Michaelis-Menten reaktionskinetik

> *restart*
> *with(Gym)* :
> *with(plots)* :

Data

Dataene stammer fra forsøget i sektion 6 på websitet:
http://www.wiley.com/college/pratt/0471393878/student/animations/enzyme_kinetics/index.html

Tube 1 ——————> Tube 6						
5	5	5	5	5	5	[E] (µM)
0	10	20	40	80	160	[S] (mM)
5	5	5	5	5	5	time (min)
10	405	610	850	1005	1096	[P] formed (µM)
2	81	122	170	201	219	$v_0 = \Delta P/\Delta t$ (µM/min)

Her anvendes de 2 grundlæggende datalister med 6 datasæt:

$[S] = [0, 10, 20, 40, 80, 160]$

$V = [2, 81, 122, 170, 201, 219]$

Michaelis-Menten plot ([*S*], *v*)

> $Xmm := [0, 10, 20, 40, 80, 160]$

$$Xmm := [0, 10, 20, 40, 80, 160] \tag{2.1}$$

> $Ymm := [2, 81, 122, 170, 201, 219]$

$$Ymm := [2, 81, 122, 170, 201, 219] \tag{2.2}$$

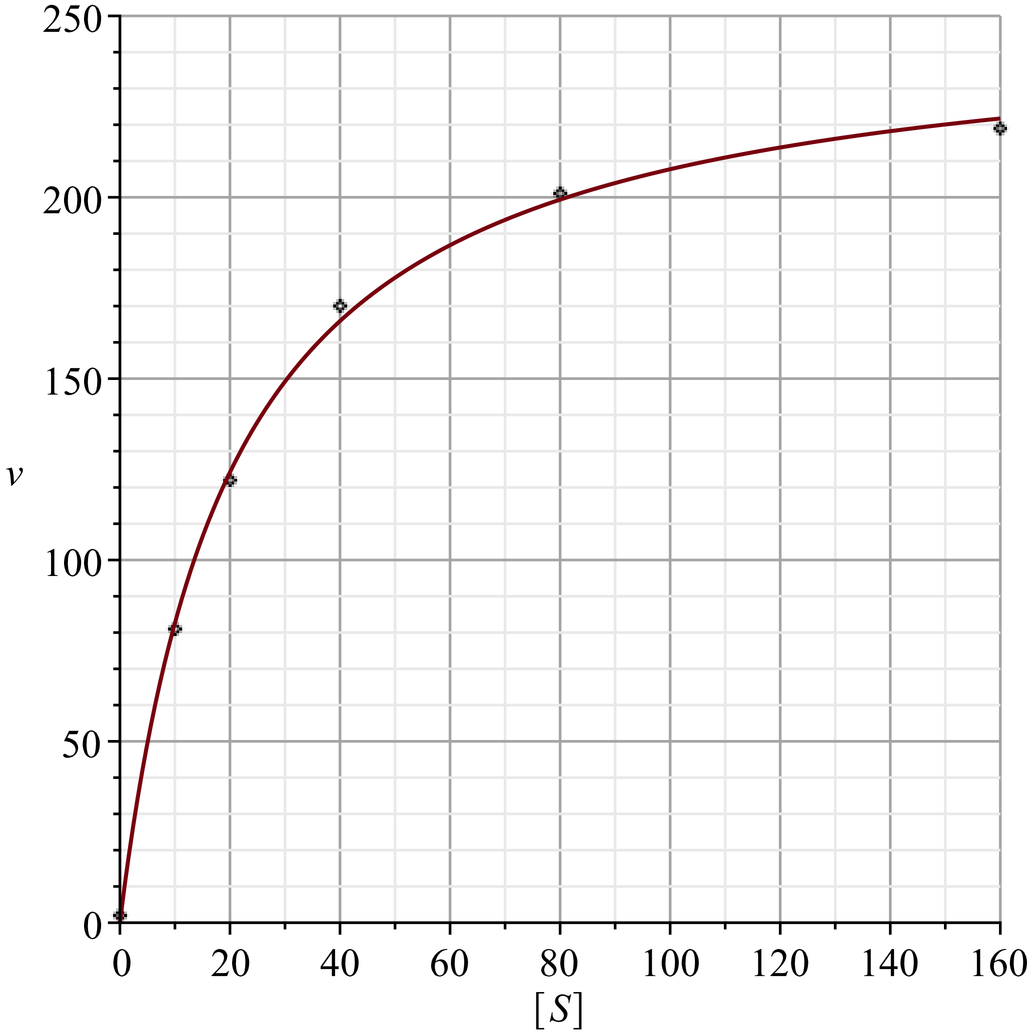
> *with(Statistics)* :

