Gaussian Quadrature

- We have 4 parameters, so we can integrate an arbitrary cubic polynomial with 4 constants!

Let $m = (a+b)/2$

- We want to pick x_1, x_2, w_1, w_2 such that we integrate without error!

$$f(x) = (x - m)^0 \quad (=1)$$
$$f(x) = (x - m)^1$$
$$f(x) = (x - m)^2$$
$$f(x) = (x - m)^3$$

- Any cubic is a linear combination of these our functions. If we get these right, we get them all right!

We get the four equations:

(1) $\int_a^b (x-m)^0 \, dx = (b-a) = w_1 + w_2$

(2) $\int_a^b (x-m)^1 \, dx = 0 = w_1(x_1 - m) + w_2(x_2 - m)$

(3) $\int_a^b (x-m)^2 \, dx = \frac{(b-a)^3}{12} = w_1(x_1 - m)^2 + w_2(x_2 - m)^2$

(4) $\int_a^b (x-m)^3 \, dx = 0 = w_1(x_1 - m)^3 + w_2(x_2 - m)^3$

The second and fourth equations enforce symmetry:

$w_1 = w_2 \quad , \quad (x_1 - m) = -(x_2 - m)$

From the first equation, $w_1 = w_2 = \frac{b-a}{2}$

and from the 3rd eqn,

$$x_1 = \frac{a+b}{2} - \frac{b-a}{2\sqrt{3}}, \quad x_2 = \frac{a+b}{2} + \frac{b-a}{2\sqrt{3}}$$

So we get the quadrature rule:

$$I \simeq \frac{b-a}{2}\left[f\left(\frac{a+b}{2} - \frac{b-a}{2\sqrt{3}}\right) + f\left(\frac{a+b}{2} + \frac{b-a}{2\sqrt{3}}\right)\right]$$

Let's use this to integrate x^4: $\left(\int_0^2 x^4 dx = 6.4\right)$

$$I = \int_0^2 x^4 dx \simeq \frac{2-0}{2}\left[\left(1 - \frac{1}{\sqrt{3}}\right)^4 + \left(1 + \frac{1}{\sqrt{3}}\right)^4\right] = \frac{56}{9} = 6.222\ldots$$

The error is just $\frac{8}{45}$ which is less than the 3pt Simpson's rule!

In general,

$$\int_a^b f(x)dx = \sum_{i=1}^{n} w_i f(x_i) + R_n$$

where $R_n = \frac{(b-a)^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{2n}(\xi)$

and $\xi \in [a,b]$

provided that $f(x)$ has $2n$ continuous derivatives on $[a,b]$

(If $f(x)$ has singularities in itself or any of its derivatives the error can be much larger.)

The gaussian quadrature rules are of polynomial degree $2n-1$. This is because it has $2n$ adjustable parameters.

Gaussian Quadrature

What are the properties of Gaussian quadrature?

1. The weights and nodes are, in general, irrational numbers. The exceptions are:

   n=1: The midpoint rule

   $w_1 = b - a$, $x_1 = m = (b+a)/2$

   n=2: $w_1 = w_2 = (b - a)/2$

   n=odd: the midpoint is a node.

   (As a consequence, lists of weights and nodes are usually provided in subroutines that do the quadrature.)

Gaussian Quadrature

2. Gaussian rules are <u>open</u>: the function is never evaluated at the edges of the domain of integration. This is convenient for integrals like:

$$\int_0^1 \sin x / x \, dx$$

which is well behaved at x=0, but may lead to errors in closed rule quadrature.

3. Nodes for the n-point rule are <u>disjoint</u> from those of the m-point rule, with the exception that the midpoint is always a node for odd n,m.

Two sets are disjoint if they have no elements in common.

Gaussian Quadrature

1. Among all rules using n-point evaluation, the n-point Gaussian rule will produce the most accurate estimate for a smooth function.
2. The weights in Gaussian quadrature are always positive. This would not be true if the nodes were evenly spaced and the weights determined optimally. Thus, increasing the number of nodes always improves accuracy. For evenly spaced nodes at large n you can get large positive and negative weights leading to roundoff error.
3. The n Gauss nodes of the n-point rule are the roots of the n^{th} Legendre polynomial.

Gaussian Quadrature

- In Gaussian quadrature routines the weights and nodes are given based on the interval (-1,1). The nodes are thus symmetric:

For the four point rule:

x_i^*	w_i^*
+/- 0.8611363…	0.3478548…
+/- 0.3399810…	0.6521452…

Gaussian Quadrature

- Suppose we have some general interval [a,b].
- We could use the stored values of x_i* and w_i* to get the values of x_i and w_i on the general interval via a mapping:

$$x_i = (a+b)/2 + (b - a)/2 * x_i^*$$

$$w_i = (b - a)/2 * w_i^*$$

and

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i).$$

yields the desired result.

Error Estimation

- It’s not enough just to compute some estimate for an integral.
- We must also estimate how accurate the estimate is!
- One approach: for the trapezoidal rule, just cut the interval in half!
- Let’s look at the example

$$\int_0^2 x^3 dx = (1/4)(2)^4 = 4$$

Error Estimation

- Suppose we use n panels:

  n=2: $I \sim 0.5(0)^3 + 1(1)^3 + 0.5(2)^3 = 5$

  n=4: $I \sim 0.5[0.5(0)^3 + (0.5)^3 + (1)^3 + (1.5)^3 + 0.5(2)^3] = 4.25$

  n=8: $I \sim 0.25[\ \ldots\ ] = 4 + 1/16$

- Each time the error was decreased by a factor of 4! This is because the error was $O(1/n^2)$.
- We can actually use this to improve our result via repeated Richardson Extrapolation.

Richardson Extrapolation

$$I = I_n + \lambda/n^2 + O(1/n^4)$$

next order in error term

- Note that odd powers in n are killed off due to symmetry.
- Suppose we took the n=2 and n=4 results:

$$I = I_2 + \lambda/4 + O(1/2^4)$$

$$I = I_4 + \lambda/16 + O(1/4^4)$$

- If we multiply the second equation by 4 and subtract from the first we can eliminate λ…

Richardson Extrapolation

$$3I = 4I_4 - I_2 + O(1/2^4)$$
$$I = (1/3)(3I_4 - I_2) + O(h^4)$$

- This gives us back Simpson's rule again!
- Note that by doubling the number of panels we only have to evaluate the function at n new points: we can use all of the points from the first evaluation over again.
- This can make a big difference if it takes a lot of time to make a function evaluation.
- If we had just increased the number of panels by one, we wouldn't have gotten a significant increase in accuracy and <u>all</u> of the interior <u>nodes</u> would change!

