- Actually, it's quadratic:
  $e_1/e_0^2 = 0.5$
  $e_2/e_1^2 = 0.333$
  $e_3/e_2^2 = 0.355$

Newton's Method

- Let's look at error in general.
- We have:

$$f(x) = f(x_i) + f'(x_i)(x^* - x_i) + 0.5f''(\xi)(x - x_i)^2$$

- Let $x = x^*$
- Thus, $0 = f(x_i) + f'(x_i)(x^* - x_i) + 0.5f''(\xi)(x^* - x_i)^2$
- Divide by $f'(x_i)$ and rearrange:

$$\overbrace{x^* - (\underbrace{x_i - f(x_i)/f'(x_i)}_{x_{i+1}})}^{e_{i+1}} = f''(\xi)/(2f'(x_i))*\underbrace{(x^* - x_i)^2}_{e_i^2}$$

Newton's Method

- Thus, $|e_{i+1}|/|e_i|^2 = |f''(\xi)/(2f'(x_i))| \sim c$

- So as $x_i \rightarrow x^*$, $c \sim |f''(x^*)/(2f'(x^*))|$

- For the example problem,

  $f''(x^*) = 2$, $f'(x^*) = 2*\mathrm{sqrt}(2)$ … $c = 0.354$

Newton's Method

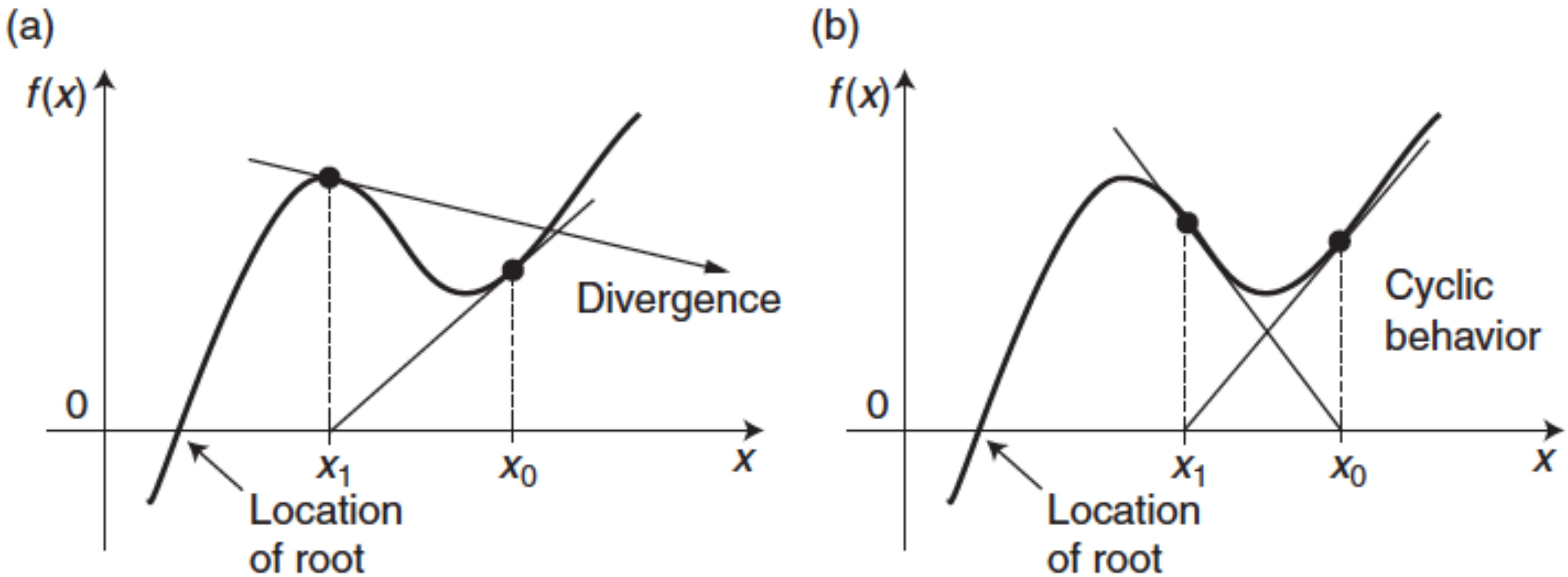
- Newton's method does not always converge!
- If $f'(x_i) \sim 0$ then $f(x_i)/f'(x_i)$ may be <u>very large</u>.
- If so, we will get a way out prediction for x_{i+1}.
- This is equivalent to $c >> 1$.
- We can fix this by requiring that:

  $|f(x_{i+1})| < |f(x_i)|$ and cutting down on the correction by halves until this is satisfied.

Newton's Method

Figure 5.10

Two situations in which Newton's method does not converge.