> $mm(x) := Fit\left(\frac{Vmax \cdot x}{Km + x}, Vector(Xmm), Vector(Ymm), x, initialvalues = [Vmax = 230, Km = 25]\right) : mm(x)$

$$\frac{249.734625639907\, x}{20.2179469970270 + x} \tag{2.3}$$

Graf med forklarende symboler på akserne:

> $punkterMM := pointplot(\langle Vector(Xmm) | Vector(Ymm) \rangle) :$
> $grafMM := plot(mm(x), x = 0..160) :$
> $display(punkterMM, grafMM, view = [0..160, 0..250], labels = [[S], v], gridlines)$



Beregner konstanterne:

> $V_{max} := \lim_{x \to \infty} mm(x)$

$$V_{max} := 249.7346256 \tag{2.4}$$

> $K_m = solve\left(mm(x) = \frac{1}{2} \cdot V_{max}, x\right)$

$$K_m = 20.21794699 \tag{2.5}$$

> $unassign('V_{max}')$

Lineweaver-Burk plot $\left(\frac{1}{[S]}, \frac{1}{v}\right)$

Dataene lineariseres.

Husk at $X = \frac{1}{[S]}$ **og** $Y = \frac{1}{v}$ **.**

NB: første værdi er 0, det kan ikke bruges, da man ikke kan dividere med 0.
Derfor er de kun 5 datasæt.

> $Xlb := \left[\frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}\right]$

$$Xlb := \left[\frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}\right] \tag{3.1}$$

> $Ylb := \left[\frac{1}{81}, \frac{1}{122}, \frac{1}{170}, \frac{1}{201}, \frac{1}{219}\right]$

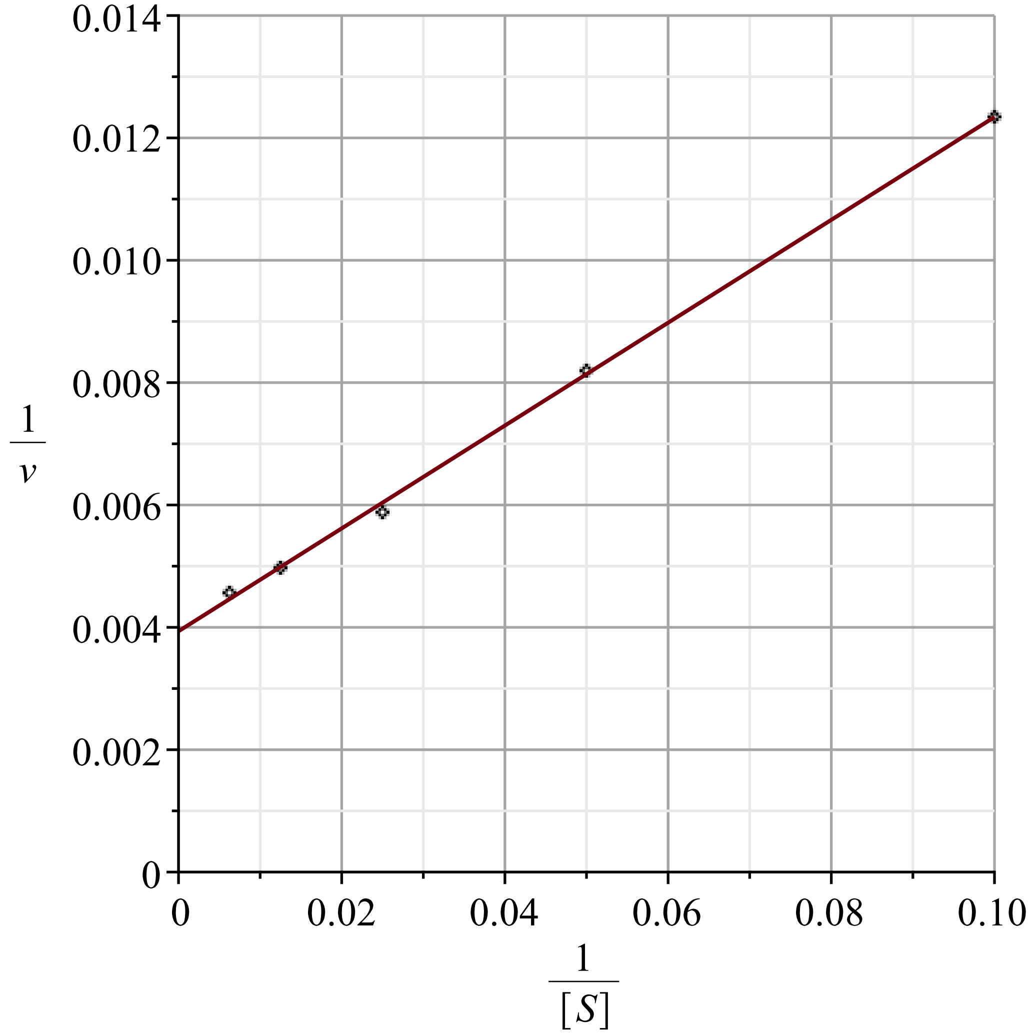
$$Ylb := \left[\frac{1}{81}, \frac{1}{122}, \frac{1}{170}, \frac{1}{201}, \frac{1}{219}\right] \quad (3.2)$$