Richardson Extrapolation

- We can take this combination process to a higher level. Suppose we have an n panel and 2n panel pair of Simpson's rule estimates. The error in each is $1/n^4$. Thus,

$$I = S_n + \lambda/n^4 + O(1/n^6)$$

$$I = S_{2n} + \lambda/(2n)^4 + O(1/n^6)$$

- We can thus get an $O(1/n^6)$ rule from the combination:

$$I = 1/(2^4-1)*(2^4 S_{2n} - S_n) + O(1/n^6)$$

Richardson Extrapolation

- This process can be repeated again and again in what is known as repeated Richardson extrapolation, or Romberg integration, and the ultimate result is known as the Newton-Cotes formula.
- Let's see how this works. Suppose we calculate an integral of f(x) over [a,b] using n=1,2,4,8,16,… panel Trapezoidal rules. This gives us the series of estimates:

$$T_1, T_2, T_4, T_8, T_{16}, \ldots$$

Richardson Extrapolation

- Note that if we quit at n=16 panels, we would only need 17 function evaluations – the nodes for the n/2 panel rule are included in those for the n-panel rule.
- We may thus combine T_1 and T_2 to get S_2; T_2 and T_4 to get S_4, and so on.

$$S_2 = 1/(2^2 - 1)*(2^2 T_2 - T_1)$$
$$S_4 = 1/(2^2 - 1)*(2^2 T_4 - T_2)$$

- The Simpson's rule estimates can be combined as well.

Richardson Extrapolation

- If we look at this in matrix form we get:

T1					
T2	S2				
T4	S4	P4			
T8	S8	P8	Q8		
T16	S16	P16	Q16	R16	
…	…	…	…	…	…

- Thus, the iteration process produces a lower triangular matrix.

Richardson Extrapolation

- The most accurate integral estimate given by the botom-right elevent, and the estimate of the error is given by the difference between the last two elements of the last row.
- If we start with 2^k panels (a total of 2^k+1 evaluations) then our extrapolation matrix is of size (k+1)x(k+1), and the error in the last estimate is:

$$\text{error} \sim O(h^{2(k+1)}f^{2(k+1)}(x)(b-a))$$

where $h = (b-a)/2^k$

- If **M** is our matrix, then an estimate for this error is:

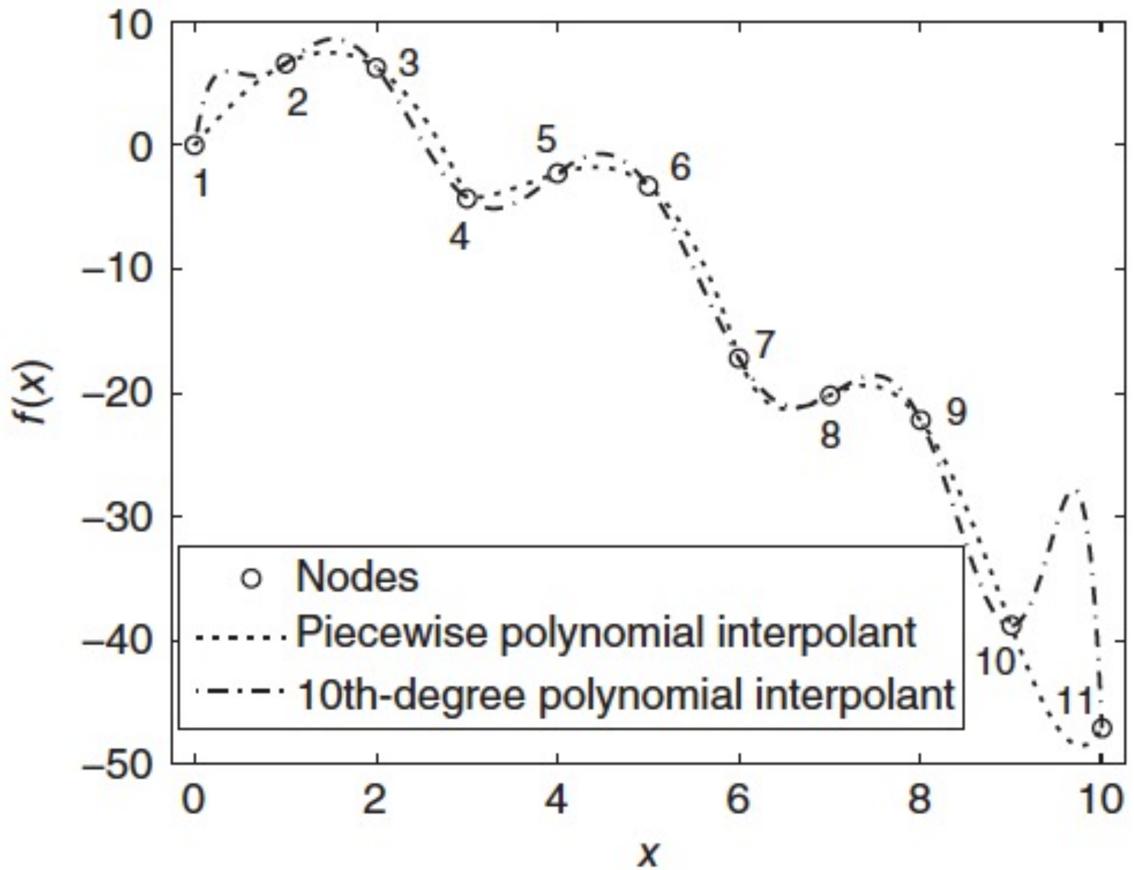
$$\text{error} < |M_{(k+1),(k+1)} - M_{(k+1),k}|$$

Q1: This graph demonstrates the numerical problem of:

A. Underdamping
B. Polynomial wiggle
C. Chaos
D. Overflow error

Figure 6.4

Piecewise polynomial interpolation versus high-degree polynomial interpolation.

