Computational Physics: Jamming of aspherical particles

Saurabh Gangwar

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1 Abstract

This project assigns energy to overlapping particles based on their specific overlap. The energy landscape defined by the sum of all particle pairs, the minima being particle positions and alignments with minimal overlaps. We want to be able to calculate these minima. I use to employ the nonlinear conjugate gradient approach for the implementation of dumbbell shape soft particles, also optimize the energy and gradient calculations. A dumbbell shaped particle is two spheres, with the distance fixed but not separated. In this research, we want to see how the jamming density varies with the L/R ratio in a system of soft dumbbell particles. Dumbbells are particles composed of two Spheres of radius R with a distance of L between their centers.The pair potential will be the same as for spherical particles. We wish to adjust the distance between the spheres that make up the dumbbells and repeat the analysis. We should next calculate the density of jamming as a function of the spacing to radius ratio. Get the jamming density for a certain dumbbell shape, then repeat for different dumbbell geometries. We will calculate the density and volume of spherical particles using various dumbbell geometries. Here, we provide short introduction to the Jamming physics demonstrated by simple method system for the jamming transition: Start with random configuration of particle soft spheres particles.

2 Introduction

Jamming physical phenomenon; the viscosity of certain mesoscopic materials, such as granular materials, glasses, foams, polymers, emulsions, and other complicated fluids, increases with particle density. The jamming transition proposed as new sort of phase transition; however,r it differs significantly from the development of crystalline solids. [1]

The jamming transition occurs as the density, or packing percentage, of the

[1] Biroli, Giulio (April 2007). "Jamming: A new kind of phase transition?". Nature Physics. 3 (4): 222–223. Bibcode:2007NatPh...3..222B. doi:10.1038/nphys580.

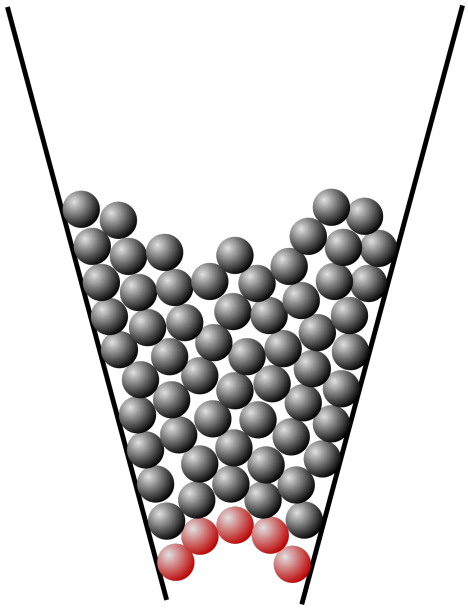

Figure 1: https://en.wikipedia.org/wiki/Jamming$_{(physics)}$/$media$/$File$: $Granular_{j}amming.svg$

particles increases. The system can be able to unjam if the volume fraction reduced or external stressors apply that surpass the yield stress. This transition nonlinear in terms of volume fractions.
The jamming phase diagram plots the jamming transition against inverse density, stress, and temperature. [2]
The shape of components, particle deformability, frictional interparticle forces, and degree of dispersity all influence the density of the system. For example, one especially intriguing aspect of the jamming transition distinction between attracting and repulsive particle systems. It's not certain whether the jamming surface diverges at sufficiently high densities or low temperatures.
Simulations of jammed systems investigate particle configurations that cause jamming in both static and stressed systems; the average cluster size may diverge after a finite amount of strain, resulting in a jammed state. A particle configuration exists in a jammed condition, requiring stress to "break" the force chains that are generating the jam.
The jamming transition occurs when the applied pressure and shear modulus are both zero, resulting in loss of stiffness. In addition, at the jamming point, system is isostatic. Above the jamming point, the applied pressure increases the volume fraction by pressing the soft spheres closer together, resulting in more

[2]Trappe, V.; et al. (14 June 2001). "Jamming phase diagram for attractive particles". Nature. 411 (6839): 772–775. Bibcode:2001Natur.411..772T. doi:10.1038/35081021. PMID 11459050. S2CID 661556. Retrieved 2008-03-28.

interactions between neighboring spheres.