> $lb(x) := LinReg(Xlb, Ylb, x) : lb(x)$

$$0.0840438296352689\, x + 0.00393651913883333 \quad (3.3)$$

Graf med forklarende symboler på akserne:

> $punkterLB := pointplot(\langle Vector(Xlb) | Vector(Ylb)\rangle) :$
> $grafLB := plot(lb(x), x = 0..0.1) :$
> $display\left(punkterLB, grafLB, view = [0..0.1, 0..0.014], labels = \left[\frac{1}{[S]}, \frac{1}{v}\right], gridlines\right)$



Afløser konstanterne:

> $a := lb(1) - lb(0)$

$$a := 0.0840438296352689 \quad (3.4)$$

> $b := lb(0)$

$$b := 0.00393651913883333 \quad (3.5)$$

> $solve\left(\left\{a = \frac{K_m}{V_{\max}}, b = \frac{1}{V_{\max}}\right\}, \{K_m, V_{\max}\}\right)$

$$\{K_m = 21.34978306, V_{\max} = 254.0315352\} \quad (3.6)$$

Hanes-Wolf plot $\left([S], \dfrac{[S]}{v}\right)$

Dataene lineariseres.

Husk at $X = [S]$ og $Y = \dfrac{[S]}{v}$:

> $Xhw := [0, 10, 20, 40, 80, 160]$

$$Xhw := [0, 10, 20, 40, 80, 160] \tag{4.1}$$

> $Yhw := \left[\frac{0}{2}, \frac{10}{81}, \frac{20}{122}, \frac{40}{170}, \frac{80}{201}, \frac{160}{219}\right]$

