CS 395T: Homework 2

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1 Programming

Problem 1. Shape deformation (Gradient Descent)

We are interested in minimizing the following equation via gradient descent.

$$\underset{p_1,\dots,p_n,R_1,\dots,R_n}{\operatorname{argmin}} \sum_{i=1}^{n} \Big(\sum_{j\in\mathcal{N}(i)} ||R_i(p_i^{rest} - p_j^{rest}) - (p_i - p_j)||^2 \Big) + \lambda \sum_{p_i \in \mathcal{H}} ||p_i - h_i||^2$$

First, we can take the derivative with respect to p_k, and for notations γ will be 1 if $p_k \in \mathcal{H}$ and 0 otherwise.

$$\begin{aligned}
&= \nabla \sum_{i=1}^{n} \Big(\sum_{j\in\mathcal{N}(i)} ||R_i(p_i^{rest} - p_j^{rest}) - (p_i - p_j)||^2 \Big) + \nabla\lambda \sum_{p_i \in \mathcal{H}} ||p_i - h_i||^2 \\
&= \sum_{j\in\mathcal{N}(k)} \nabla ||R_k(p_k^{rest} - p_j) - (p_k - p_j)||^2 + \sum_{j\in\mathcal{N}(k)} \nabla ||R_j(p_j^{rest} - p_k) - (p_j - p_k)||^2 + \gamma\lambda||p_k - h_k||^2 \\
&= \sum_{j\in\mathcal{N}(k)} -2(R_k(p_k^{rest} - p_j)) + \sum_{j\in\mathcal{N}(k)} 2(R_j(p_k^{rest} - p_j)) + 2\gamma\lambda(p_k - h_k)
\end{aligned}$$

Next, to take the derivative with respect to R, we have to reparameterize R_i by $c_i \in \mathbb{R}^3$. For notation, let $[c]_x$ denote the skew symmetric matrix formed by c. From homework 1 we can see that $R = I + \frac{1-\cos\theta}{\theta^2}[c]_x^2 + \frac{\sin\theta}{\theta}[c]_x$, where $\theta = ||c||$.

For this exercise, note that $\frac{d\theta}{c_i} = \frac{c_i}{d\theta}$ first let us take $\frac{dR}{dc_x}$.

$$\frac{dR}{dc_x} = \frac{\theta^2\sin\theta\frac{d\theta}{dc_x} - 2(1-\cos\theta)\theta\frac{d\theta}{dc_x}}{\theta^4}[c]_x^2 + \frac{1-\cos\theta}{\theta^2}A_x + \frac{-\theta\cos\theta\frac{d\theta}{dc_x} - \sin\theta\theta\frac{d\theta}{dc_x}}{\theta^2}[c]_x + \frac{\sin\theta}{\theta}B_x$$

where

$$A_x = \begin{bmatrix} 0 & c_y & c_z \\ c_y & -2c_x & 0 \\ c_z & 0 & -2c_x \end{bmatrix} B_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

Next, consider $\frac{dR}{dc_y}$.

$$\frac{dR}{dc_x} = \frac{\theta^2\sin\theta\frac{d\theta}{dc_y} - 2(1-\cos\theta)\theta\frac{d\theta}{dc_y}}{\theta^4}[c]_x^2 + \frac{1-\cos\theta}{\theta^2}A_y + \frac{-\theta\cos\theta\frac{d\theta}{dc_y} - \sin\theta\theta\frac{d\theta}{dc_y}}{\theta^2}[c]_x + \frac{\sin\theta}{\theta}B_y$$

where

$$A_y = \begin{bmatrix} -2c_y & c_x & 0 \\ c_x & 0 & c_z \\ 0 & c_z & -2c_y \end{bmatrix} B_y = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

Finally, consider $\frac{dR}{dc_z}$.

$$\frac{dR}{dc_z} = \frac{\theta^2\sin\theta\frac{d\theta}{dc_z} - 2(1-\cos\theta)\theta\frac{d\theta}{dc_z}}{\theta^4}[c]_x^2 + \frac{1-\cos\theta}{\theta^2}A_z + \frac{-\theta\cos\theta\frac{d\theta}{dc_z} - \sin\theta\theta\frac{d\theta}{dc_z}}{\theta^2}[c]_x + \frac{\sin\theta}{\theta}B_z$$

where

$$A_z = \begin{bmatrix} -2c_z & 0 & c_x \\ 0 & -2c_z & c_y \\ c_x & c_y & 0 \end{bmatrix} B_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Next, we must compute $\frac{df}{dR}$ for simplicity, we will now compute this element wise.