In general, you get into trouble if the first guess is too far off.

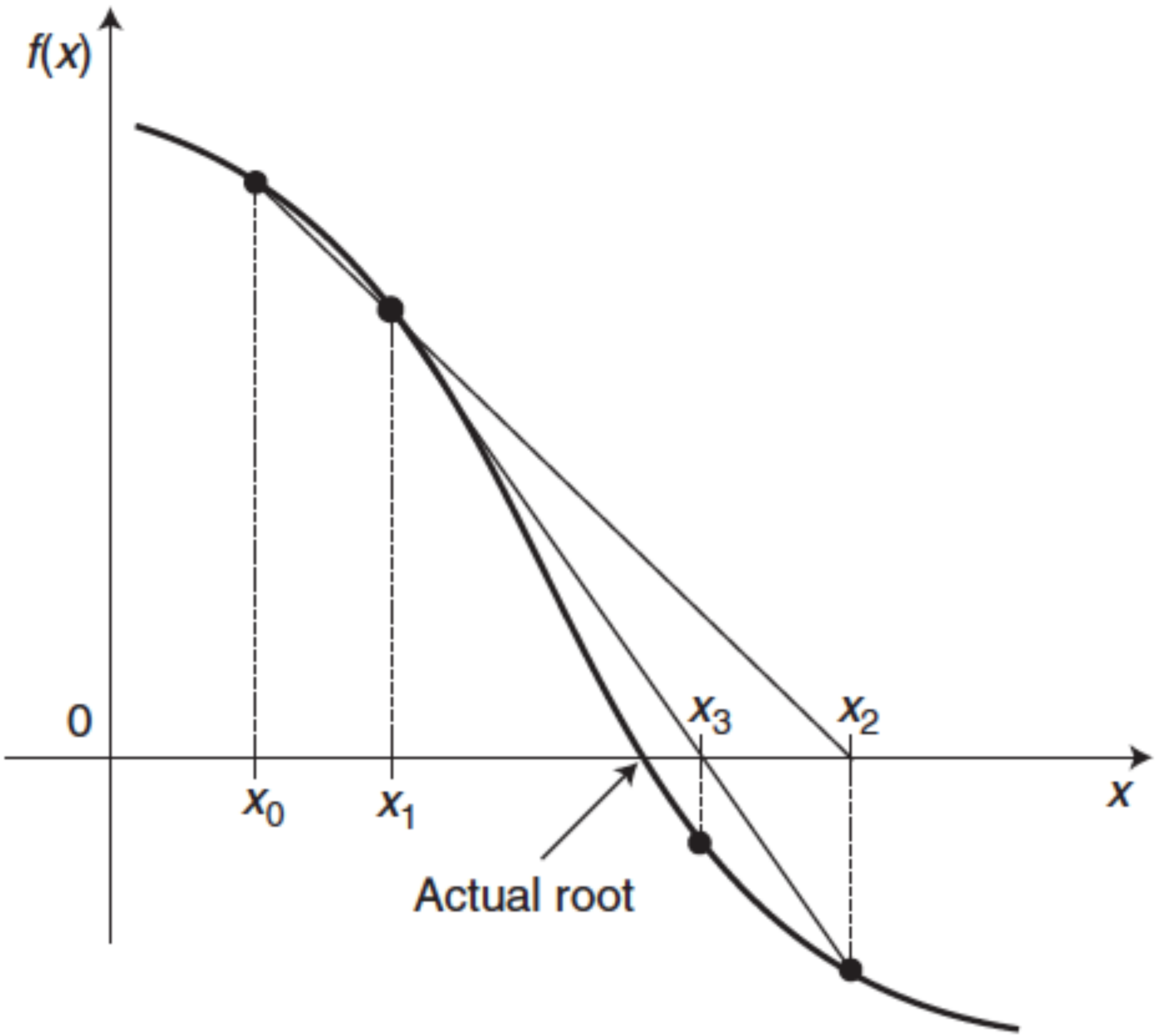
Secant Method

- Newton's method has the drawback that it requires <u>derivatives</u>.
- We can avoid this using the <u>secant method</u>.
- Start with two points x_{i-1}, x_i
- Compute the line through the points:

  $(x_{i-1}, f(x_{i-1})),\ (x_i, f(x_i))$
- Find the intercept to get x_{i+1} and then repeat.

Figure 5.13

Illustration of the secant method.



Secant Method

- The line is given by:

$$y = f(x_i) + (x - x_i)*(f(x_i) - f(x_{i-1}))/(x_i - x_{i-1})$$

- Thus,

$$\boxed{x_{i+1} = x_i - f(x_i)*(x_i - x_{i-1})/(f(x_i) - f(x_{i-1}))}$$

- This is just Newton's method where we approximate the derivative by:

$$f'(x_i) \sim (f(x_i) - f(x_{i-1}))/(x_i - x_{i-1})$$

- This converges a bit more slowly.

