FYS4411/9411, Feb 21, 2025

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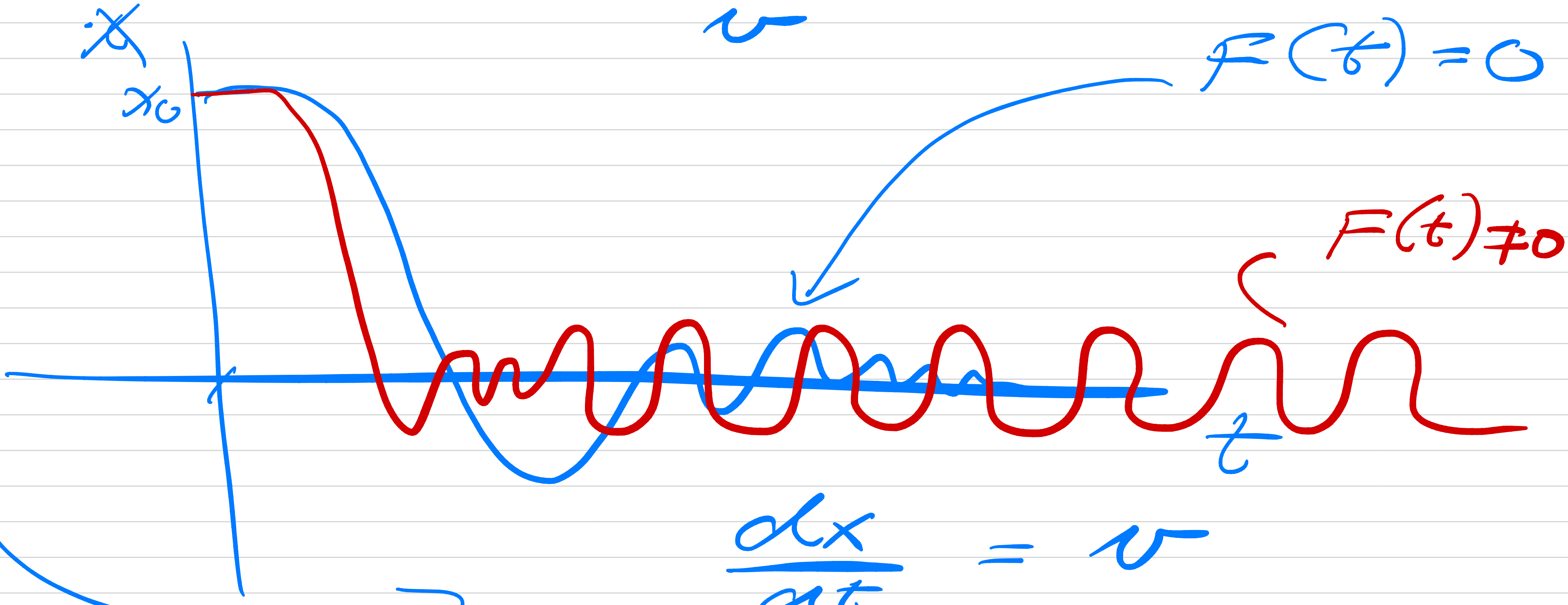
$$m\frac{d^2x}{dt^2} + \eta \underbrace{\frac{dx}{dt}}_{v} + x(t) = F(t)$$



