

$$Z = \frac{P\bar{V}}{RT} = 1 \text{ when ideal behavior}$$

$$\neq 1 \text{ when non-ideal behavior}$$

~ a dozen non-ideal gas equations of state

Van der Waals equation

$$P\bar{V} = RT \text{ (ideal)}$$

$$\left(P + \frac{a}{\bar{V}^2}\right)(\bar{V} - b) = RT \text{ (VDW)}$$

a, b are spec. fic parameters for each gas

$a \rightarrow$ accounts for interactions

$b \rightarrow$ accounts for size not being zero

If no interactions ($a=0$) and size is infinitely small ($b=0$)
VDW reduces to ideal gas law

Consider N_2 gas $a = 1.3483 \frac{L^2 \text{ atm}}{\text{mol}}$ $b = 0.038577 \frac{L}{\text{mol}}$

5.85 g N_2 in a container with 100.0 mL volume and temp is 300.0 K

$P_{\text{ideal}}?$ 51.4 atm

$P_{\text{VDW}}?$ 50.06 atm $P + \frac{a}{\bar{V}^2} = \frac{RT}{\bar{V} - b}$

$$P = \frac{RT}{\bar{V} - b} - \frac{a}{\bar{V}^2}$$

Consider N_2 again 1.000 moles at 300.0 K and $P = 100.0$ atm

$\bar{V}_{\text{ideal}}?$ 0.246 $\frac{L}{\text{mol}}$

$\bar{V}_{\text{VDW}}?$ Ugh

$$\left(P + \frac{a}{\bar{V}^2}\right)(\bar{V} - b) = RT$$

$$P\bar{V} - Pb + \frac{a\bar{V}}{\bar{V}^2} - \frac{ab}{\bar{V}^2} = RT$$

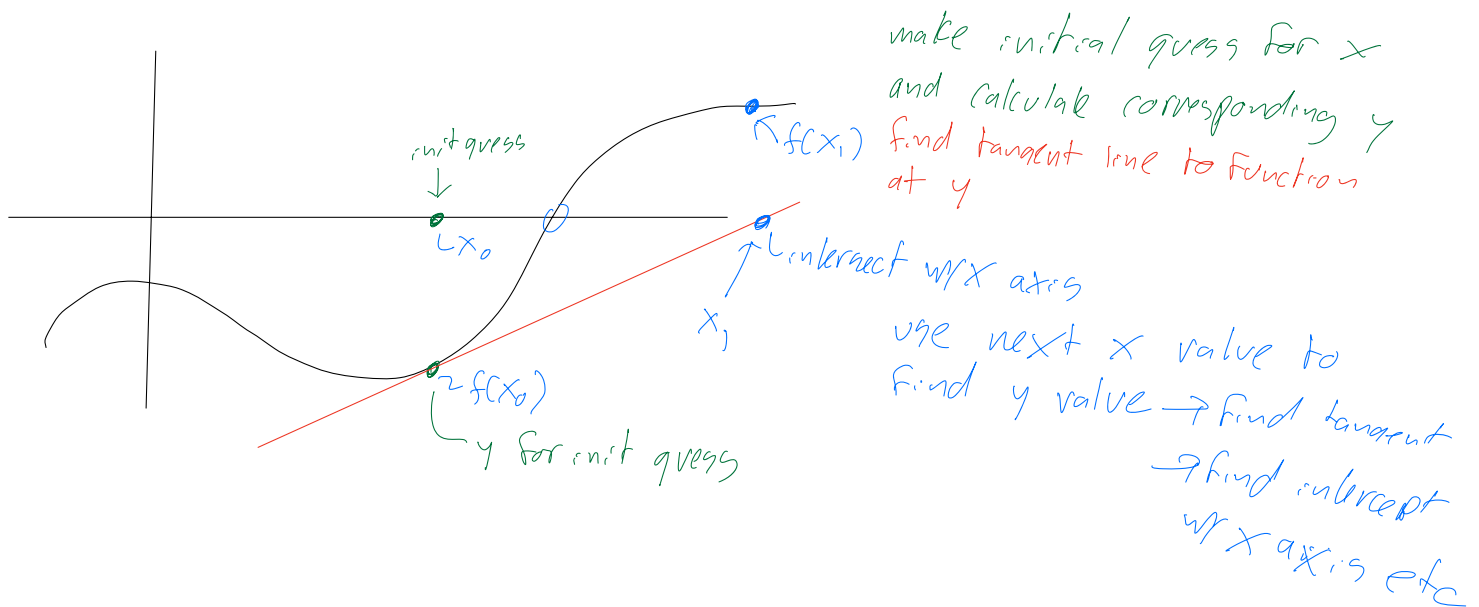
$$P\bar{V}^3 - Pb\bar{V}^2 + a\bar{V} - ab = RT\bar{V}^2$$

$$P\bar{V}^3 - (RT + Pb)\bar{V}^2 + a\bar{V} - ab = 0$$

need to solve for $\bar{V}$ - lots of ways to do with technology

How was it done 200+ years ago?

Newton-Raphson method



trial (n)	x_n	$f(x_n)$	$f'(x_n)$
0	$x_0 = \text{init guess for } x$	$f(x_0)$	$f'(x_0)$
1	$\left[x_0 - \frac{f(x_0)}{f'(x_0)}\right] = x_1$	$f(x_1)$	$f'(x_1)$
2	$\left[x_1 - \frac{f(x_1)}{f'(x_1)}\right] = x_2$	$f(x_2)$	$f'(x_2)$

continue until $X_{n+1} \approx X_n$