3 Methodology

We use our CG method to optimize the non-linear convex functions. The nonlinear CG method can discover the minimum point of a quadratic form or minimize any continuous function f(x) with the computed gradient f'.
Outline for the non-linear conjugate gradient method
To obtain non-linear CG, three adjustments are made to the linear approach.The residual in nonlinear CG is always set to the inverse of the gradient $r_(i) = f'(x_(i))$.I use two methods: the Fletcher-Reeves formula and the Polak-Ribiere formula.

$$\beta_{i+1}^{FR} = \frac{r_{(i+1)}^T r_{(i+1)}}{r_{(i)}^T r_{(i)}}, \qquad \beta_{i+1}^{PR} = \frac{r_{(i+1)}^T (r_{(i+1)-r_{(i)}})}{r_{(i)}^T r_{(i)}}$$

To ensure convergence of the Polak-Ribi'ere approach, choose $\beta = max\beta^{PR}, 0$. Using this value is equivalent to CG if $\beta^{PR} < 0$. Here is outline for the nonlinear CG method:

$$d_{(0)} = r_{(0)} = -f'(x_{(0)})$$

,
Find $\alpha_{(i)}$ that minimizes $f(x_{(i)} + \alpha_{(i)} d_{(i)})$,

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)}$$

,

$$r_{(i+1)} = -f'(x_{(i+1)})$$

,

$$\beta_{(i+1)} = \frac{r_{(i+1)}^T r_{(i+1)}}{r_{(i)}^T r_{(i)}} \quad or \quad \beta_{(i+1)} = \max\left\{ \frac{r_{(i+1)}^T (r_{(i+1)} - r_{(i)})}{r_{(i)}^T r_{(i)}}, 0 \right\}$$

,

$$d_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} d_{(i)}$$

Nonlinear CG, search directions lose conjugacy faster compared to quadratic functions. Figure 37 shows non-linear CG. Figure 37(a) depicts a function with several local minima. Figure 37(b) shows the convergence of non-linear CG to the Fletcher-Reeves formula.Figure 37 (c) depicts a cross section of the surface,

corresponding to the first-line search in Figure 37(b).The line search yields the value of α corresponding to the nearby minimum. Figure 37(d) demonstrates the higher convergence of the Polak-Ribi'ere CG.Figure 38 illustrates the effect of restarting nonlinear CG every second iteration.

4 General Line Search

It depends on the value of (f'), a quick technique could be used to identify the zeros of $f^T d$. For example, if it (f') is polynomial in (α), a **efficient technique for polynomial zero-finding** can be applied. We solely consider general-purpose algorithms.

Two iterative methods for zero-finding are the **Newton-Raphson method** and the **Secant method** . Both methods require that (f) be twice continuously differentiable. Newton-Raphson also requires that it be possible to compute the second derivative of $(f(x+\alpha d))$ with respect to (α) .
The Newton-Raphson approach uses the Taylor series approximation:

$$\begin{aligned} f(x+\alpha d) &\approx f(x) + \alpha \left[\frac{d}{d\alpha} f(x+\alpha d)\right]_{\alpha=0} + \frac{\alpha^2}{2}\left[\frac{d^2}{d\alpha^2} f(x+\alpha d)\right]_{\alpha=0} \qquad (56) \\ &= f(x) + \alpha \left[f'(x)\right]^T d + \frac{\alpha^2}{2} d^T f''(x) d, \end{aligned}$$

$$\frac{d}{d\alpha} f(x+\alpha d) \approx \left[f'(x)\right]^T d + \alpha d^T f''(x) d.$$

where, $(f''(x))$ is the **Hessian matrix** : $f''(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}$.
The function $f(x+\alpha d)$ approximately minimized by setting Expression 57 to zero, giving

$$\alpha = -\frac{f'^T d}{d^T f'' d}.$$

The truncated Taylor series approximates $f(x+\alpha d)$ with parabola, and we step to the bottom of it (Figure 39). In reality, if f is quadratic form, then this parabolic approximation is exact, because f'' simply the familiar matrix A).$Generally,$**search directions**$are conjugate if they are f''$-orthogonal. The meaning of **"conjugate"** changes as f'' varies with x. The faster f'' changes with x, the faster the search directions lose conjugacy. In contrast, the closer $x_{(i)}$ is to the solution, the less f'' changes from iteration to iteration. The convergence

