Physics-based Animation: A Mathematical Perspective

Based on Ladislav Kavan's CS6660 with annotations from wxgopher

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Contents

This lecture note is based on Dr. Ladislav Kavan's Physics-based Animation course CS6660, originally taught at the University of Utah. I also try to include some supplementary materials from other resources.

Warning: Although as I strive to make this material useful, there are certain bugs, use this material at your own risk. I would also be grateful to hear feedbacks.

1 Classical Mechanics

1.1 Basics: a harmonic oscillator

2 Time Integration

3 Optimization

3.1 Implicit Newmark

$$x_{n+1} = x_n + \frac{h}{2}(v_n + v_{n+1}), \tag{1a}$$

$$v_{n+1} = v_n = \frac{h}{2}(f_n + f_{n+1}), \tag{1b}$$

where x and v are positions and velocities, and $f_n \equiv f(x_n)$. Thus we have

$$x_{n+1} - x_n - hv_n = \frac{h^2}{4}(f_n + f_{n+1}). \tag{2}$$

Let $y = x_n + h_n v_n + \frac{h^2}{4} f_n$, $x_{n+1} = x$, note that $\nabla E = -f$, then (2) becomes

$$x - y = \frac{h^2}{4} f \Rightarrow x - y + \frac{h^2}{4} f \nabla E = 0. \tag{3}$$

Let $g(x) = \frac{1}{2}\|x - y|^2 + \frac{h^2}{4} E$, then solving g equals to solve x for

$$\min_x \quad g(x). \tag{4}$$

3.2 Optimization Problems

Problem formulation:

$$\min_x \quad g(x), \quad x \in R^n, \quad g \in R. \tag{5}$$

Optimization problems can be categorized into constrained or unconstrained problems, or convex or non-convex problems.

Theorem 1. *For a convex problem (where both objective and feasible set are convex), if the objective is C^2, then the Hessian $H \succeq 0$, and the local minimum is the global minimum.*

Definition 1. *A **linear programming (LP)** is a problem with linear objective and linear equality or inequality constraints. A **quadratic programming (QP)** is* **the same as LP** *except with a quadratic objective.*

Note 1. *Convex QP has polynomial time solver but non-convex QP is NP-hard.*

Example 1. *A non-convex QP:*

$$\min_x \quad \frac{1}{2}\|Ax\|^2, \tag{6a}$$

$$s.t. \quad \|x\|_2 = 1. \tag{6b}$$

Note 2. *Software package for solving non-convex problem:* IpOPT, KNITRO, *or* NEOS-Guide

3.2.1 Solving unconstrained problems

There are two ways to solve an unconstrained problem: descent method or trust-region method.

Descent method refers to pick a descent direction d and do an exact or inexact line search (LS) to determine descent distance αd.

Definition 2. ***Descent direction***: $\forall \alpha \in (0, \alpha_0)$, $\alpha_0 > 0$, $g(x + \alpha d) < g(x)$.

Definition 3. ***Exact LS*** *refers to solving the following problem:*

$$\arg\min_{\alpha > 0} g(x + \alpha d).$$

Backtracking LS

3.2.2 Newton's method

A usual descent direction is called **gradient descent** (GD), denoted by $d = -\nabla g$. It doesn't work well sometime, for example:

Example 2.

$$\min_{x_1, x_2} g(x1, x2) = \frac{1}{2}(x_1^2 + \gamma x_2^2), \quad \gamma > 0. \tag{7}$$

If we do exact LS, we get

$$x_1^k = \gamma(\frac{\gamma - 1}{\gamma + 1})^k, \tag{8a}$$

$$x_2^k = (-\frac{\gamma - 1}{\gamma + 1})^k. \tag{8b}$$

If gamma becomes huge, we can tell GD converges slowly (as two GD directions are perpendicular).