Secant Method

- One can show that:

$$|e_{i+1}|/|e_i|^{0.5(1+\mathrm{sqrt}(5))} = |f''(x^*)/(2f'(x^*))|^{1/0.5(1+\mathrm{sqrt}(5))}$$

- Where 0.5(1+sqrt(5)) = 1.618… > 1
- This method can fail to converge in the same ways as Newton’s method.

Q1: Linear equations can be solved in a finite number of steps.

A. True

B. False

Q1: Linear equations can be solved in a finite number of steps.

A. True

B. False

$\mathbf{Ax} = \mathbf{b}$ is solved in $O(N^3)$ number of steps.

Q2: Consider the temperature dependence of an irreversible chemical reaction.

$$k = ae^{-E_a / k_B T}$$

The modeling functions will define the A matrix in linear regression.

They are:

A. 1, $e^{-1/T}$

B. 1, 1/T

C. 1, $e^{-1/T}$, 1/T

D. a, E_a/kT

Q3: Consider the temperature dependence of an irreversible chemical reaction.

$$k = ae^{-E_a / k_B T}$$

The column vector of the dependent variable ("the data") is equal to:

A. $\mathbf{b} = (k_1, k_2, k_3, \ldots)^T$
B. $\mathbf{b} = (a_1, a_2, a_3, \ldots)^T$
C. $\mathbf{b} = (1/T_1, 1/T_2, 1/T_2, \ldots)^T$
D. $\mathbf{b} = (\log k_1, \log k_2, \log k_3, \ldots)^T$

Q4: If the chemical substance can follow 2 reaction pathways, then we are stuck with a nonlinear system:

$$k = a_1 e^{-E_{a1}/k_B T} + a_2 e^{-E_{a2}/k_B T}$$

The model (regression) parameters for this model are:

A. a_1, E_{a1}, k_B, a_2, E_{a2}
B. a_1, E_{a1}, T, a_2, E_{a2}
C. a_1, E_{a1}, a_2, E_{a2}
D. k, a_1, E_{a1}, a_2, E_{a2}

Langmuir **2003**, *19*, 1573−1579

Endothelial Cell Traction Forces on RGD-Derivatized Polyacrylamide Substrata[†]

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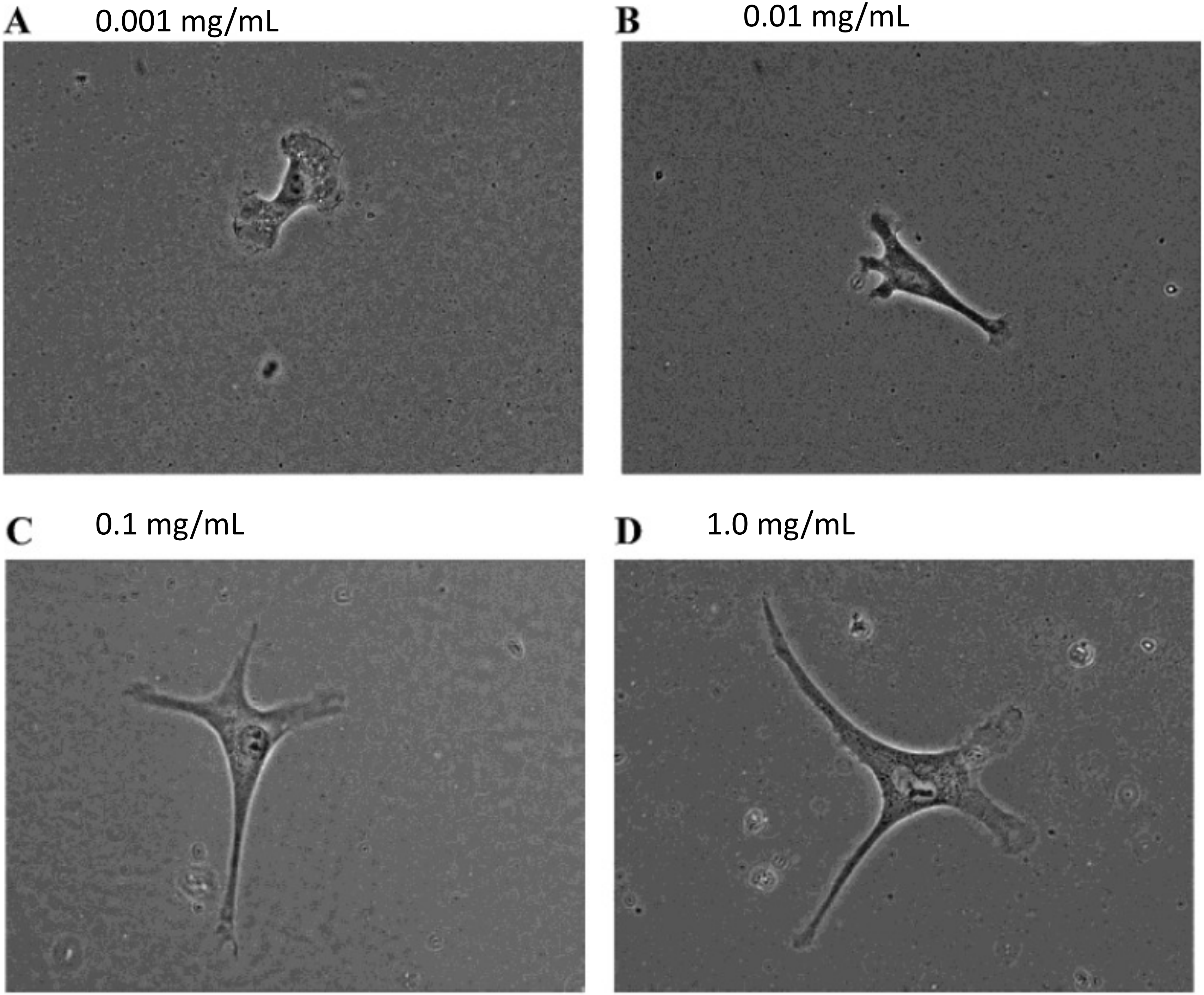
Received June 28, 2002. In Final Form: October 11, 2002