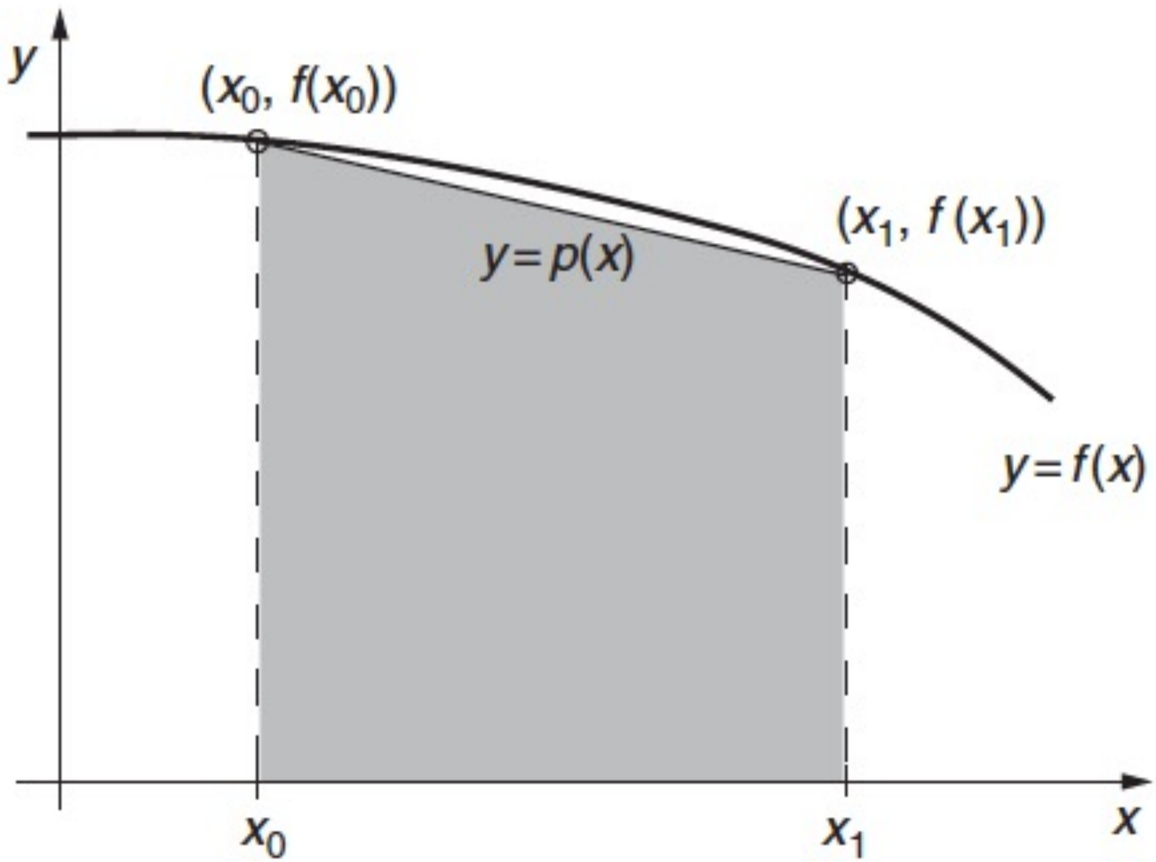


Q2: When the second derivative of f is negative, then trapezoidal rule will overpredict the integral.

A. True **B. False**

Figure 6.10

The trapezoidal rule for numerical integration. The shaded area is a trapezoid.



Q3: Suppose trapezoidal rule is used to integrate a <u>linear polynomial</u>. If the number of panels is doubled from 4 to 8, the error would be reduced by which amount?

A. zero
B. factor of 2
C. factor of 4
D. factor of 8

Q4: Suppose trapezoidal rule is used to integrate a <u>cubic polynomial</u>. If the number of panels is doubled from 4 to 8, the error would be reduced by which amount?

A. zero

B. factor of 2

C. factor of 4

D. factor of 8

RESTRICTED TRANSPORT IN SMALL PORES

A Model for Steric Exclusion and Hindered Particle Motion

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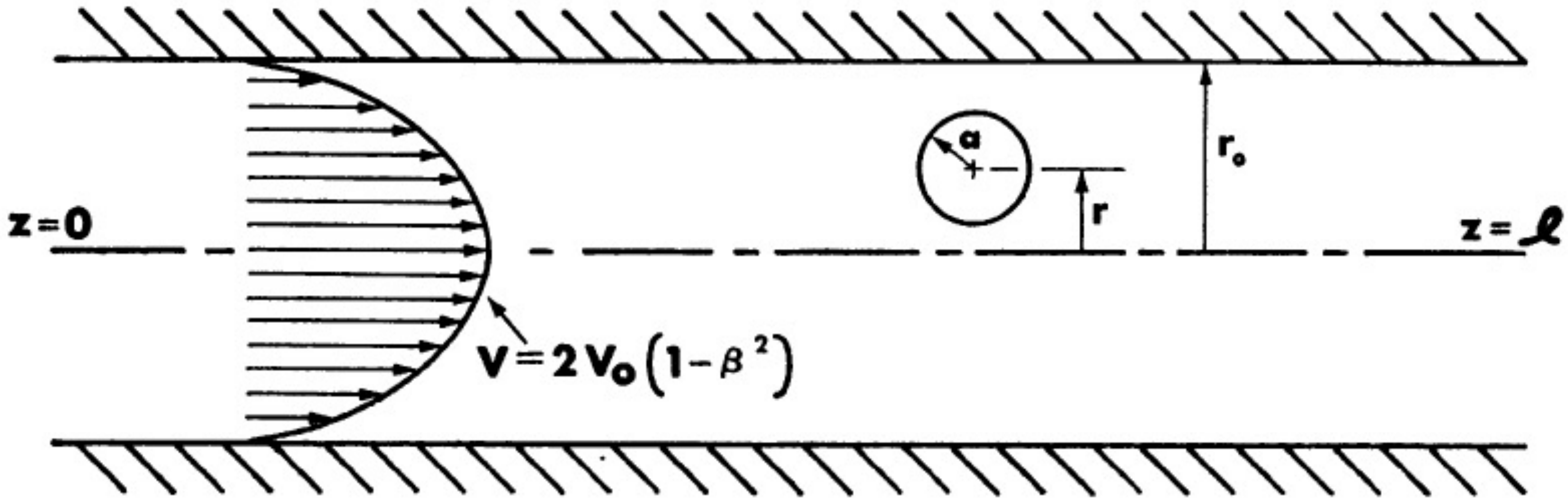
ABSTRACT The basic hydrodynamic equations governing transport in submicron pores are reexamined. Conditions necessary for a simplified, one-dimensional treatment of the diffusion/convection process are established. Steric restrictions and Brownian motion are incorporated directly into the resulting model. Currently available fluid mechanical results are used to evaluate an upper limit on hindered diffusion; this limit is valid for small particle-to-pore ratios. Extensions of the analysis are shown to depend on numerical solutions of the related hydrodynamic problem, that of asymmetrical particle motion in a bounded fluid.



$$\lambda = {}^{a}/_{r_0} \quad ; \quad \beta = {}^{r}/_{r_0}$$

FIGURE 1 Particle located off the centerline of a long, cylindrical pore with a parabolic velocity profile.

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Macromolecule transport across glomerular capillaries: Application of pore theory

