

Projecting chains of constrained points

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1 Formulation

We're going to solve

$$\begin{aligned} \min_{\mathbf{x}} \quad & \frac{1}{2} (\mathbf{x} - \mathbf{p})^\top \mathbf{M} (\mathbf{x} - \mathbf{p}) \\ \text{s.t} \quad & \mathbf{z} = \mathbf{R}\mathbf{x} \quad \text{and} \quad \mathbf{z}_i^\top \mathbf{z}_i = 1 \end{aligned} \tag{1}$$

where

- $n \in \mathbb{N}$ is the number of particles between links
- $m \in \mathbb{N}$ is the $n - 1$ of links between particles
- $\mathbf{x} \in \mathbb{R}^{3n}$ is the solution vector,
- $\mathbf{p} \in \mathbb{R}^{3n}$ is target/free moving positions,
- $\mathbf{z} \in \mathbb{R}^{3m}$ is the vector of difference vectors in the chain,
- $\mathbf{z}_i \in \mathbb{R}^3$ is the i th 3-vector in \mathbf{z} ,
- $\mathbf{R} \in \mathbb{R}^{3m \times 3n}$ is the per vector finite-difference matrix so that $(\mathbf{R}\mathbf{x})_i = \mathbf{x}_i - \mathbf{x}_{i+1}$
- $\mathbf{M} \in \mathbb{R}^{3n \times 3n}$ is the mass matrix, simply having the mass (or weight) of each particle in each 3x3 block diagonal

We want to be working only on the difference vectors in \mathbf{z} . To do that, we need to eliminate \mathbf{x} , and we do this by holding \mathbf{z} constant and deriving the optimality conditions for (1). We first state the Lagrangian:

$$\mathcal{L}(\mathbf{x}, \lambda) = \frac{1}{2} (\mathbf{x} - \mathbf{p})^\top \mathbf{M} (\mathbf{x} - \mathbf{p}) + \lambda^\top (\mathbf{z} - \mathbf{R}\mathbf{x})$$

with the optimality conditions:

$$\begin{aligned} \mathbf{M}(\mathbf{x} - \mathbf{p}) - \mathbf{R}^\top \lambda &= 0 \\ \mathbf{z} - \mathbf{R}\mathbf{x} &= 0 \end{aligned}$$

solving for λ gives us:

$$\lambda = (\underbrace{\mathbf{R}\mathbf{M}^{-1}\mathbf{R}^\top}_{\mathbf{S}})^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p})$$

where $\mathbf{S} = \mathbf{R}\mathbf{M}^{-1}\mathbf{R}^\top \in \mathbb{R}^{3m \times 3m}$ is a block tridiagonal SPD matrix. We use this to give us an expression for \mathbf{x} :

$$\mathbf{x} = \mathbf{p} + \mathbf{M}^{-1}\mathbf{R}^\top\mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p})$$

Inserting this into (1) eliminates $\mathbf{z} = \mathbf{R}\mathbf{x}$ and we are left with

$$\begin{aligned} \min_{\mathbf{x}} \quad & \frac{1}{2} (\mathbf{z} - \mathbf{R}\mathbf{p})^\top \mathbf{S}^{-1} (\mathbf{z} - \mathbf{R}\mathbf{p}) \\ \text{s.t.} \quad & \mathbf{z}_i^\top \mathbf{z}_i = 1 \quad i = 1 \dots m \end{aligned} \tag{2}$$

In this reformulated problem we must find a \mathbf{z} that consist of unit length 3-vectors that minimize the distance to $\mathbf{R}\mathbf{p}$ under the \mathbf{S}^{-1} -norm. Note that it is trivial to project \mathbf{z} to satisfy the unit length constraints (under the regular \mathbf{I} -norm, known as normalization), and likewise it is trivial to obtain \mathbf{x} given any \mathbf{z} . This means that whenever we take a newton step on \mathbf{z} we can trivially reign it in to its feasible solution, and in effect only change the directions of each \mathbf{z}_i vector, never their lengths.