Receptor-mediated adhesion involves both mechanical and chemical signals occurring at the cell−substrate interface. Using a relatively new technique called traction force microscopy, the magnitude, direction, and spatial location of mechanical forces exerted by endothelial cells on a RGD-peptide-derivatized hydrogel substrate were measured. We constructed a surface with a controlled density of cell adhesion nonapeptide containing RGD, which can ligate endothelial cell integrin receptors and induce cell spreading. Increasing the concentration of the RGD peptide increases cell spreading on an otherwise nonadhesive surface of polyacrylamide, and cell area is a monotonically increasing function of peptide concentration. Correlating the force exerted by the cell to the cell area reveals that force is a linear, increasing function of cell area, with a mean increase in cell force of 10^4 dyn/cm^2 cell area. Additionally, we have found that tractions exerted by endothelial cells are concentrated at the ends of pseudopodia and are almost negligible under the nucleus. These results indicate that endothelial cells may have an internal structure that contacts and pulls on the substrate at concentrated locations within the tips of cell extensions and that the strength in adhesion increases with cell spreading.


A
0.001 mg/mL
B
0.01 mg/mL
C
0.1 mg/mL
D
1.0 mg/mL

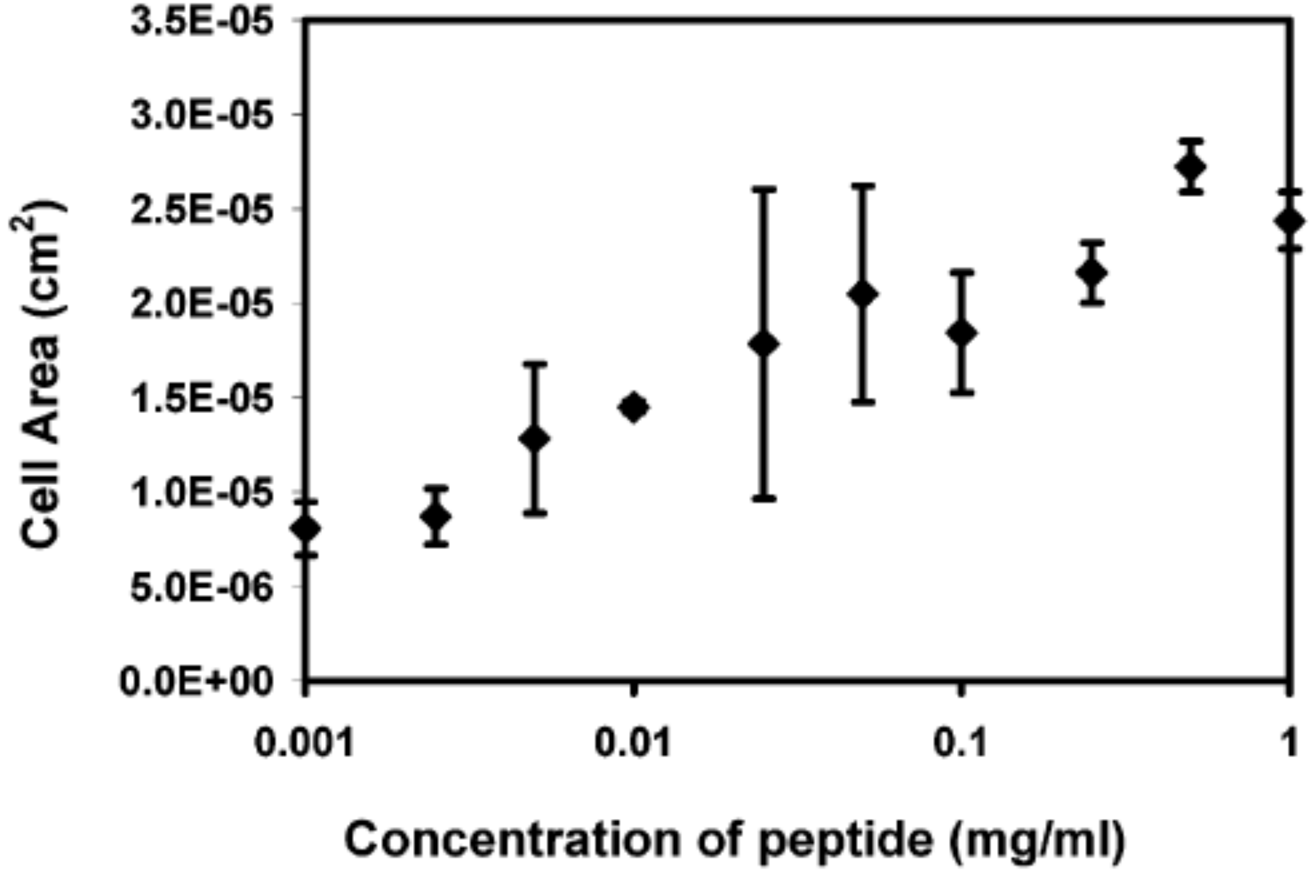


Figure 4. Cells were plated on polyacrylamide derivatized with an RGD-containing peptide. The graph shows the relationship between the RGD-peptide concentration and spread cell area. $n = 3$.