$$\begin{aligned} \frac{dF}{dR_{rc}} &= \nabla \sum_{j \in \mathcal{H}} ||R(p^{rest} - p_j) - (p - p_j)||^2 \\ &= \sum_{j\ in \mathcal{H}} 2\Big((R(p^{rest} - p_j) - (p - p_j))_r (p^{rest} - p_j)_c\Big) \end{aligned}$$

Now, we collect all the partials into a vector $\frac{df}{dR} \in \mathbb{R}^9$, we collect all the partials with respect to c_i, $\frac{dR}{dc_i} \in \mathbb{R}^9$, and do chain rule to get $\frac{df}{dc_i}$, and finally turn this into a vector $\frac{df}{dc} \in \mathbb{R}^3$.

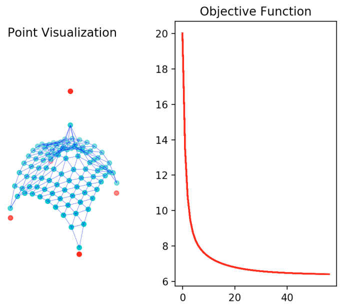

Figure 1: Results of gradient descent

Problem 2. Shape deformation (Alternating Minimization)

First, to calculate $p_1, \dots, p_n$ that minimize the equation, we can write this the energy as a least squares system $Ax = b$, where $x \in \mathbb{R}^{3n}$, is a block vector of $p_1, \dots, p_n$, and A is a "selector matrix", and b is a vector of block vectors of knowns.

To be more precise,

$$x = \begin{bmatrix} p_1 \\ p_2 \\ \dots \\ p_n \end{bmatrix}$$

where $p_i \in \mathbb{R}^3$.

$$A = \begin{bmatrix} —A_1— \\ —A_2— \\ \dots \\ —A_m— \end{bmatrix}$$

where $A_k \in \mathbb{R}^{3\times 3n}$, and m is the total number of squared norm terms.

Now, consider a single term in the left hand term of the energy function $R_i(p_i^{rest} - p_j^{rest}) - (p_i - p_j)$. We will decompose this into a block matrix A_k and b_k vector.

Clearly, for the known $b_k \in \mathbb{R}^3$,

$$b_k = \begin{bmatrix} & | & \\ p_i^{rest} & - & p_j^{rest} \\ & | & \end{bmatrix}$$

Now, A_k will consist of a single block I for p_i, and a $-I$ for p_j.

$$A_k = \begin{bmatrix} \cdots & 1 & 0 & 0 & \cdots & -1 & 0 & 0 & \cdots \\ \cdots & 0 & 1 & 0 & \cdots & 0 & -1 & 0 & \cdots \\ \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & -1 & \cdots \end{bmatrix}$$

To finish the least squares formulation, consider a single of the right hand terms $\lambda||p_i - h_i||^2$. Clearly, this is equivalent to $||\lambda^{\frac{1}{2}}p_i - \lambda^{\frac{1}{2}}h_i||^2$, which we can write in a block form.

$$b_k = \begin{bmatrix} | \\ \lambda^{\frac{1}{2}}h_i \\ | \end{bmatrix}$$

$$A_k = \begin{bmatrix} \cdots & \lambda^{\frac{1}{2}} & 0 & 0 & \cdots \\ \cdots & 0 & \lambda^{\frac{1}{2}} & 0 & \cdots \\ \cdots & 0 & 0 & \lambda^{\frac{1}{2}} & \cdots \end{bmatrix}$$

Now, we solve $Ax = b$ with our favorite least squares solver (note that A will be sparse due to the connectivity of the mesh) and update p_i with the corresponding block in x.

Next, we need to compute optimal R_k. This is equivalent the orthogonal Procustes problem (constrained version).

$$\underset{R_k}{\operatorname{argmin}} \sum_{j \in \mathcal{N}(\|)} ||R_k(p_k^{rest} - p_j^{rest}) - (p_k - p_j)||^2$$

We can form two matrices $P, Q \in \mathbb{R}^{3\times m}$, where $m = |\mathcal{N}(k)|$ such that

$$P = \begin{bmatrix} | & & | \\ p_k^{rest} - p_1^{rest} & \cdots & p_k^{rest} - p_m^{rest} \\ | & & | \end{bmatrix}$$

and

$$Q = \begin{bmatrix} | & & | \\ p_k - p_1 & \cdots & p_k - p_m \\ | & & | \end{bmatrix}$$

From this we can reformulate this into block form.