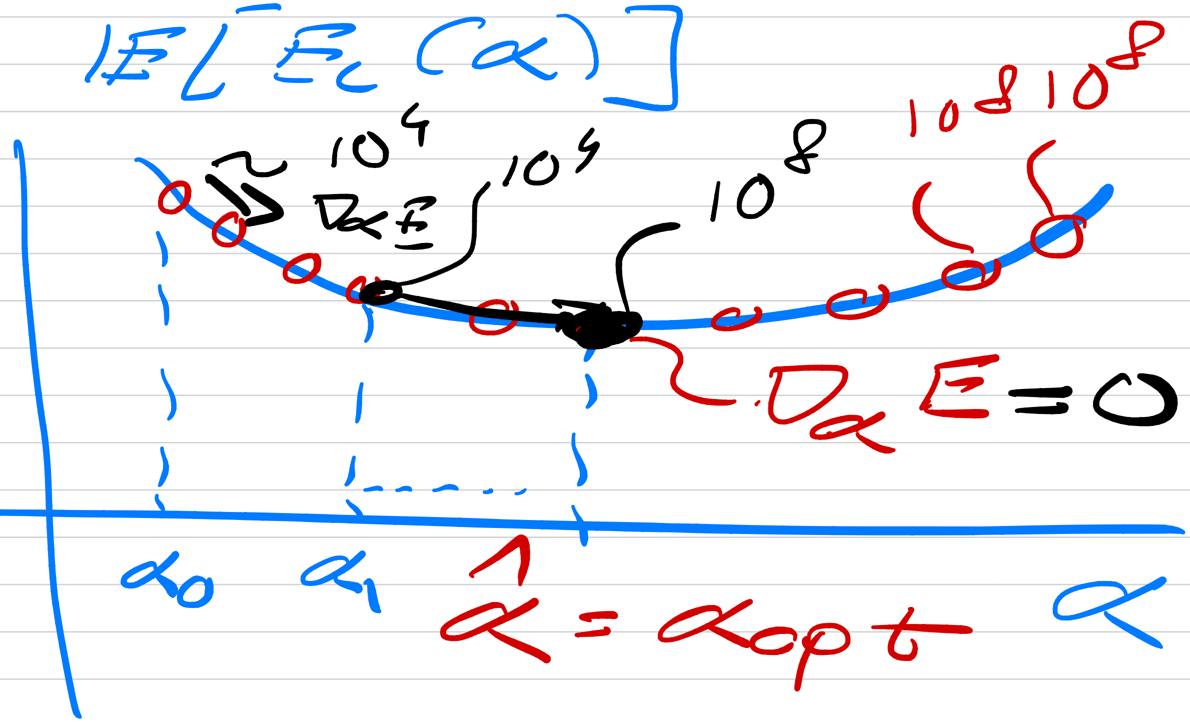
$$\frac{dx}{dt} = v$$

$$m\frac{dv}{dt} + \eta v + x = F(t)$$

$$\underbrace{\mathbb{E}\left[E_L(\vec{\alpha})\right]}_{E} = \int_{\vec{R}\in D} d\vec{R}\, P_{\vec{\alpha}}(\vec{R})\, E_L(\vec{R};\vec{\alpha})$$

$$P_{\vec{\alpha}}(\vec{R}) = \frac{|\psi_T(\vec{R};\vec{\alpha})|^2}{\int d\vec{R}\, |\psi_T(\vec{R};\vec{\alpha})|^2}$$

$$\vec{\alpha} = \{\alpha\}$$



$$\mathbb{E}\left[E_L(\vec{\alpha})\right] = E(\vec{\alpha})$$

$$\vec{\nabla}_{\vec{\alpha}} E(\vec{\alpha}) = g(\vec{\alpha})$$

$$\vec{\alpha} \Rightarrow \alpha \, ; \quad g(\vec{\alpha}) \rightarrow g(\alpha)$$

$$\alpha_{opt} = \hat{\alpha}$$

Prepare for Taylor expansion

$$\hat{\alpha} - \alpha_n = b_n \, ; \quad g(\alpha) = g(\alpha_n)$$

iteration -n- $\quad = g_n$

$$\nabla_\alpha^2 E(\alpha) \rightarrow \nabla_\alpha^2 E(\alpha_n) = A_n$$

Taylor expand around $\hat{\alpha}$

$$E(\hat{\alpha}) = \underset{\underset{E(\alpha_n)}{\shortparallel}}{E_n} + \underbrace{(\hat{\alpha}-\alpha_n)}_{b_n} g_n$$

$$+ \frac{1}{2} A_n (\hat{\alpha}-\alpha_n)^2 + O((\hat{\alpha}-\alpha_n)^3)$$

with more than one α.