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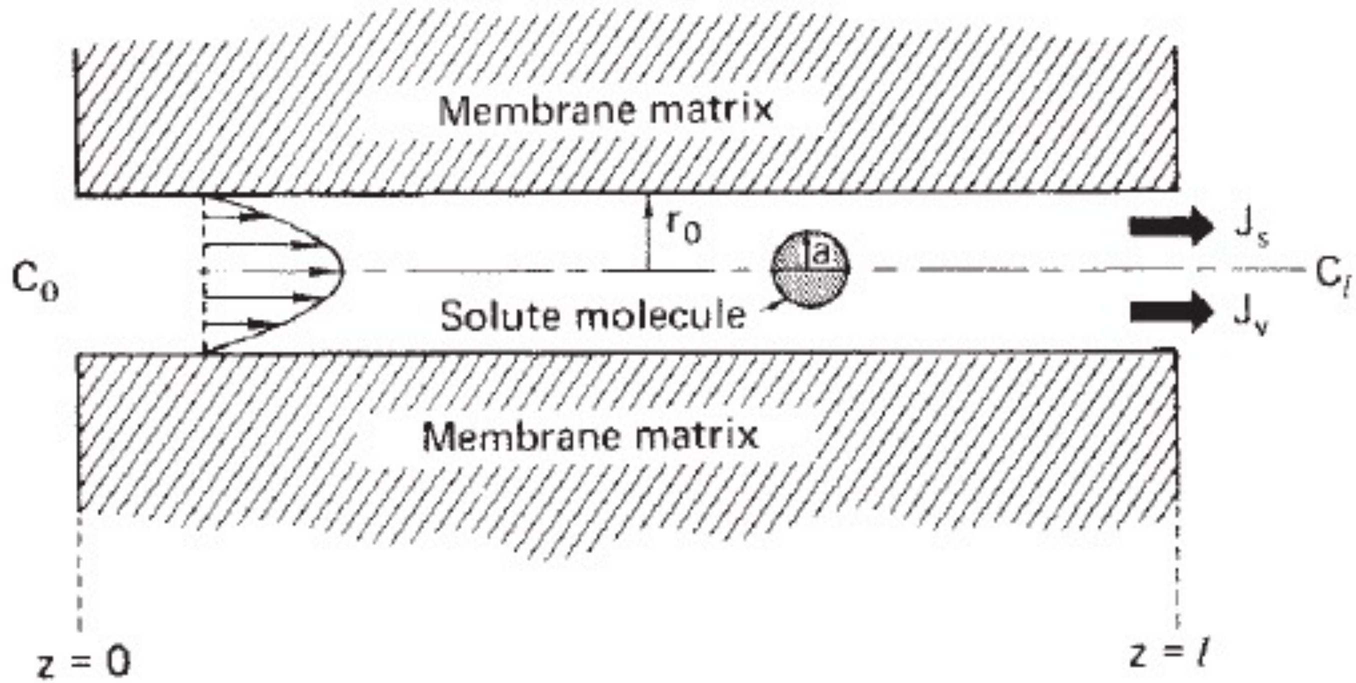

Fig. 1. *Schematic representation of a solute molecule traversing a membrane through a cylindrical pore*. Symbols are defined in the text. Reproduced with permission of *Biophys J* [22].

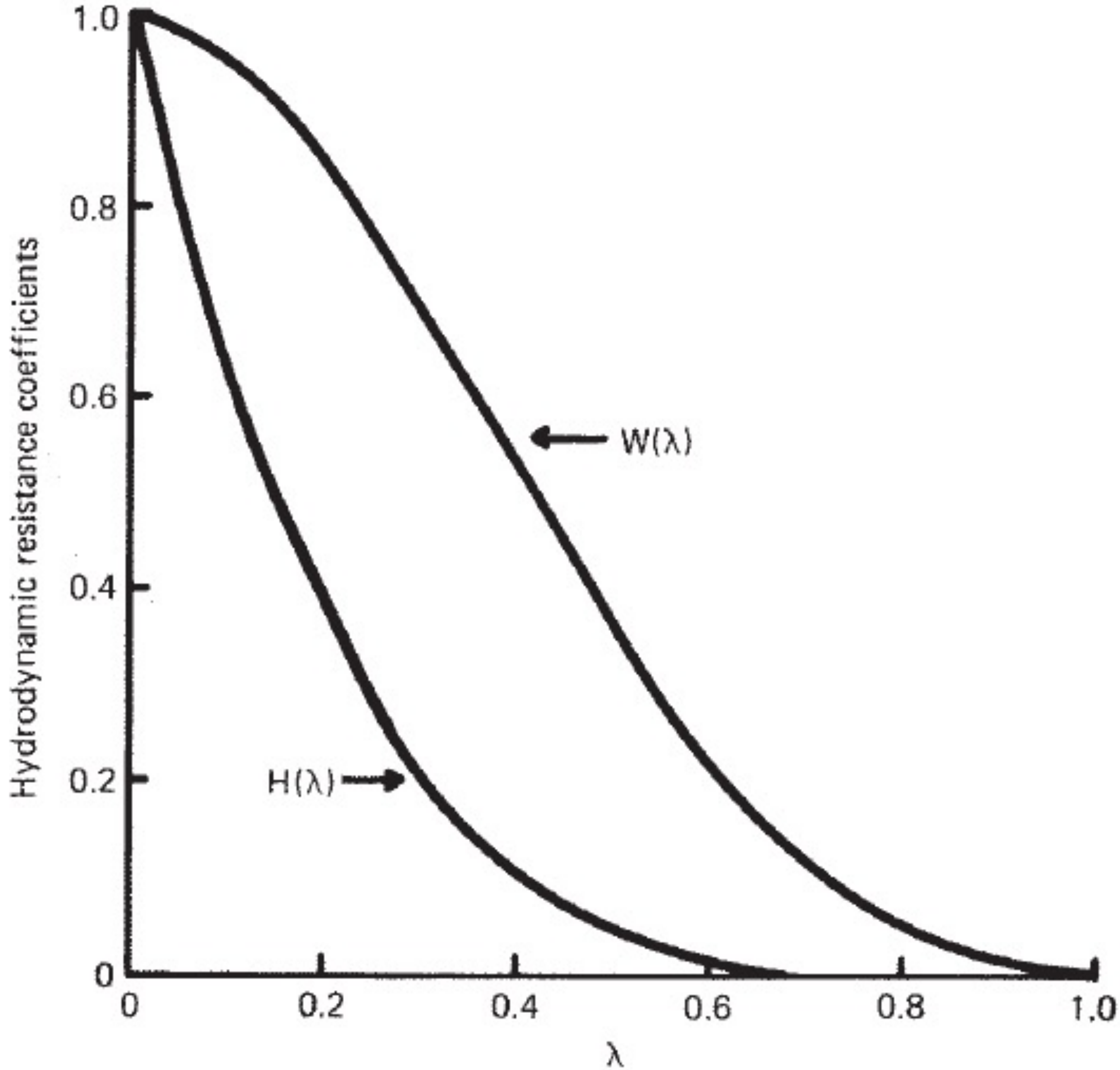

Fig. 2. *Restriction factors for convection (W) and diffusion (H) as a function of the ratio of solute radius to pore radius (λ).*