Newton's method refers to do a quadratic approximation to problem (5), given by

$$g(x + p) = g(x) + \nabla g^{\mathrm{T}}(x)p + \frac{1}{2}p^{\mathrm{T}}\nabla^2 g(x)p + O(\|p\|^2) \equiv \tilde{g}(x) + O. \tag{9}$$

Thus we have

$$\frac{\partial \tilde{g}}{\partial p} = 0 \Longleftrightarrow \nabla g + \nabla^2 g p = 0.$$

The **Newton descent direction** is given by

$$p = -(\nabla^2 g)^{-1}\nabla g. \tag{10}$$

Note 3. *Newton's method is affine invariant. Let $x = Ty$ with T being a nonsingular matrix, so problem (5) is equivalent to problem*

$$\min_y \tilde{g}(y). \tag{11}$$

We also have

$$\nabla \tilde{g} = T^2 \nabla g, \quad \nabla^2 \tilde{g} = T^{\mathrm{T}} \nabla^2 g T.$$

Newton direction Δy of $\tilde{g}$ and Δx of g is given by

$$\Delta y = -T^{-1} \nabla^2 g \nabla g = T^{-1} \Delta x.$$

Definition 4. ***Newton decrement****: substitute Newton descent direction (10) into (9), we get the* ***Newton decrement***

$$\lambda^2 = g - \frac{1}{2} \nabla g^{\mathrm{T}} (\nabla^2 g)^{-1} \nabla g. \tag{12}$$

A stopping criteria for Newton's method would be

$$\frac{\lambda^2}{2} \leq \epsilon.$$

Note that Newton decrement is also affine invariant.

Convergence analysis of the Newton's method is given as follows:

Theorem 2. ***Kantorovich****: if g is strictly convex and $\nabla^2 g$ is Lipschitz continuous, then $\exists \epsilon > 0, \eta > 0, \gamma > 0$, s.t.*

Damped phase I *If $\|\nabla g\| \geq \eta$, then $\|g^{k+1}\| \leq \|g^k\| - \gamma$;*

Quadratic phase II *If $\|\nabla g\| < \eta$, then $\|g^{k+1}\| \leq c\|g^k\|^2$.*

Some cases where Newton's method doesn't work well:

1. If g is highly nonlinear, the damped phase will be long;
2. If g is non-convex, solution might not converge to a minimum.

In practical implementations, the Hessian might not always be positive definite. A possible Hessian modification is:

Note 4. ***Hessian modification****: Consider $A = \nabla^2 g + cI$, where $c > 0$. It is shown that if $\nabla^2 g = Q \Lambda Q^{\mathrm{T}}$ ($\nabla^2 g$ is symmetric, hence it is always diagonalizable), then $A = Q(\Lambda + cI)Q^{\mathrm{T}}$, hence A is positive definite given sufficiently large $c > 0$.*

Solving Newton's direction (10) refers to solving a linear system. We introduce several techniques to tackle this.

3.3 Numerical Linear Algebra

We consider solving a linear system $Ax = b$.

3.3.1 Direct solvers

We can prefactor A into $A = UV^{\mathrm{T}}$, with U and V being low rank matrices.

Common factorization methods are

LU If A is nonsingular, then there exist L, P, U, where they are lower-triangular matrix, permutation matrix (hence orthogonal), and upper-triangular matrix, respectively, s.t. $A = PLU$.

Sparse LU $A = P_1 L U P_2$, where P_1 and P_2 are permutations to utilize sparse information of A.

Cholesky For symmetric positive-definite matrix, we have $A = LL^{\mathrm{T}}$ with unique L. Note that for positive semi-definite matrix, Cholesky is not unique.

LDLT

3.3.2 Iterative solvers

Iterative solvers includes:

1. Classical method: Jacobian, Gauss-Seidel, SOR (super over-relaxation), etc.;
2. Krylov subspace method: CG (conjugate gradient)[1], GMRES (generalized minimal residual), etc.;
3. multigrid method.

Classical method Suppose P is easy to invert, let $A = P + A - P$, then

$$Ax = b \quad \Leftrightarrow \quad Px = (P - A)x + b.$$

$P = diag(A)$ gives us Jacobian method, and it's GPU-friendly; $P = lower(A)$ gives us GS method; $P = diag(A) + w \cdot lower(A)$ gives us SOR method where $w < 2$.

The residual term follows

$$r_k \equiv A(x^\star - x_k) = b - Ax_k \quad \Leftrightarrow \quad r_{k+1} = (I - P^{-1}A)r_k.$$

To make classical method converge, we need $\rho(I - P^{-1}A) < 1$, where $\rho(\cdot)$ is the spectrum radius.