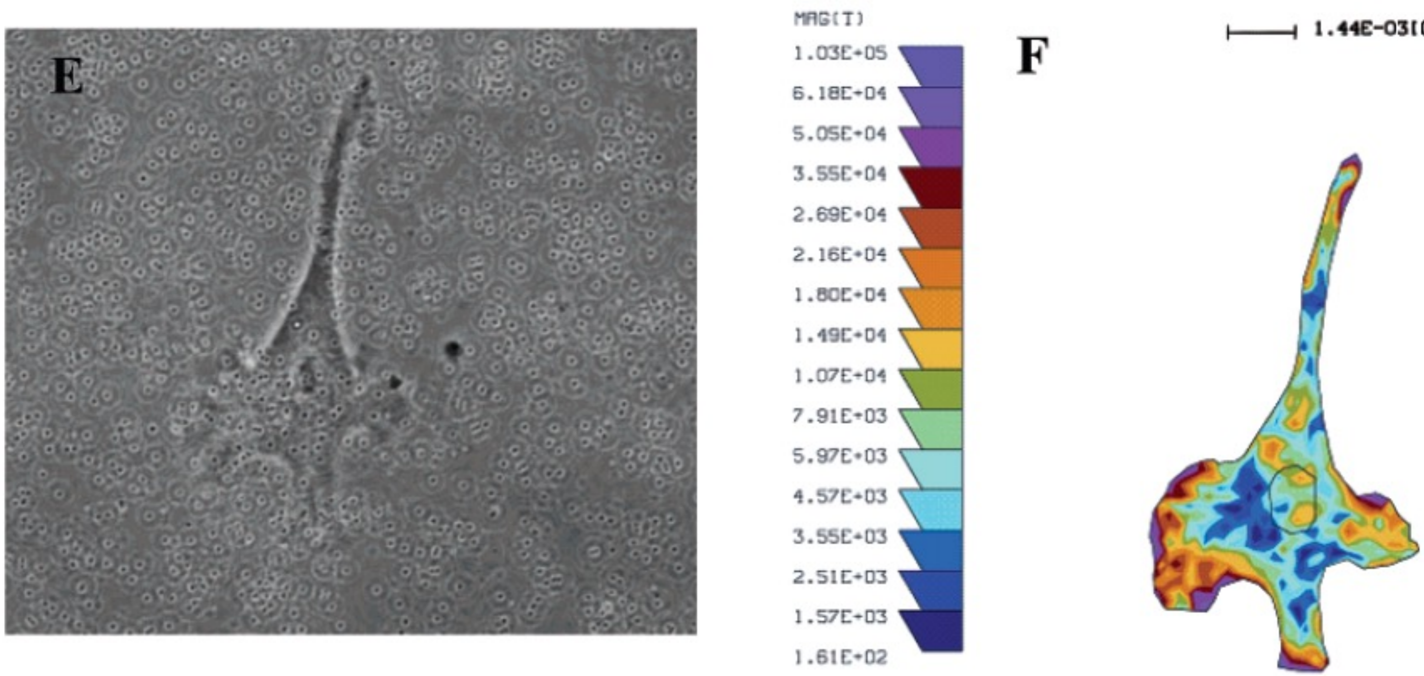


Figure 5. Traction forces of cells plated in polyacrylamide derivatized with an RGD-containing peptide were determined using traction force microscopy. (A,C,E) Phase images of BAECs taken at 40× magnification on (A) 0.001 mg/mL of RGD peptide, (C) 0.01 mg/mL of RGD peptide, and (E) 0.25 mg/mL of RGE peptide. (B,D,F). Color contour plot of the