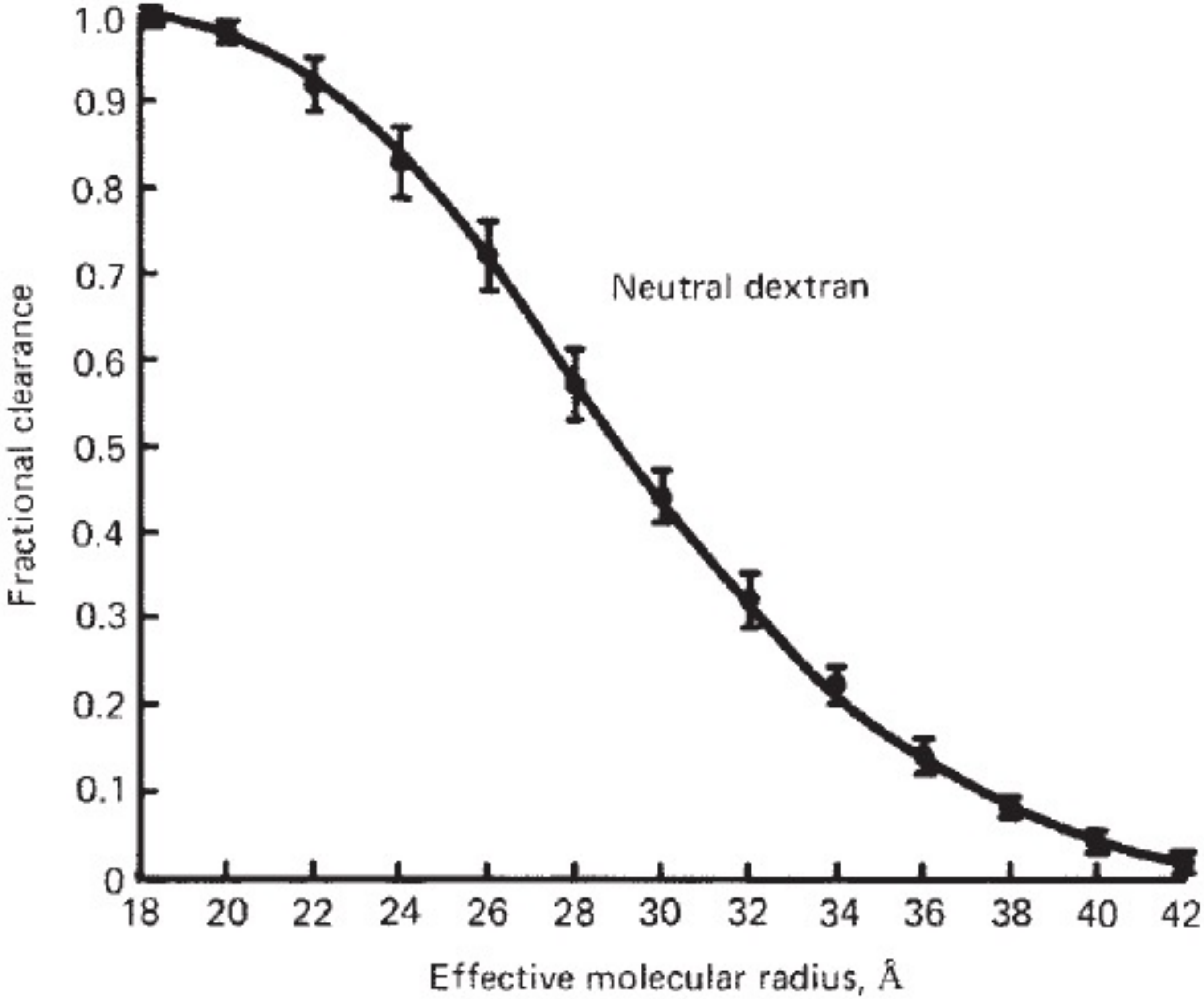

Fig. 3. *Fractional clearance of tritiated, neutral dextran as a function of effective molecular radius*. Values are expressed as means ± 1 SEM for 14 normal hydropenic rats. Data are from Refs. 23 and 25.

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Microvascular Permeability

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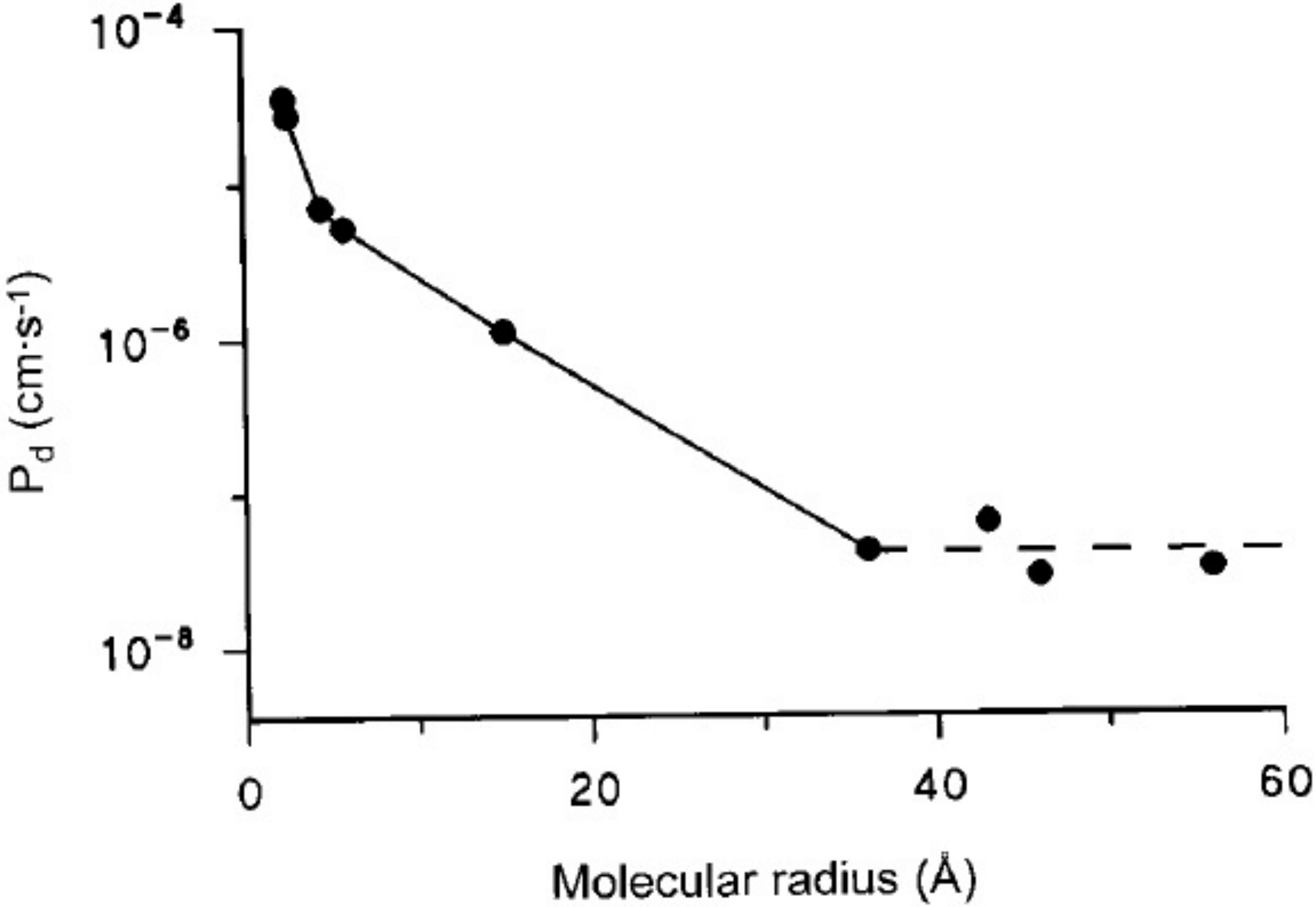

FIG. 1. Relation between permeability (P_d) of microvessels in skeletal muscle to hydrophilic solutes and solute molecular radius. Permeability has been plotted on a logarithmic scale to show range of values, although it is possible that values of P_d for the largest molecules are overestimates (see text). [Data from Renkin (238a).]