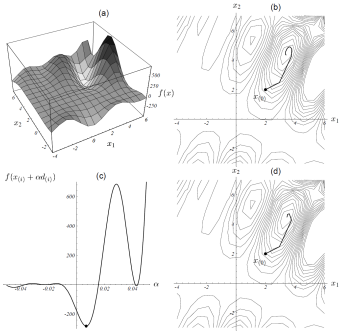

Figure 37: Convergence of the nonlinear Conjugate Gradient Method. (a) A complicated function with many local minima and maxima. (b) Convergence path of Fletcher-Reeves CG. Unlike linear CG, convergence does not occur in two steps. (c) Cross-section of the surface corresponding to the first line search. (d) Convergence path of Polak-Ribière CG.

Figure 2:

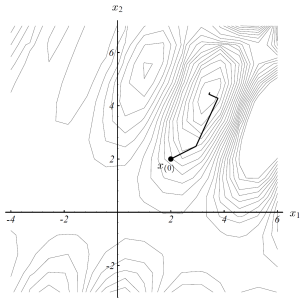

Figure 38: Nonlinear CG can be more effective with periodic restarts.

Figure 3:

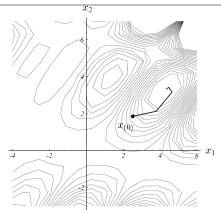

Figure 41: The preconditioned nonlinear Conjugate Gradient Method, using the Polak-Ribière formula and a diagonal preconditioner. The space has been "stretched" to show the improvement in circularity of the contour lines around the minimum.

Figure 4:

of nonlinear CG is more similar to linear CG as the starting point approaches the solution.

To complete an exact line search of a non-quadratic function, repeated steps must be taken along the line until $f'^T d$ 0; thus, **one CG iteration may comprise several Newton-Raphson iterations**. Each step requires evaluating the values of $f'^T d$ and $d^T f'' d$. These evaluations may be inexpensive if $d^T f'' d$ can be analytically simplified, but if the complete matrix f'' must be evaluated repeatedly, the procedure becomes prohibitively slow. In some cases, an approximation line search using only the diagonal elements of f'' can solve this issue. Some functions cannot be evaluated using f''.

To perform an exact line search without computing f'', the **Secant method** approximates the second derivative of $f(x + \alpha d)$ by evaluating the first derivative at distinct points $\alpha = 0$ and $\alpha = \sigma$, where σ is an arbitrary small nonzero number.

As α and σ approach 0, the approximation to the second derivative improves. If we replace Expression 58 for the third term of the Taylor expansion (Equation 56), we get Minimize $f(x + \alpha d)$ by setting its derivative to zero:

The Secant technique, like Newton-Raphson, approximates $f(x+\alpha d)$ with a parabola. However, instead of obtaining the first and second derivatives at a location, it finds the first derivative at two distinct points (Figure 40). Typically, we will choose an arbitrary σ on the first Secant method iteration; on following iterations, we will choose $x + \sigma d$ as the value of x from the preceding Secant method iteration. In other words, let $\alpha_{[i]}$ denote the value of α calculated during Secant iteration i, then $\sigma_{[i+1]} = -\alpha_{[i]}$.

If $f''(x)$ changes significantly with x, it will converge quickly. As a result, a speedy but inexact line search is frequently the best approach (for example, limit the amount of Newton-Raphson or Secant method iterations). Unfortunately, inexact line searches might result in the creation of a search direction that is not a descending direction. A popular method is to test for this possibility (is $r^T d$ nonpositive?) and restart CG if needed by setting $d = r$.