magnitudes of the traction stress exerted by the corresponding cells in panels A, C, and E.

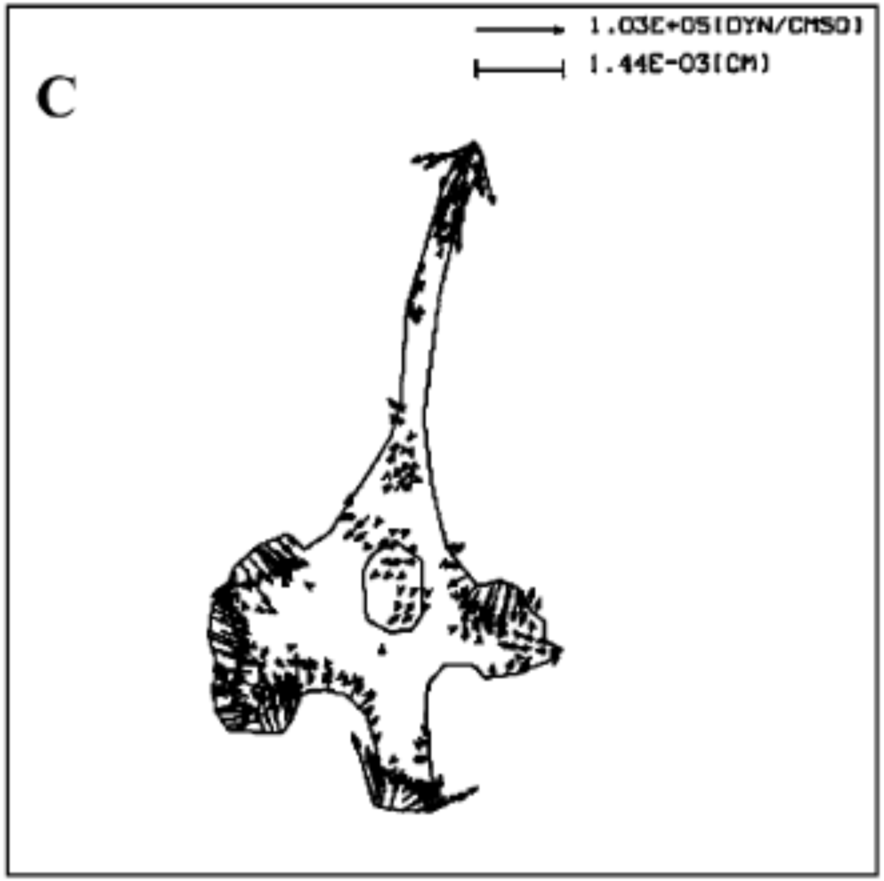


Figure 6. Traction stress renderings of the stresses exerted by the cells in Figure 5 represented by vectors within the cell boundary: (A) corresponds with cell A of Figure 5, (B) corresponds with cell C of Figure 5, and (C) corresponds with cell E of Figure 5.