2 Solution

We want to solve this system using a newton-like method, so to make sense of that we first derive the full newton step. The Lagrangian of (2) is

$$\mathcal{L}_{(\mathbf{z}, \lambda)} = \frac{1}{2} (\mathbf{z} - \mathbf{R}\mathbf{p})^\top \mathbf{S}^{-1} (\mathbf{z} - \mathbf{R}\mathbf{p}) + \frac{1}{2} \sum_{i=1}^m \lambda_i (\mathbf{z}_i^\top \mathbf{z}_i - 1) \tag{3}$$

The optimality conditions for (3) are:

$$\begin{aligned} \mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) + \mathbf{Q}_z^T \lambda &= 0 \\ \mathbf{z}_i^T \mathbf{z}_i - 1 &= 0 \quad i = 1, \dots, m \end{aligned}$$

and the newton step to find a stationary point (\mathbf{z}, λ) for (3) is

$$\underbrace{\begin{bmatrix} \mathbf{S}^{-1} + \mathbf{D}_\lambda & \mathbf{Q}_z^T \\ \mathbf{Q}_z & \end{bmatrix}}_{H\mathcal{L}_{(\mathbf{z}, \lambda)}} \begin{bmatrix} \Delta \mathbf{z} \\ \Delta \lambda \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) + \mathbf{Q}_z^T \lambda \\ \mathbf{Q}_z \mathbf{z} - \mathbf{1} \end{bmatrix}}_{\nabla \mathcal{L}_{(\mathbf{z}, \lambda)}} \quad (4)$$

where

$$\mathbf{Q}_z = \begin{bmatrix} \mathbf{z}_1^T & 0 & \cdots & 0 \\ 0 & \mathbf{z}_2^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{z}_m^T \end{bmatrix} \in \mathbb{R}^{m \times 3m} \quad \mathbf{D}_\lambda = \begin{bmatrix} \mathbf{I}_{\lambda_1} & 0 & \cdots & 0 \\ 0 & \mathbf{I}_{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{I}_{\lambda_m} \end{bmatrix} \in \mathbb{R}^{3m \times 3m}$$

There are many interesting ways to go about solving this system, but in our case the goal is to exploit the tri-diagonal structure of \mathbf{S} , in order to use fast direct solves. Instead of solving the full step, we first solve just for $\Delta \lambda$ at $\lambda = \mathbf{0}$, effectively resetting the multipliers in each iteration. After that we solve for $\Delta \mathbf{z}$ to update the solution variables.

2.1 Solving for λ

To derive the solution for $\Delta \lambda$ we eliminate $\Delta \mathbf{z}$ by using $\lambda = \mathbf{0}$ and solving the first row in (4). Interestingly, because we will project the vectors in \mathbf{z} in each iteration the $\mathbf{Q}_z \mathbf{z} - \mathbf{1}$ term is always 0, which will simplify things a bit:

$$\Delta \mathbf{z} = \mathbf{S}(\mathbf{Q}_z^T \Delta \lambda + \mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}))$$

Substitute $\Delta \mathbf{z}$ into the second row in (4):

$$\mathbf{Q}_z(\mathbf{S}(\mathbf{Q}_z^T \Delta \lambda + \mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}))) = \underbrace{\mathbf{Q}_z \mathbf{z} - \mathbf{1}}_0$$

Simplify to solve for $\Delta \lambda$ we get:

$$\mathbf{Q}_z \mathbf{S} \mathbf{Q}_z^T \Delta \lambda = -\mathbf{Q}_z(\mathbf{z} - \mathbf{R}\mathbf{p})$$

This system is tridiagonal because the operator $\mathbf{Q}_z(\cdot)\mathbf{Q}_z^T$ collapses each 3×3 block in \mathbf{S} to a scalar value $\mathbf{z}_i^T \mathbf{S}_{(i,j)} \mathbf{z}_j$. This operation effectively reduces the block tridiagonal structure of \mathbf{S} to the plain tridiagonal structure in $\mathbf{Q}_z \mathbf{S} \mathbf{Q}_z^T \in \mathbb{R}^{m \times m}$. Also note that $\mathbf{Q}_z \mathbf{z} = \mathbf{1}$ appears in the RHS and so it could be further reduced to $\mathbf{Q}_z \mathbf{R}\mathbf{p} - \mathbf{1}$ but since the vector $\mathbf{z} - \mathbf{R}\mathbf{p}$ is needed elsewhere this has neglectable practical benefit.

2.2 Solving for $\Delta \mathbf{z}$

To solve for $\Delta \mathbf{z}$, we substitute $\Delta \lambda = 0$ into the first row of (4):

$$(\mathbf{S}^{-1} + \mathbf{D}_\lambda) \Delta \mathbf{z} = \mathbf{S}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) - \mathbf{Q}_z^T \lambda \quad (5)$$