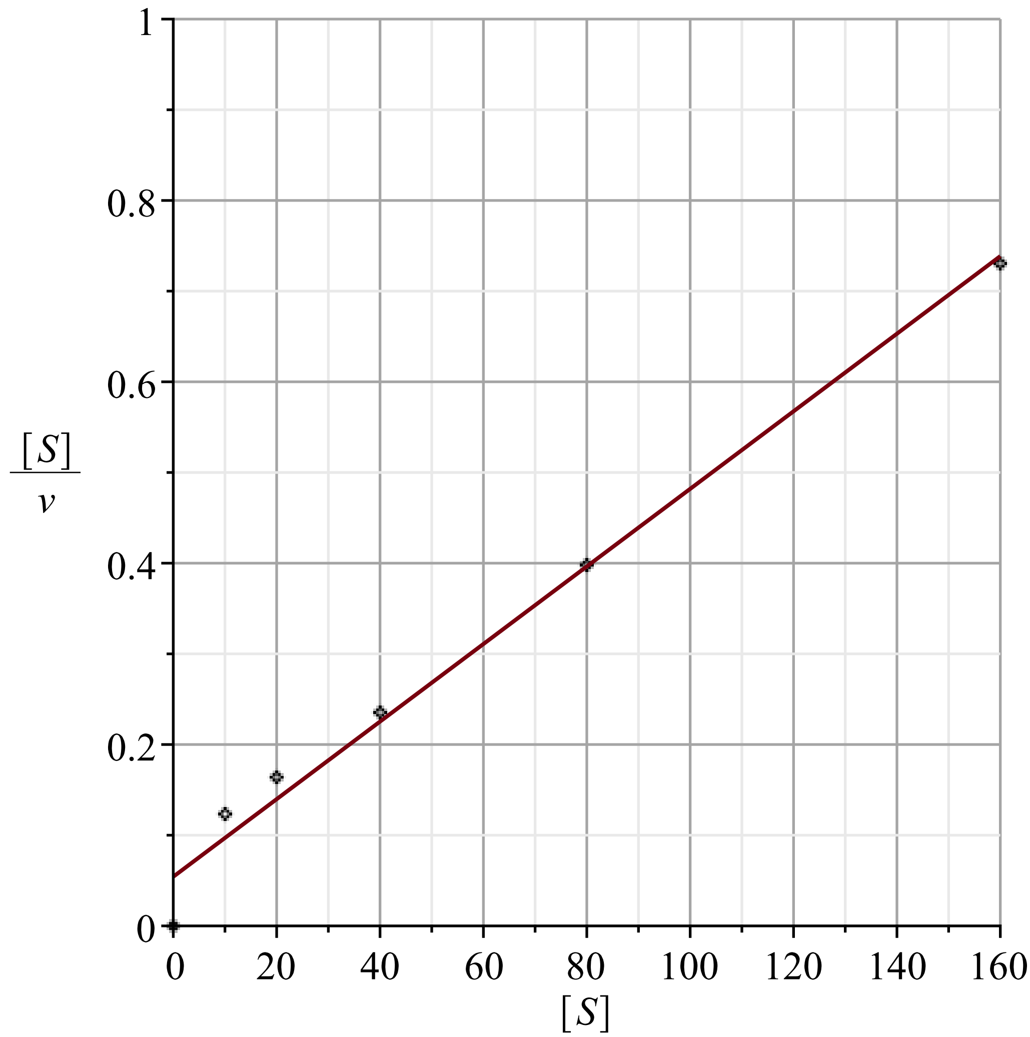
$$Yhw := \left[0, \frac{10}{81}, \frac{10}{61}, \frac{4}{17}, \frac{80}{201}, \frac{160}{219}\right] \tag{4.2}$$

> $hw(x) := LinReg(Xhw, Yhw, x) : hw(x)$

$$0.00427709870547465\, x + 0.0542313821171430 \tag{4.3}$$

Graf med forklarende symboler på akserne:

> $punkterHW := pointplot(\langle Vector(Xhw) | Vector(Yhw) \rangle) :$
$grafHW := plot(hw(x), x = 0..160) :$
$display\left(punkterHW, grafHW, view = [0..160, 0..1], labels = \left[[S], \frac{[S]}{v}\right], gridlines\right)$



Aflæser konstanterne:

> $a := hw(1) - hw(0)$

$$a := 0.00427709870547465 \tag{4.4}$$

> $b := hw(0)$

$$b := 0.0542313821171430 \tag{4.5}$$

> $solve\left(\left\{a = \frac{1}{V_{\max}}, b = \frac{K_m}{V_{\max}}\right\}, \{K_m, V_{\max}\}\right)$

$$\{K_m = 12.67947874, V_{\max} = 233.8033487\} \tag{4.6}$$

Eadie-Hofstee diagram $\left(\frac{v}{[S]}, v\right)$

Dataene lineariseres.

Husk at $X = \frac{v}{[S]}$ og $Y = v$.

NB: første værdi er 0, det kan ikke bruges, da man ikke kan dividere med 0.
Derfor er de kun 5 datasæt.

> $Xeh := \left[\frac{81}{10}, \frac{122}{20}, \frac{170}{40}, \frac{201}{80}, \frac{219}{160}\right]$

$$Xeh := \left[\frac{81}{10}, \frac{61}{10}, \frac{17}{4}, \frac{201}{80}, \frac{219}{160}\right] \tag{5.1}$$