Krylov subpace method Assuming $A^{\mathrm{T}} = A$ and $A \succeq 0$, then

$$\arg\min_x g(x) = \frac{1}{2}x^{\mathrm{T}}Ax - x^{\mathrm{T}}b \quad \Leftrightarrow \quad solve\ Ax = b. \tag{13}$$

Let $\nabla g_k = Ax_k - b = -r_k$[2] as a descent direction, the line search for (13) is as follows:

1. Solve α from $\arg\min_\alpha(\frac{1}{2}(x + \alpha r)^{\mathrm{T}}A(x + \alpha r) - (x + \alpha r)^{\mathrm{T}}b \equiv \frac{1}{2}\|x + \alpha r\|_A^2 - (x + \alpha r)^{\mathrm{T}}b)$ by letting $\frac{\partial E}{\partial \alpha} = 0$, where E is the objective;
2. α follows $\alpha = -\frac{\|r\|^2}{|r\|_A^2}$;
3. $x_{k+1} = x_k + \alpha_k r_k$.

This is the gist of CG from gradient descent.

CG Assuming solving problem (13).

Definition 5. ***A-conjugate*** *A set of vectors $\{p_i\}$ are A-conjugate iff $\forall i, j, i \neq j, p_i^{\mathrm{T}}Ap_j = 0$.*

The CG algorithm is as follows:

1. We define $r_k = Ax_k - b$;
2. Let $p_1 = r_1$[3];
3. $p_k = r_k + \beta_k p_{k-1}, \beta_k = \frac{r_k^{\mathrm{T}}Ap_{k-1}}{p_{k-1}^{\mathrm{T}}Ap_{k-1}}$;
4. Do LS along direction p_k, we have $\alpha_k = \frac{r_k^{\mathrm{T}}p_k}{p^{\mathrm{T}}Ap_k}$;
5. $x_{k+1} = x_k + \alpha_k p_k$.

[1] A good reference on CG is [8].
[2] Ax is computed on-fly, we don't need the whole A.
[3] r_1 is usually chosen as a GD step

Preconditioning CG If A is ill-conditioned, we consider adding preconditioner M to A, s.t. $cond(MA) < cond(A)$.

The Jacobian preconditioner is given by $M = diag(A)^{-1}$. The incomplete Cholesky is given by pref-actoring A into $L_a L_a^{\mathrm{T}}$ where -L_a is an approximation of L of the Cholesky decomposition of A given by $A = LL^{\mathrm{T}}$.

4 Elastic Materials and Finite Element Simulation

4.1 Kinetic energy

Consider kinetic energy

$$k = \frac{1}{2} v^{\mathrm{T}} M v.$$

Assuming unit mass, we have

$$k = \frac{1}{2} \int_{\Omega} \rho(p) \|v(p)\|^2 \mathrm{d}p, \tag{14}$$

where $p \in \Omega$ is the material point. We discretize Ω, and for every node p_i we define piece-wise shape function $s_i : \Omega \mapsto [0, 1]$, s.t. $\sum_i s_i = 1$. For every region E_t, we also define

$$r_t(p) = \begin{cases} 1 & p \in E_t, \\ 0 & otherwise. \end{cases}$$

We have

$$v(p) = \sum_i v_i s_i(p), \tag{15a}$$

$$\rho(p) = \sum_t \rho_t r_t(p). \tag{15b}$$

The kinetic energy follows

$$k = \frac{1}{2} \int_{\Omega} \sum_t \rho_t r_t \|v(p)\|^2 \mathrm{d}p \tag{16a}$$

$$= \frac{1}{2} \sum_t \rho_t \int_{\Omega} r_t(p) \|v(p)\|^2 \mathrm{d}p \tag{16b}$$

$$= \frac{1}{2} \sum_t \rho_t \int_{E_t} \|v\|^2 \mathrm{d}p \tag{16c}$$

$$= \frac{1}{2} \sum_t \rho_t \sum_{i,j} v_i^{\mathrm{T}} v_j \int_{E_t} s_i s_j \mathrm{d}p. \tag{16d}$$

$$\tag{16e}$$

We define

$$\int_{E_t} s_i s_j \mathrm{d}p = s_{i,j}^t, \tag{17}$$

for different methods of discretization, we have

Triangal element (2-dimension)

$$s_{i,j}^t = \begin{cases} \frac{Area(t)}{6} & i = j, \\ \frac{Area(t)}{12} & i \neq j. \end{cases}$$