A greater issue with both techniques is that they cannot distinguish between

minima and maxima. The outcome of nonlinear CG is often significantly dependent on the beginning point, and if CG with the Newton-Raphson or Secant method begins near a local maximum, it is likely to converge there.

The Newton-Raphson approach has a higher convergence rate and is favored if $d^T f'' d$ can be determined (or well approximated) fast (i.e., in $\mathcal{O}(n)$ time). The **Secant method** just requires first derivatives of f, but its performance may depend on a suitable selection of the parameter σ. Other ways can be easily derived as well. For example, sampling f at three distinct places can build a parabola that approximates $f(x + \alpha d)$ without calculating the first derivative of f.

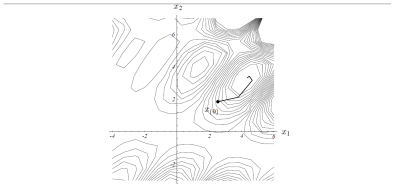

Figure 41: The preconditioned nonlinear Conjugate Gradient Method, using the Polak-Ribière formula and a diagonal preconditioner. The space has been "stretched" to show the improvement in circularity of the contour lines around the minimum.

Figure 5: https://en.wikipedia.org/wiki/Jamming$_{(physics)}$/$media$/$File$: $Granular_{j}amming.svg$

5 Nonlinear Conjugate Gradients with Newton-Raphson and Fletcher-Reeves

Consider a function f, a beginning value x, a maximum number of CG iterations $i_{\max}$, CG error tolerance $\varepsilon < 1$, a maximum number of Newton-Raphson iterations $j_{\max}$, and Newton-Raphson error tolerance $\epsilon < 1$.

$i \leftarrow 0$
$k \leftarrow 0$
$r \leftarrow -f'(x)$
$d \leftarrow r$
$\delta_{\text{new}} \leftarrow r^T r$
$\delta_0 \leftarrow \delta_{\text{new}}$
while $i < i_{\max}$ and $\delta_{\text{new}} > \varepsilon^2 \delta_0$ **do**
    $j \leftarrow 0$
    $\delta_d \leftarrow d^T d$
Do $\alpha \leftarrow -\frac{[f'(x)]^T d}{d^T f''(x) d}$
    $x \leftarrow x + \alpha d$
    $j \leftarrow j + 1$
while $j \geq j_{\max}$ or $\alpha^2 \delta_d \leq \varepsilon^2$
    $r \leftarrow -f'(x)$
    $\delta_{\text{old}} \leftarrow \delta_{\text{new}}$
    $\delta_{\text{new}} \leftarrow r^T r$
    $\beta \leftarrow \frac{\delta_{\text{new}}}{\delta_{\text{old}}}$
    $d \leftarrow r + \beta d$
    $k \leftarrow k + 1$
    if $k = n$ or $r^T d \leq 0$ **then**
        $d \leftarrow r$
        $k \leftarrow 0$
        $i \leftarrow i + 1$

This algorithm ends when the maximum number of iterations $i_{\max}$ is reached, or

$$\|r_{(i)}\| \leq \varepsilon \|r_{(0)}\|.$$

Each Newton-Raphson iteration adds αd to x; iterations are halted when each update αd falls below the stated tolerance ($\|\alpha d\| \leq \varepsilon$), or when the number of iterations exceeds $j_{\max}$. A quick inexact line search is achieved by utilizing a short $j_{\max}$ and/or approximating the Hessian $f''(x)$ with its diagonal.
Nonlinear CG restarts (by setting $d \leftarrow r$) anytime a search direction other than descent is computed. It is additionally restarted every n iteration to promote convergence for small n.
The calculation of α yields divide-by-zero error. This occurs when the beginning point $x_{(0)}$ is not close enough to the required minimum, or if f is not twice continuously differentiable. In the former scenario, the remedy is to select a better starting point or conduct a more sophisticated line search. In the latter scenario, CG may not be the most suitable minimization algorithm.

