Gradient Dynamics Relaxiation Method

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1 The motivating idea behind GD

Suppose we have a potential field $\phi = \phi(\boldsymbol{x})$, where $\boldsymbol{x}$ is the postion vector of all the degrees of freedom (dof) of the system, and we are interested in finding the minimum of ϕ. The GD method is motivated by the fact that at the minimum potential energy the system is at equilibrium, meaning $\boldsymbol{F} = \boldsymbol{0}$, where $\boldsymbol{F}$ is the net force vector (also known as the residual when we are looking for equilibrium). We also know for a conservative system that $\boldsymbol{F} = -\nabla_{\boldsymbol{x}}\phi$. The idea of GD is to move the system, from an initial guess, in the direction of $-\nabla_{\boldsymbol{x}}\phi$, the direction of the maximum decrease of $\phi(\boldsymbol{x})$, to get to a local minimum or in the opposite direction $+\nabla_{\boldsymbol{x}}\phi$, the direction of the maximum increase of $\phi(\boldsymbol{x})$, to reach a maxima. In other words, moving the dof in a direction proportional to the forces, or $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \gamma \boldsymbol{F_t}$, $\gamma \in \boldsymbol{R}^+$, we are guaranteed to reach a local mimima, provided that we choose small enough values of γ at each step and ϕ is not pathological within the problem domain. γ is also refered to as the time step Δt for obvious reasons, although it is a numerical parameter and not the physical time step precisely.

2 The algorithm of GD

Starting from an initial point $\boldsymbol{x} = \boldsymbol{x}_o$ at t = 0:

- Calculate $\boldsymbol{F}_t = -\nabla_{\boldsymbol{x}}\phi(\boldsymbol{x}_t)$
- Check for convergence. For example if L2Norm($\boldsymbol{F}_t$) <= Tol, then break
- Take a time step, $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \gamma \boldsymbol{F_t}$
- t= t+1
- Repeat