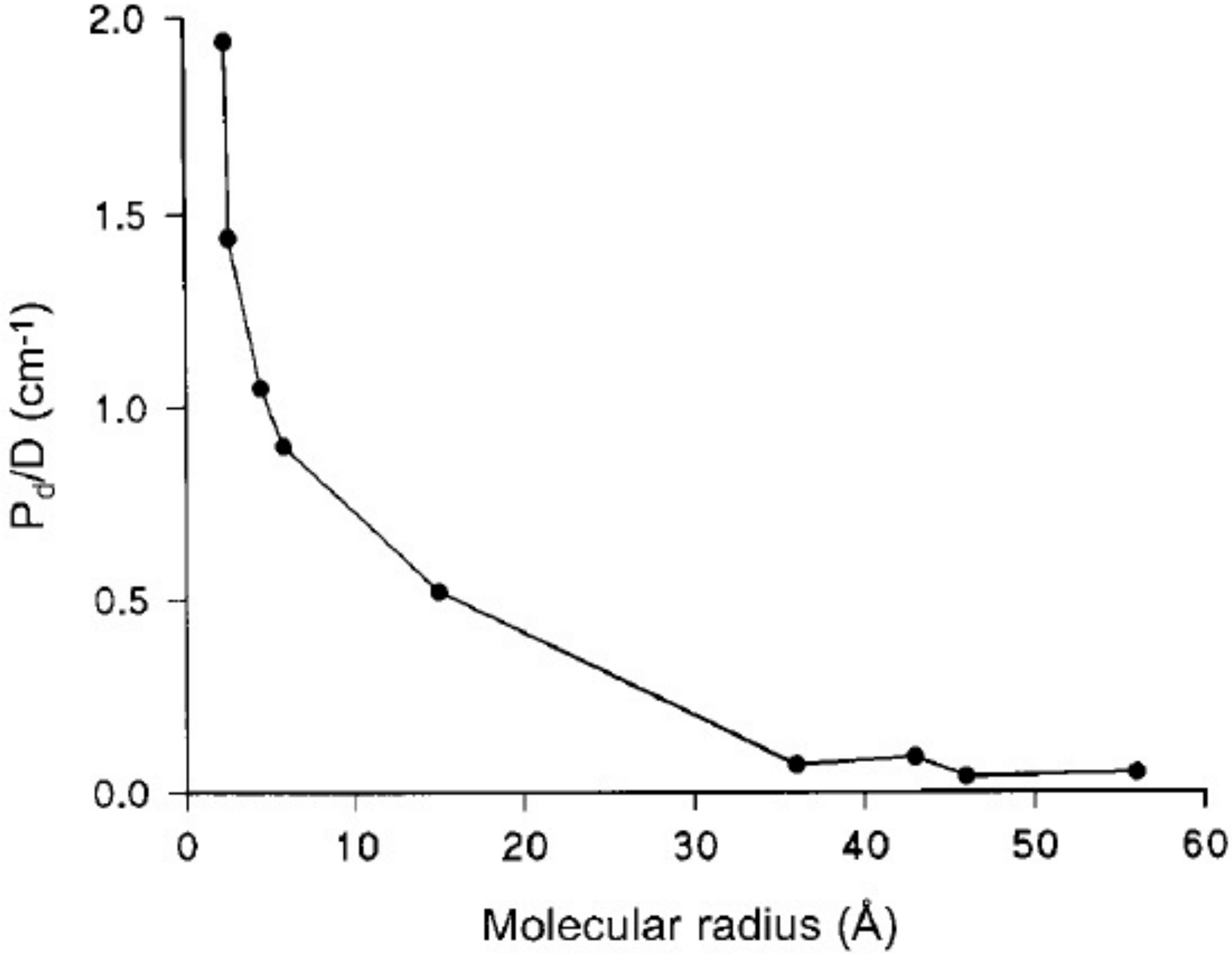

FIG. 2. Restricted diffusion of hydrophilic solutes at walls of microvessels in skeletal muscle. Values of P_d shown in Figure 1 have been divided by free diffusion coefficient (D) of same solute. If fall in P_d with increasing molecular radius were due to reduction in D alone, then P_d/D would be a constant. It is seen that P_d/D falls by nearly 2 orders of magnitude as molecular radius rises from 2.4 to 36.