6 Preconditioned Nonlinear Conjugate Gradients with Secant and Polak-Ribi‘ere

Given a function f, starting value x, maximum number of CG iterations $i_{\max}$, CG error tolerance $\varepsilon < 1$, Secant method step parameter σ_0, maximum number of Secant method iterations $j_{\max}$, and Secant method error tolerance $\epsilon < 1$:

$i \leftarrow 0$
$k \leftarrow 0$
$r \leftarrow -f'(x)$
Calculate a preconditioner $M \approx f''(x)$
$s \leftarrow M^{-1}r$
$d \leftarrow s$
$\delta_{\text{new}} \leftarrow r^T d$
$\delta_0 \leftarrow \delta_{\text{new}}$
While $i < i_{\max}$ **and** $\delta_{\text{new}} > \epsilon^2 \delta_0$ **do**
    $j \leftarrow 0$
    $\delta_d \leftarrow d^T d$
    $\alpha \leftarrow -\sigma_0$
    $\eta_{\text{prev}} \leftarrow [f'(x + \sigma_0 d)]^T d$
    Do
        $\eta \leftarrow [f'(x)]^T d$
        $\alpha \leftarrow \alpha \dfrac{\eta}{\eta_{\text{prev}} - \eta}$
        $x \leftarrow x + \alpha d$
        $\eta_{\text{prev}} \leftarrow \eta$
        $j \leftarrow j + 1$
    while $j < j_{\max}$ **and** $\alpha^2 \delta_d > \epsilon^2$
    $r \leftarrow -f'(x)$
    $\delta_{\text{old}} \leftarrow \delta_{\text{new}}$
    $\delta_{\text{mid}} \leftarrow r^T s$

Calculate a preconditioner $M \approx f''(x)$
$s \leftarrow M^{-1}r$
$\delta_{\text{new}} \leftarrow r^T s$
$\beta \leftarrow \dfrac{\delta_{\text{new}} - \delta_{\text{mid}}}{\delta_{\text{old}}}$
$k \leftarrow k + 1$
If $k = n$ **or** $\beta \leq 0$
$d \leftarrow s$
$k \leftarrow 0$
else
$d \leftarrow s + \beta d$
$i \leftarrow i + 1$

This algorithm ends when the maximum number of iterations $i_{\max}$ is reached or when $\|r(i)\| \leq \epsilon \|r(0)\|$.
Each iteration of the Secant method adds αd to x; iterations are halted when each update αd falls below a set tolerance ($\|\alpha d\| \leq \epsilon$), or when the number of iterations exceeds $j_{\max}$. Using tiny $j_{\max}$ allows for a quick but inexact line search. The parameter σ_0 sets the value of σ in Equation 59 during the first phase of Secant method minimization. It may be essential to change this parameter to obtain convergence.
The Polak-Ribière β parameter is defined as:

$$\beta = \frac{\delta_{\text{new}} - \delta_{\text{mid}}}{\delta_{\text{old}}} = \frac{r_{(t+1)}^T s_{(t+1)} - r_{(t+1)}^T s_{(t)}}{r_{(t)}^T s_{(t)}} = \frac{r_{(t+1)}^T M^{-1}(r_{(t+1)} - r_{(t)})}{r_{(t)}^T M^{-1} r_{(t)}}$$

Ensure the preconditioner M always positive-definite. The preconditioner does not need take the shape of a matrix. Nonlinear CG resumed (by setting $d \leftarrow r$) when the Polak-Ribière β parameter is negative. It additionally restarts every n iterations to promote convergence for small n.

7 Reference

1) Biroli, Giulio (April 2007). "Jamming: A new kind of phase transition?". Nature Physics. 3 (4): 222–223. Bibcode:2007NatPh...3..222B. doi:10.1038/nphys580. Retrieved 2008-03-28.
2) Trappe, V.; et al. (14 June 2001). "Jamming phase diagram for attractive particles". Nature. 411 (6839): 772–775. Bibcode:2001Natur.411..772T. doi:10.1038/35081021. PMID 11459050. S2CID 661556. Retrieved 2008-03-28.
methodologyShewchuk, J. R. (August 1994). "An Introduction to the Conjugate Gradient Method Without the Agonizing Pain"