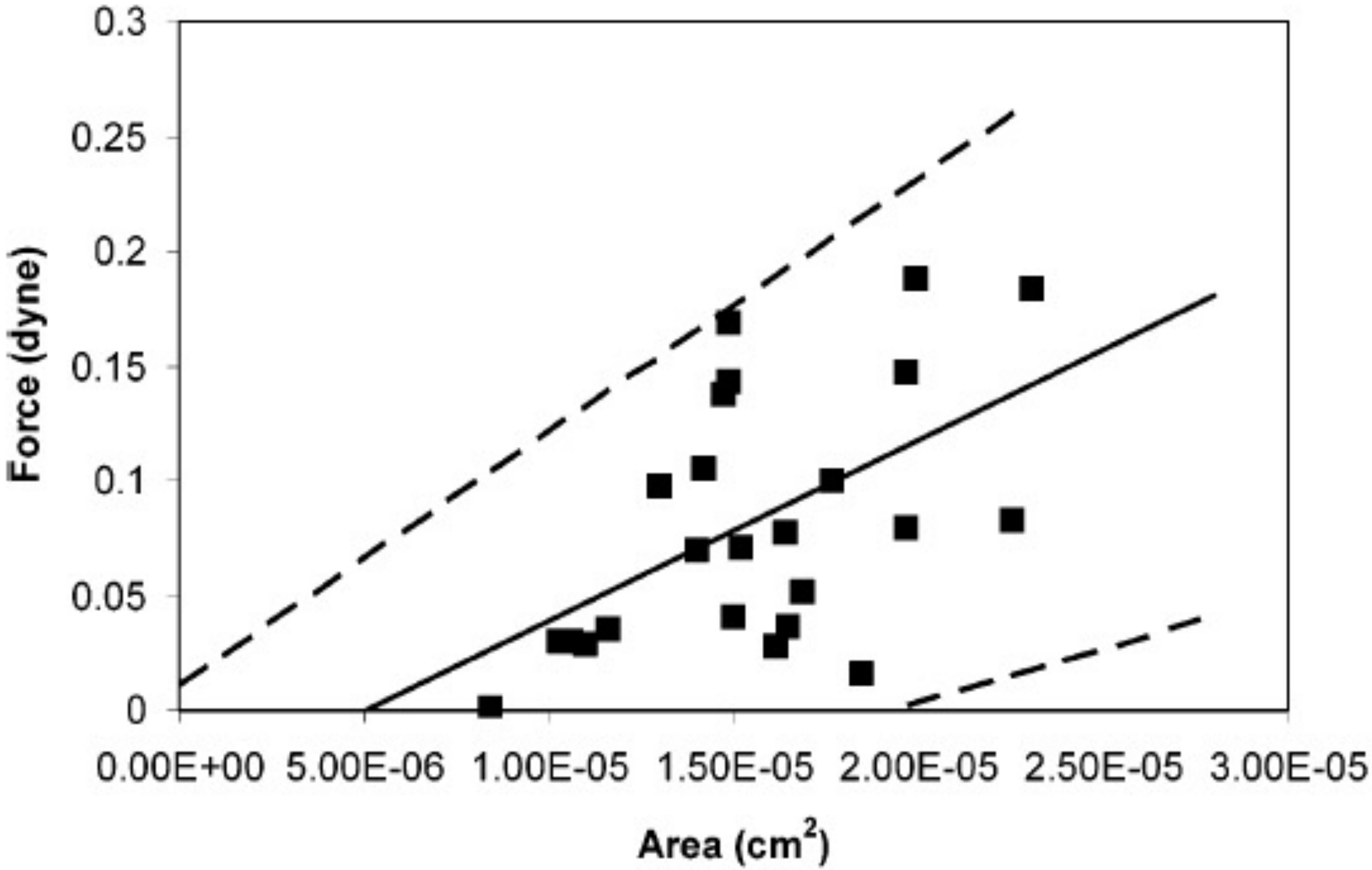


Figure 7. Graph of force exerted by a cell versus the spread cell area for cells on 0.2−0.5 mg/mL of RGD peptide. The solid line represents the linear best fit with an R^2 value equal to 0.29 and a slope of 7878 dyn/cm^2. The dashed lines represent the regression line $\pm 2\sigma$.