To avoid having to solve the dense system $\mathbf{S}^{-1} + \mathbf{D}_\lambda$ we exploit that we can cheaply compute the cholesky decomposition $\mathbf{L}\mathbf{L}^T = \mathbf{S}$ and make use of the identity

$$\mathbf{S}^{-1} + \mathbf{D}_\lambda = \mathbf{L}^{-T}(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L}) \mathbf{L}^{-1} \quad (6)$$

we insert (6) into (5)

$$\mathbf{L}^{-T}(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L}) \mathbf{L}^{-1} \Delta \mathbf{z} = \mathbf{L}^{-T} \mathbf{L}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) - \mathbf{Q}_z^T \lambda$$

then multiplying with the invertible \mathbf{L}^T

$$(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L}) \mathbf{L}^{-1} \Delta \mathbf{z} = \mathbf{L}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) - \mathbf{L}^T \mathbf{Q}_z^T \lambda$$

means we can solve for $\mathbf{u} = \mathbf{L}^{-T} \Delta \mathbf{z}$ and then obtain $\Delta \mathbf{z}$ like so

$$(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L}) \mathbf{u} = \mathbf{L}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p}) - \mathbf{L}^T \mathbf{Q}_z^T \lambda$$

and then finally

$$\Delta \mathbf{z} = \mathbf{L}^T \mathbf{u}$$

The great advantage here is that $(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L})$ remains block tridiagonal and so it's fast to solve. The disadvantage is that we need one extra solve of the block bidiagonal \mathbf{L} to compute $\mathbf{L}^{-1}(\mathbf{z} - \mathbf{R}\mathbf{p})$. This is annoying but still greatly outweighs the pain of solving a dense system using iterative methods. Note also that in the trivial case where $\lambda = \mathbf{0}$ the system reduces to the identity. In an effort to keep the eigenvalues of $(\mathbf{I} + \mathbf{L}^T \mathbf{D}_\lambda \mathbf{L})$ positive, we clamp λ to positive values before we compute \mathbf{D}_λ . This is a hack but seems to work well in practice. We now proceed to list the full algorithm.

3 Algorithm

Here we'll outline the algorithm in full before explaining each step in detail:

```
01  $\mathbf{L} = \text{cholesky}(\mathbf{S})$ 
02  $\mathbf{z} = \mathbf{R}\mathbf{x}$ 
03 while true do
04      $\mathbf{Q}_{\cdot \mathbf{z}} = \text{normalize}(\mathbf{z})$ 
05      $\mathbf{y} = \mathbf{R}\mathbf{p} - \mathbf{z}$ 
06      $\lambda = \text{solve}(\mathbf{Q}\mathbf{S}\mathbf{Q}^T, \mathbf{Q}\mathbf{y})$ 
```

```

07    $\mathbf{b}_z = \text{solve}(\mathbf{L}, \mathbf{y})$ 
08    $\mathbf{b}_\lambda = \mathbf{L}^\top \mathbf{Q}^\top \lambda$ 
09   if  $\|\mathbf{b}_z - \mathbf{b}_l\|^2 < \epsilon$  then
10        $\mathbf{s} = \text{solve}(\mathbf{L}^\top, \mathbf{b}_z)$ 
11        $\mathbf{x} = \mathbf{p} - \mathbf{M}^{-1} \mathbf{R}^\top \mathbf{s}$ 
12       return  $\mathbf{x}$ 
13    $\mathbf{D} = \text{diagonal}(\max(0, \lambda))$ 
14    $\Delta \mathbf{z} = \mathbf{L} \text{ solve}(\mathbf{I} + \mathbf{L}^\top \mathbf{D} \mathbf{L}, \mathbf{b}_z - \mathbf{b}_\lambda)$ 
15    $\mathbf{z} = \mathbf{z} + \Delta \mathbf{z}$ 

```

Each iteration the algorithm does these main steps:

1. Normalize the 3-vectors in \mathbf{z}
2. Compute the $n - 1$ Lagrange multipliers of the system at \mathbf{z}
3. Check the solution residual, if below threshold compute and return \mathbf{x}
4. Compute the Newton step on \mathbf{z} and go to step 1

Note the following:

- we compute the cholesky decomposition $\mathbf{L}\mathbf{L}^\top = \mathbf{S}$ to keep the systems we need to solve sparse and symmetric. See more details bellow. Computing cholesky for a block-tridiagonal SPD matrix is simple and fast, and if \mathbf{M} is fixed it can be done off-line/once.
- every `solve()` is at least a block tri-diagonal system (or simpler), which are fast and easy to solve
- to compute the Lagrange multipliers we build the Jacobian matrix $\mathbf{Q} \in \mathbb{R}^{3m \times m}$, which is simply the \mathbf{z}_i vectors vertically stacked

- the matrix \mathbf{D} is the contribution to the Hessian stemming from the non-linear unit length constraints. We clamp it to be positive to keep the Hessian PD. This is a hack but seems to play out well in practice