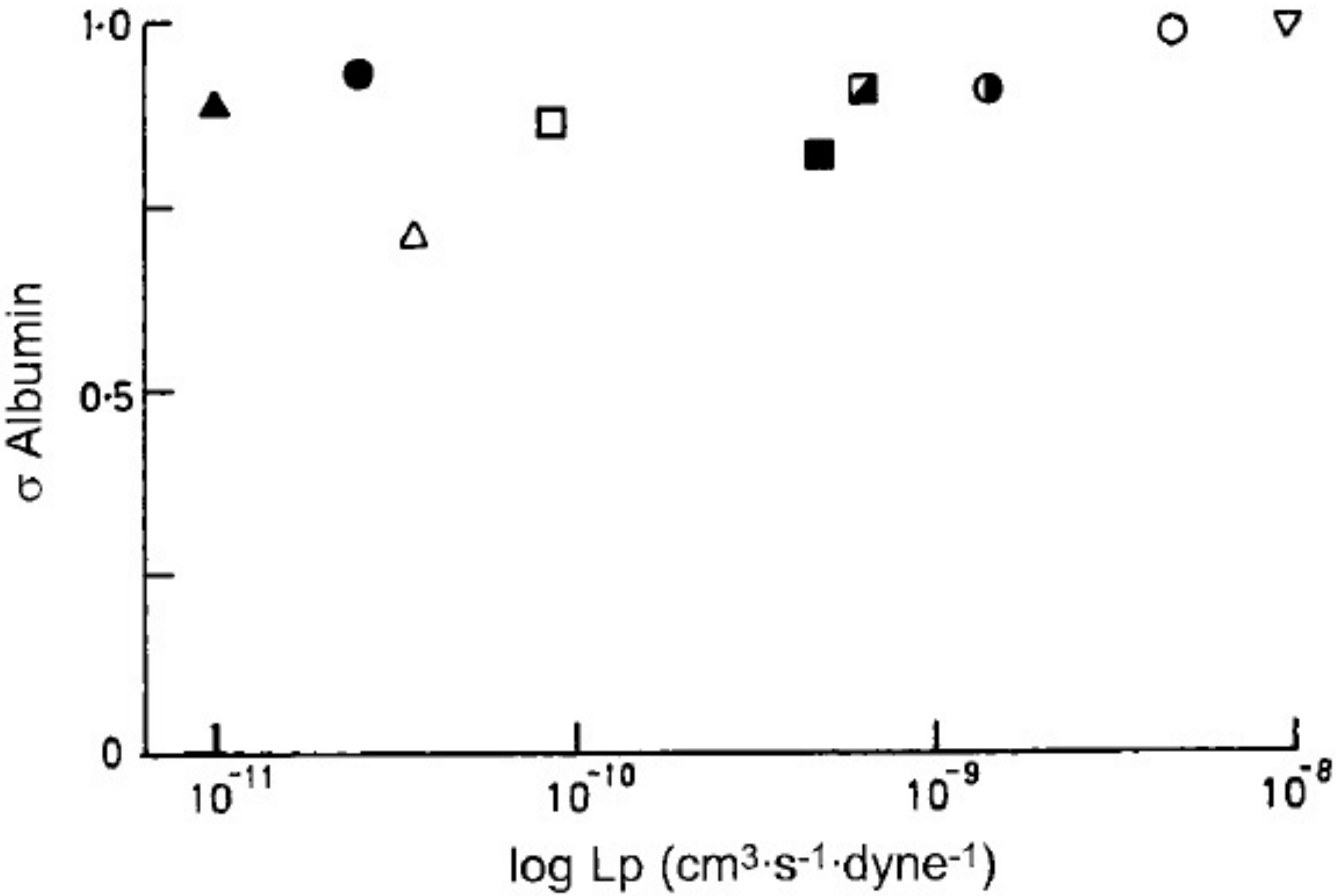

FIG. 3. Reflection coefficient to serum albumin ($\sigma_{albumin}$) and hydraulic permeability (L_p) in different microvascular beds. Each point represents mean value of $\sigma_{albumin}$ and L_p for microvessels in a particular tissue: ▲, cat hindlimb; ●, rat hindlimb; △, dog lung; □, dog heart; ■, frog mesentery; ◪, rabbit salivary gland; ◑, dog small intestine; ○, dog glomerulus; ▽, rat glomerulus. [From Michel (186).]

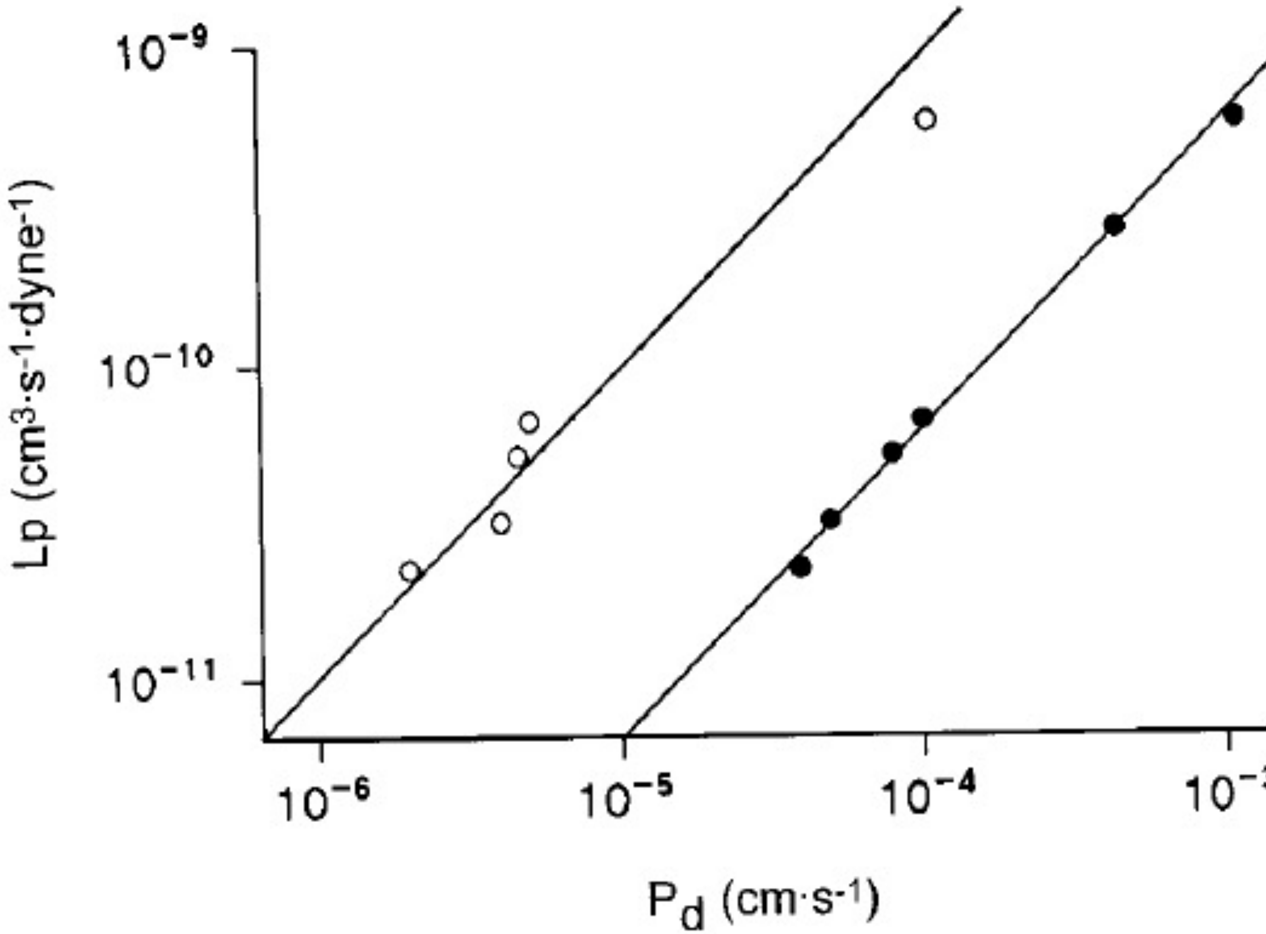

FIG. 4. Relations between hydraulic permeabilities (L_p) of microvessels in different tissues and their diffusional permeabilities to small and intermediate-sized molecules (P_d). Solid circles are values for L_p plotted against values for P_d to either sodium or potassium from same vessel. Open circles are corresponding data for P_d to inulin. Values of L_p and P_d have been plotted on logarithmic scales to show a range of 2 orders of magnitude. Lines are not regression lines but have been constructed through points with a slope of unity to indicate direct proportionality.