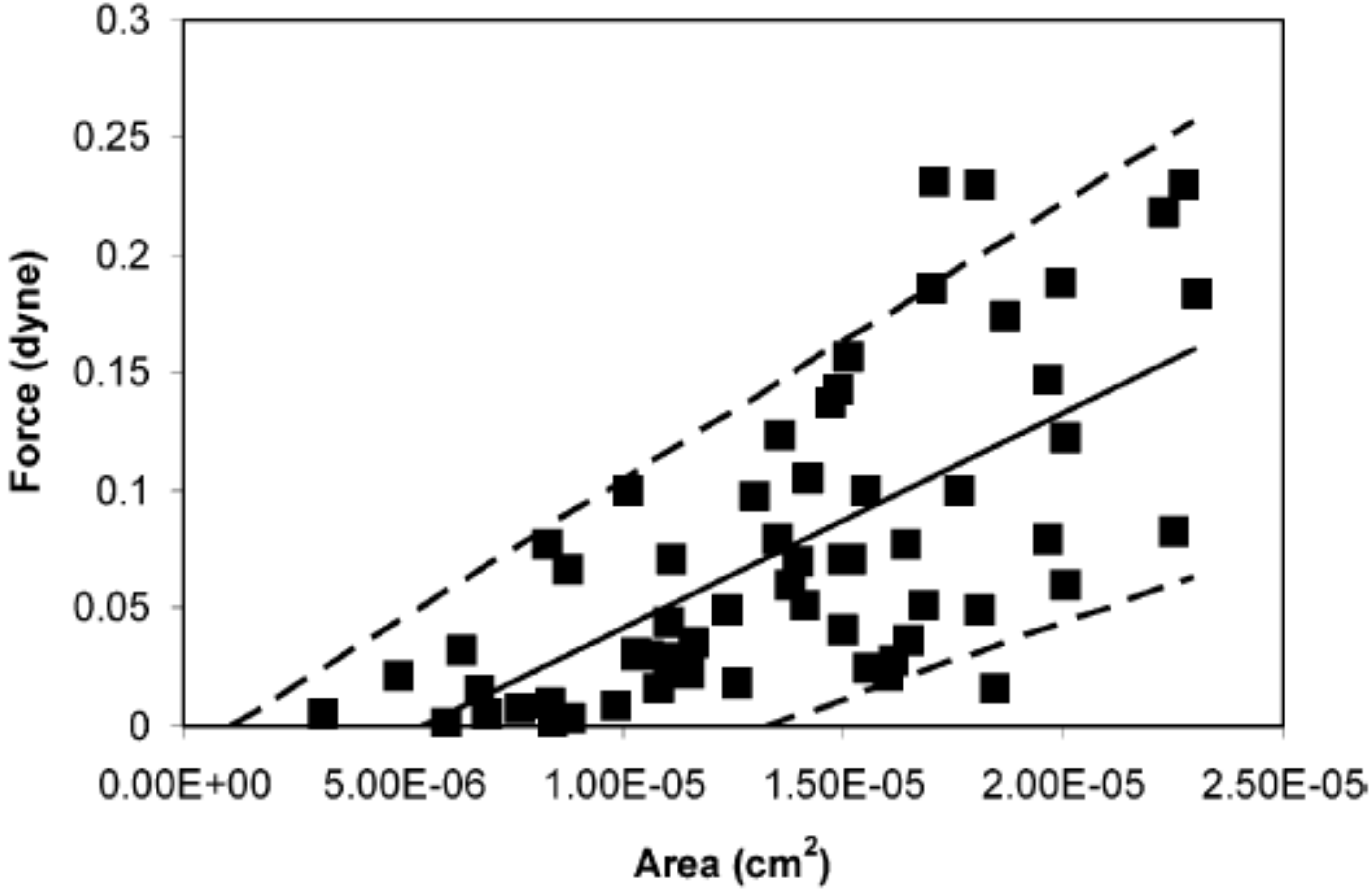


Figure 8. Graph of the relationship between cell area and overall force exerted by the cell. The solid line represents the linear best fit with an R^2 value equal to 0.45 and a slope of 9146 dyn/cm^2. The dashed line represents the regression line $\pm 2\sigma$.

Systems of Equations

- So far we have just looked at a single equation. What if we had a <u>system</u> of equations?
- Suppose we have the set:

$$f_1(x_1, \ldots , x_n) = 0$$

$$\ldots \qquad\qquad\qquad \text{or} \qquad \mathbf{f}(\mathbf{x}) = \mathbf{0}$$

$$f_n(x_1, \ldots , x_n) = 0$$

Systems of Equations

- We wish to determine **x** $= (x_1, \dots, x_n)$ such that **f**(**x**) $= (f_1, f_2, \dots, f_n) = \mathbf{0}$
- We shall use Newton's method: expand **f**(**x**) in a Taylor series about $\mathbf{x}^{(k)}$.
- Note: $x^{(k)}$ is the k^{th} guess for the root.
- So… (written notes)

So: $f(\underset{\sim}{x}) = \underset{\sim}{f}(\underset{\sim}{x}^{(k)}) + \nabla \underset{\sim}{f}\Big|_{\underset{\sim}{x}^{(k)}} \cdot (\underset{\sim}{x} - \underset{\sim}{x}^{(k)}) + \cdots$

The matrix $\underset{\sim}{\nabla} \underset{\sim}{f}$ is known as the <u>Jacobian</u> of $\underset{\sim}{f}$:

$$\underset{\approx}{J} \equiv \underset{\sim}{\nabla} \underset{\sim}{f}$$

or,

$$\underset{\approx}{J} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & & \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

We truncate the Taylor series after the linear term & set it equal to zero to get the next guess!

$$\underset{\sim}{0} = \underset{\sim}{f}^k + \underset{\approx}{J}^k(\underset{\sim}{x}^{k+1} - \underset{\sim}{x}^k)$$

Thus:

$$\underset{\sim}{x}^{k+1} = \underset{\sim}{x}^k - [\underset{\approx}{J}^k]^{-1} \underset{\sim}{f}^k$$

Actually, this should be solved using Gaussian elimination.