Tetrahderal element (3-dimension)

$$s_{i,j}^t = \begin{cases} \frac{Area(t)}{10} & i = j, \\ \frac{Area(t)}{20} & i \neq j. \end{cases}$$

Let's consider practical implementation of FEM. From discussions above, we have

$$\int_{E_t} \|v(p)\|^2 \mathrm{d}p = \sum_{i,j} v_i^{\mathrm{T}} v_j \int_{E_t} s_i s_j \mathrm{d}p \tag{18a}$$

$$= \sum_{i,j} v_i^{\mathrm{T}} v_j s_{i,j}^t \tag{18b}$$

$$= V^{\mathrm{T}} S_t V, \tag{18c}$$

where $V = (v_1, v_2, \cdots, v_n)^{\mathrm{T}}$, and

$$S_t = \begin{pmatrix} s_{1,1}^t \cdot I_3 & \cdots & s_{1,n}^t \cdot I_3 \\ \vdots & \ddots & \vdots \\ s_{n,1}^t \cdot I_3 & \cdots & s_{n,n}^t \cdot I_3 \end{pmatrix}.$$

The kinetic energy follows

$$k = \frac{1}{2} \sum_t \rho_t (V^{\mathrm{T}} S_t V) \tag{19a}$$

$$= \frac{1}{2} V^{\mathrm{T}} (\sum_t \rho_t S_t) V \tag{19b}$$

We denote *mass matrix* M_t with $M_t = \sum_t \rho_t S_t$. For triangle element we have

$$M_t = \sum_t \rho_t S_t = \rho_t Area(t) P \otimes I_3, \tag{20}$$

where P is defined by

$$P_{m,n} = \begin{cases} \frac{1}{6} & m = n \in i, j, k \\ \frac{1}{12} & m \neq n \in i, j, k \\ 0 & otherwise \end{cases},$$

where i, j and k are triangle vertex indices[4].

4.2 Elastic energy

In this section we only consider hyperelastic materials.

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Consider a deformation f from n-points d-dimensional material (rest pose) space Ω to world (deformed) space $f(\Omega) \in \mathbb{R}^{\mathrm{nd} \times \mathrm{nd}}$, for every spatial point p, the deformation gradient is $\nabla f(p)$. Elastic energy can be represented by

$$E = \int_\Omega \psi(\nabla f(p)) \nabla f(p) \mathrm{d}p, \tag{21}$$

where $\psi \in \mathbb{R}^{\mathrm{n} \times \mathrm{n}} \mapsto \mathbb{R}^+$ is the *energy density function*.

The energy density function can be further decomposed into

$$\psi = \psi_{material} \circ \psi_{strain}, \tag{22}$$

[4]In practical implementation, sometimes the *mass lumping* technique is used. This technique aggregates matrix element to its diagonal and to facilitate computations.

where $\psi_{material}$ describes material property and ψ_{strain} describes geometric measure of distortion of this material.

Let's consider how to use FEM to discretize the elastic energy.

elaborate on this

We consider 3-dimensional problem, where $\psi \in \mathbb{R}^{3\times3} \mapsto \mathbb{R}^{+}$ is given. For every tetrahedron (tet), we define $F = \nabla f \in \mathbb{R}^{3\times3}$. For every deformed vertex $\mathbf{x}$ and material vertex $\tilde{\mathbf{x}}$[5], we have $\mathbf{x} = f(\tilde{\mathbf{x}}) = F\tilde{\mathbf{x}} + b$, where $\mathbf{b}$ is a constant. For the whole tet, we have

$$\mathbf{x}_i - \mathbf{x}_4 = F(\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_4), \tag{23}$$