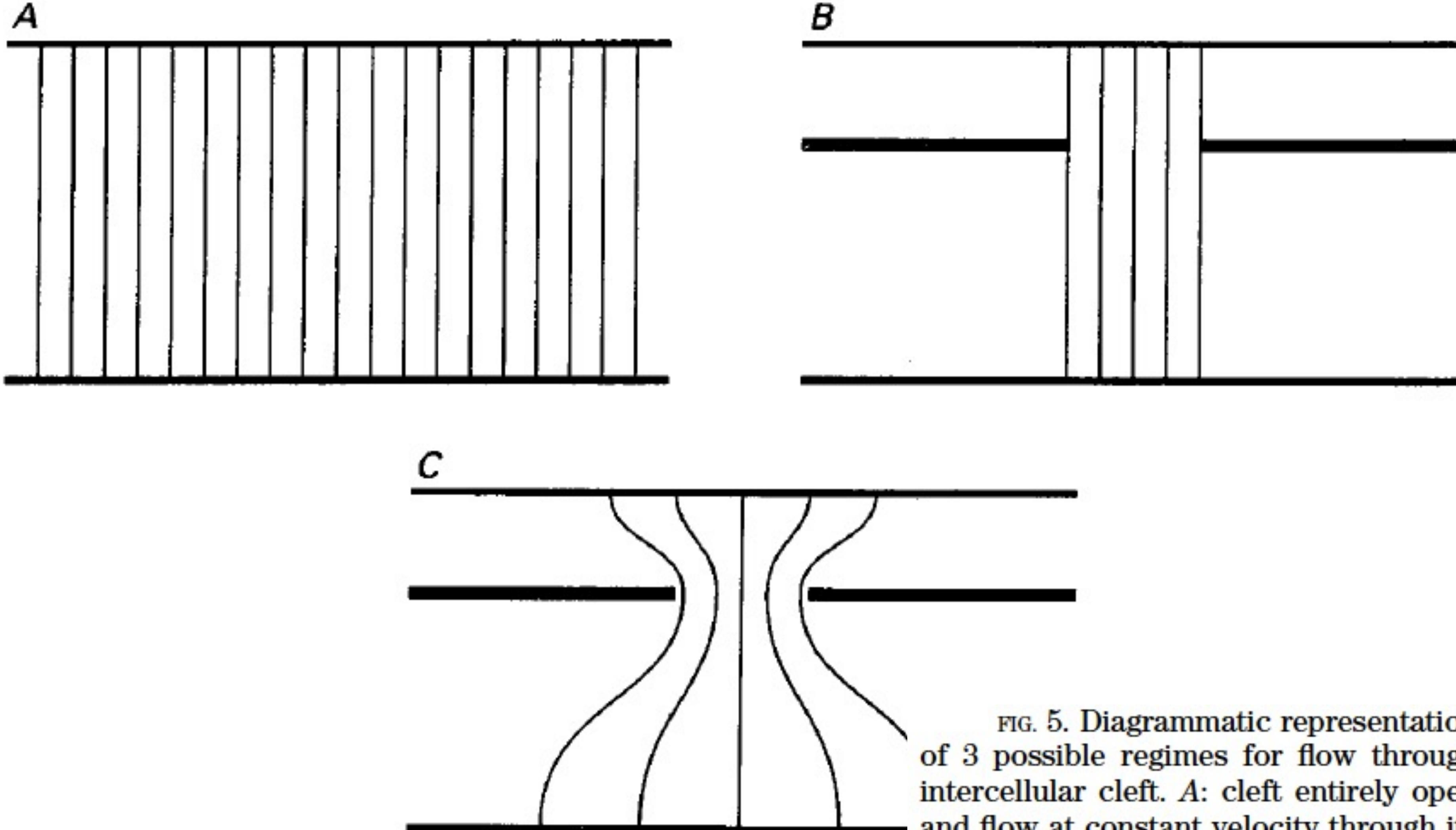

FIG. 5. Diagrammatic representation of 3 possible regimes for flow through intercellular cleft. *A*: cleft entirely open and flow at constant velocity through its entire length. *B*: 1-dimensional flow limited to area of discontinuities in tight junction and wide region of cleft immediately above and below break. *C*: 2-dimensional convergent and divergent flow through wide regions of cleft above and below discontinuities in tight junction. [From Adamson and Michel (9).]

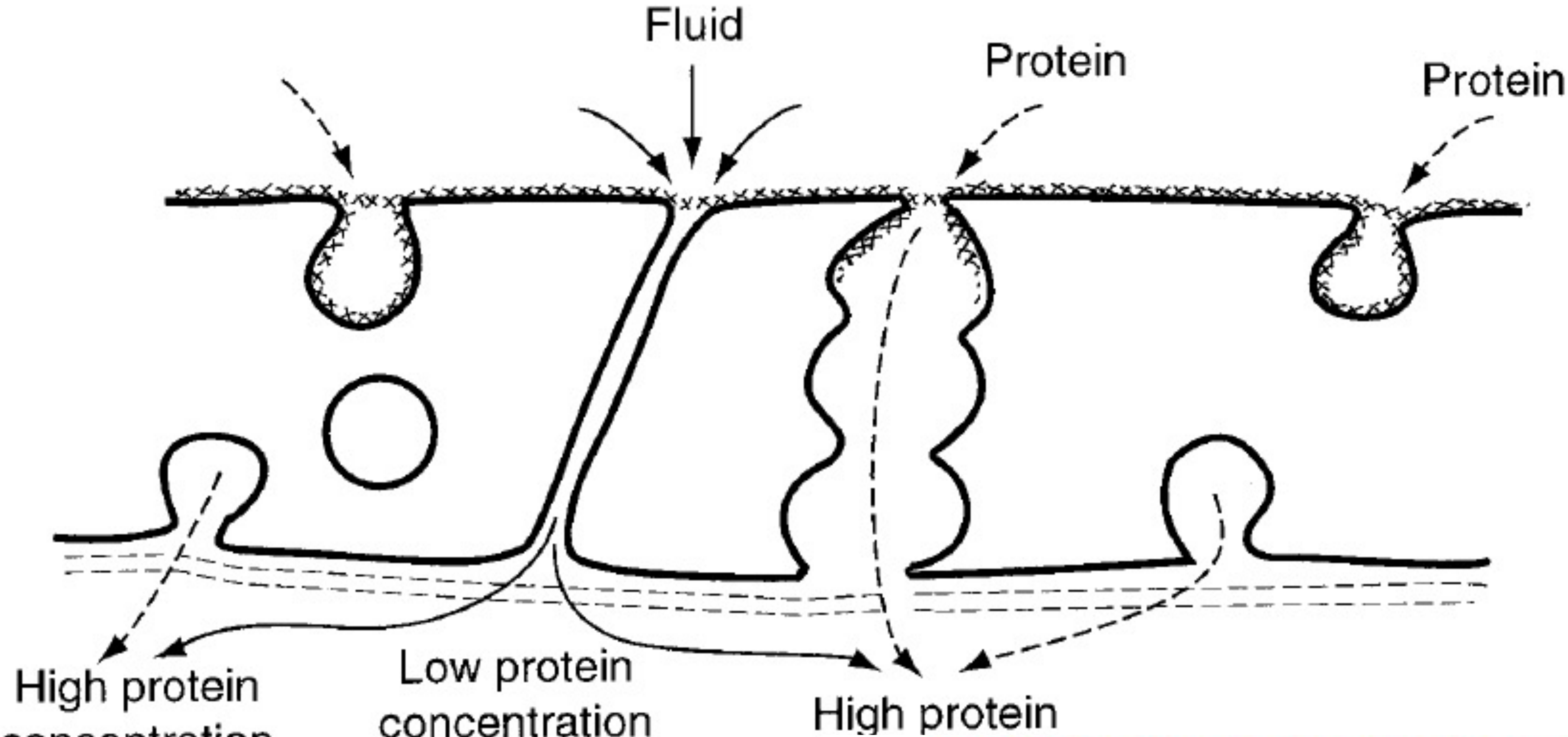

FIG. 10. Diagram of microvascular endothelium to show how separate pathways for fluid (through intercellular cleft containing a fiber matrix at luminal entrance) and protein (through vesicular system) can lead to differences between mean osmotic pressure between plasma and interstitium (and lymph) and plasma and fluid in intercellular cleft downstream from sieving matrix. [From Michel (188).]