$$E(\hat{\alpha}) = E_n + g_n^T \underbrace{b_n}_{(\hat{\alpha}-\vec{\alpha}_n)}$$

$$+ \frac{1}{2} b_n^T A_n b_n + O((b_n)^3)$$

$$\alpha = \{\alpha_0, \alpha_1\} \qquad \alpha_n = \{\alpha_0^n, \alpha_1^n\}$$

$$A_n = \begin{bmatrix} \left.\dfrac{\partial^2 E}{\partial \alpha_0^2}\right|_{\alpha=\alpha_n} & \left.\dfrac{\partial^2 E}{\partial \alpha_0 \, \partial \alpha_1}\right|_{\alpha=\alpha_n} \\ \left.\dfrac{\partial^2 E}{\partial \alpha_1 \, \partial \alpha_0}\right|_{\alpha=\alpha_n} & \left.\dfrac{\partial^2 E}{\partial \alpha_1^2}\right|_{\alpha=\alpha_n} \end{bmatrix}$$

Neglect $O(b_n^3)$

$$E(\alpha) = E_n + g_n^T b_n + \frac{1}{2} b_n^T A_n b_n$$

$$\left(f(\vec{x}) = c + \vec{g}^T \vec{x} + \frac{1}{2} \vec{x}^T A \vec{x} \right)$$

$$\frac{\partial f}{\partial x} = 0 = Ax + g \Rightarrow$$

$$x = A^{-1} g$$

g and A are known at iteration x_n

simple example

$$f(x_1, x_2) = x_1^2 + x_1 x_2 + 10 x_2^2 - 5x_1 - 3x_2$$

$$\left(x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right) \Rightarrow = \frac{1}{2} x^T \begin{bmatrix} 2 & 1 \\ 1 & 20 \end{bmatrix} x -$$

$$- \begin{bmatrix} 5 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\frac{\partial f}{\partial x} = 0$$

$$\frac{\partial f}{\partial x_1} = 0 = 2x_1 + x_2 - 5$$

$$\frac{\partial f}{\partial x_2} = 0 = x_1 + 20x_2 - 3$$

our guess for an iterative

$$x_0 = \begin{bmatrix} -3 \\ 1 \end{bmatrix}$$

what we need is

$$\nabla_{\vec{\alpha}} E(\vec{\alpha}) \qquad \hat{\alpha} = \alpha_{n+1}$$

$$\nabla_{\vec{\alpha}} E(\alpha_{n+1}) = 0 = \underbrace{g_n}_{\nabla_{\vec{\alpha}} E(\vec{\alpha}_n)} + A_n b_n$$

$$b_n = \alpha_{n+1} - \alpha_n$$

$$\alpha_{n+1} - \alpha_n = -A_n^{-1} g_n \implies$$

$$\boxed{\alpha_{n+1} = \alpha_n - A_n^{-1} g_n}$$

Newton-Raphson's method

Solve iteratively, starting with x_0 and repeat till

$$\| x_{n+1} - x_n \|_2 \leq \varepsilon \sim 10^{-5}$$
$$\sim 10^{-8}$$

A_n is a second derivative (can be difficult and time consuming to evaluate)

common (simplest approach) to replace by a constant

$$A_n \Rightarrow \gamma_n$$

$$\hat{\alpha} = \alpha_{n+1} = \boxed{\alpha_n - \gamma_n g_n}$$

plain gradient descent

How do we find an optimal γ_n

Expand

$$E(\alpha_n - \gamma_n g_n) =$$

$$E_n - \gamma_n g_n^T g_n + \frac{1}{2}\gamma_n^2 g_n^T A_n g_n + \cancel{O((\alpha_n - \gamma_n g_n)^3)}$$

$\alpha_{n+1} = \alpha_n - \gamma_n g_n$ depends on γ_{n-1}

$$\frac{dE}{d\gamma_n} = 0 \Longrightarrow$$

$$\gamma_n = \frac{g_n^T g_n}{g_n^T A_n g_n}$$

matrix

vector

Steepest descent

we want to avoid to calculate

$$A_n = \nabla_x^2 E_n$$

we need to show that

$$\nabla_{\vec{\alpha}} E_{\vec{\alpha}} =$$

$$2\left[\left\langle \frac{1}{\psi_T(\alpha)} \frac{d\psi_T}{d\alpha} E_L(\vec{\alpha}) \right\rangle\right.$$

one - integral

$$\left. - \left\langle \frac{1}{\psi_T(\alpha)} \left(\frac{d\psi_T}{d\alpha}\right) \right\rangle \langle E_L(\vec{\alpha}) \rangle \right]$$

one integral

integral