where $i \in 1, 2, 3, 4$ are vertex indices. This can be written as

$$D_s = FD_m, \tag{24}$$

where

$$D_s = \begin{pmatrix} x_1 - x_4 & x_2 - x_4 & x_3 - x_4 \\ y_1 - y_4 & y_2 - y_4 & y_3 - y_4 \\ z_1 - z_4 & z_2 - z_4 & z_3 - z_4 \end{pmatrix}, \quad D_m = \begin{pmatrix} \tilde{x}_1 - \tilde{x}_4 & \tilde{x}_2 - \tilde{x}_4 & \tilde{x}_3 - \tilde{x}_4 \\ \tilde{y}_1 - \tilde{y}_4 & \tilde{y}_2 - \tilde{y}_4 & \tilde{y}_3 - \tilde{y}_4 \\ \tilde{z}_1 - \tilde{z}_4 & \tilde{z}_2 - \tilde{z}_4 & \tilde{z}_3 - \tilde{z}_4 \end{pmatrix}, \tag{25}$$

thus

$$F = D_s(x)D_m^{-1}. \tag{26}$$

The elastic energy (21) can be discretized with

$$E = \sum_t \int_{E_t} \psi_t(F_t)\mathrm{d}t \tag{27a}$$

$$= \sum_t w_t \psi_t(F_t), \tag{27b}$$

where

$$w_t = \frac{1}{6} det\|D_m\|, \tag{28}$$

is the volume of the tet t.

4.3 Vectorization

Before we get to the actual material property, we would introduce a vectorization scheme frequently seen in practical implementations.

Recall that $\nabla f \equiv F$ is linear w.r.t. x, where x is a collection of material space points, we have $F = Gx$, where $F \in \mathbb{R}^{3\times3}$, $x \in \mathbb{R}^{3n\times1}$, and G is a tensor.

Definition 6. *Let $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{k\times l}$, we denote the **Kronecker product** $A \otimes B$ (which is an $mk \times nl$ matrix) with*

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix}. \tag{29}$$

Definition 7. *We denote a **vectorization** of a matrix A with*

$$vec(A) = (a_1, a_2, \cdots, a_n)^{\mathrm{T}}. \tag{30}$$

We further derives some lemmas:

Lemma 1. *For any given matrices A, B, C and D, assuming the matrix dimensions agree, we have*

[5] $\mathbf{x} = (x, y, z)$

1. $(A \otimes B) \cdot (C \otimes D) = A \cdot C \otimes B \cdot D$;
2. $(A \otimes B)^{\mathrm{T}} = A^{\mathrm{T}} \otimes B^{\mathrm{T}}$;
3. $vec(AX) = (I_p \otimes A) \cdot vec(X) = (X^{\mathrm{T}} \otimes I_m) \cdot vec(A)$, *where* $A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^{n \times p}$.

Then for each tet, $vec(F) \in \mathbb{R}^{9 \times 1}$, $G \in \mathbb{R}^{9 \times 3n}$, $x \in \mathbb{R}^{3n \times 1}$, and

$$vec(F) = vec(D_s \cdot D_m^{-1}) = (D_m^{-\mathrm{T}} \otimes I_3) \cdot vec(D_s), \tag{31}$$

where[6]

$$vec(D_s) = \begin{pmatrix} x_1 - x_4 \\ x_2 - x_4 \\ x_3 - x_4 \end{pmatrix} = (S \cdot I_3) \cdot x \in \mathbb{R}^{9 \times 1}, \tag{32}$$

where we define a selector matrix S on each tet. S is defined by

$$S = \begin{pmatrix} \cdots & 1 & \cdots & -1 & \cdots \\ 1 & \cdots & \cdots & -1 & \cdots \\ \cdots & \cdots & 1 & -1 & \cdots \end{pmatrix}, \tag{33}$$

where the column indices of 1s are from x_1, x_2, and x_3; the column index of -1 is from x_4.

To sum up, for each tet:

$$vec(F) = (D_m^{-\mathrm{T}} \otimes I_3)(S \otimes I_3)x = (D_m^{-\mathrm{T}} \cdot S \otimes I_3)x. \tag{34}$$

4.4 Material property ψ

5 Fluids and Partial Differential Equations

6 Something more...

7 Papers and books

Numerical optimization can refer to [2] [6].

[1] and [9] are great references for continuum mechanics and FEM.

An awesome book on fluids simulation is [3].

Vector calculus can be found in [7].

Useful tips of C++ programming can be found in C++ core guidelines, [4], and [5].

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