> $Yeh := [81, 122, 170, 201, 219]$

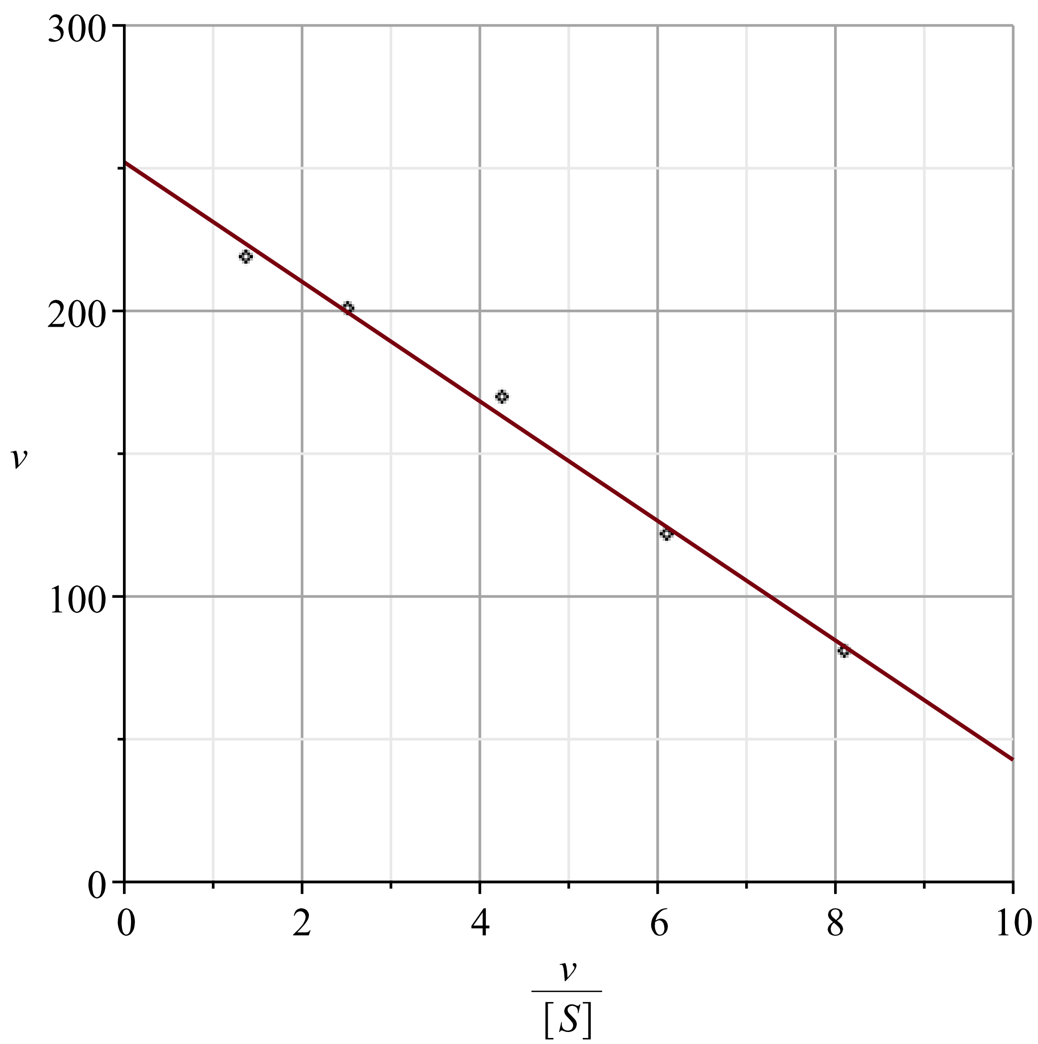
$$Yeh := [81, 122, 170, 201, 219] \tag{5.2}$$

> $eh(x) := LinReg(Xeh, Yeh, x) : eh(x)$

$$-20.9387032369004\,x + 252.117483331806 \tag{5.3}$$

Graf med forklarende symboler på akserne:

> $punkterEH := pointplot(\langle Vector(Xeh) | Vector(Yeh)\rangle) :$
> $grafEH := plot(eh(x), x = 0..10) :$
> $display\left(punkterEH, grafEH, view = [0..10, 0..300], labels = \left[\frac{v}{[S]}, v\right], gridlines\right)$



Aflæser konstanterne:

> $a := eh(1) - eh(0)$

$$a := -20.9387032369004 \quad (5.4)$$

> $b := eh(0)$

$$b := 252.117483331806 \quad (5.5)$$

> $solve(\{a = -K_m, b = V_{max}\}, \{K_m, V_{max}\})$

$$\{K_m = 20.93870324, V_{max} = 252.1174833\} \quad (5.6)$$

Konstanterne

NB: alle 4 metoder giver forskellige værdier af konstanterne!

Plottype	Michaelis-Menten	Lineweaver-Burk	Hanes-Wolf	Eadie-Hofstee
K_m	20.2	21.3	12.7	20.9
V_{max}	249.7	254.0	233.8	252.1