$$\begin{aligned}
\underset{R_k}{\operatorname{argmin}} \sum_{j \in \mathcal{N}(\|)} ||R_k(p_k^{rest} - p_j^{rest}) - (p_k - p_j)||^2 &= \underset{R_k}{\operatorname{argmin}}\, ||R_kP - Q||_F \\
&= \underset{R_k}{\operatorname{argmin}}\, tr\Big((R_kP - Q)^\intercal(R_kP - Q)\Big) \\
&= \underset{R_k}{\operatorname{argmin}}\, tr\Big(P^\intercal R_k^\intercal R_kP - P^\intercal R_k^\intercal Q - Q^\intercal R_kP + Q^\intercal Q\Big) \\
&= \underset{R_k}{\operatorname{argmin}}\, tr\Big(P^\intercal P - P^\intercal R_k^\intercal Q - Q^\intercal R_kP + Q^\intercal Q\Big) \\
&= \underset{R_k}{\operatorname{argmin}}\, tr(P^\intercal P) - tr(P^\intercal R_k^\intercal Q) - tr(Q^\intercal R_kP) + tr(Q^\intercal Q) \\
&= \underset{R_k}{\operatorname{argmin}} -tr(P^\intercal R_k^\intercal Q) - tr(Q^\intercal R_kP) \\
&= \underset{R_k}{\operatorname{argmin}} -2tr(Q^\intercal R_kP) \\
&= \underset{R_k}{\operatorname{argmax}}\, tr(Q^\intercal R_kP) \\
&= \underset{R_k}{\operatorname{argmax}}\, tr(R_kPQ^\intercal)
\end{aligned}$$

Now, taking the SVD of $QP^\intercal$, let $U\Sigma V^\intercal = QP^\intercal$.

$$\underset{R_k}{\operatorname{argmax}}\, tr(RU\Sigma V^\intercal) = \underset{R_k}{\operatorname{argmax}}\, tr(V^\intercal RU\Sigma)$$

Lemma 1.1. *For $R \in SO(3)$, $\Sigma \in \mathbb{R}^{3\times 3}$, $tr(R\Sigma)$ is maximized if $R = I$.*

Let Σ consist of column vectors u_1, u_2, u_3, R consist of row vectors $R_1^\intercal, R_2^\intercal, R_3^\intercal$. We can see that

$$\begin{aligned}
tr(R\Sigma) &= R_1^\intercal u_1 + R_2^\intercal u_2 + R_3^\intercal u_3 \\
&= ||R_1||||u_1||cos\theta_1 + ||R_2||||u_2||cos\theta_2 + ||R_3||||u_3||cos\theta_3 \\
&= \sigma_1^2 cos\theta_1 + \sigma_2^2 cos\theta_2 + \sigma_3^2 cos\theta_3
\end{aligned}$$

Since σ_i^2 are positive, we can see this term is maximized if R_i is aligned with u_i. Since we have that $||R_i|| = 1$ by orthogonality, and $u_i = \sigma_i b_i$, where b_i is a basis vector, we can see this is maximized by $R_i = b_i$. This gives us our result that $R = I$.

□

Using the lemma, we can see that $R = VU^\intercal$ will maximize the optimization problem. However, we only have guarantees that $R \in O(3)$, not necessarily that $R \in SO(3)$. So now we have two cases. If $det(VU^\intercal) = 1$, we are done. If $det(VU^\intercal) = -1$, then we have to modify R by $\hat{R} = V\hat{\Sigma}U^\intercal$, where $\hat{\Sigma}$ is the identity matrix I with a slight modification, that $\hat{\Sigma}_{33} = -1$. $\hat{R}$ has a determinant of 1 and is clearly orthogonal; moreover, $\hat{R} \in SO(3)$.

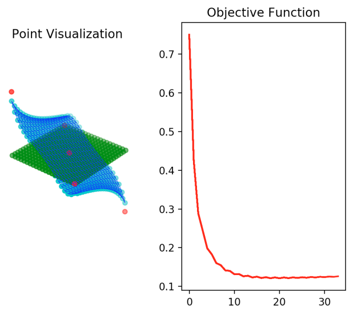

Figure 2: Results of gradient descent

Problem 3a. Finding peaks of a density (Gradient Descent)

This is a straightforward differentiation exercise.

$$\begin{aligned}
\nabla f(x) &= \nabla\Big(\sum_{i=1}^{n} \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)\Big) \\
&= \sum_{i=1}^{n} \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)\Big(-\frac{1}{2\sigma^2}\nabla(||x - x_i^2||^2)\Big) \\
&= \sum_{i=1}^{n} \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)\Big(-\frac{1}{\sigma^2}(x - x_i)\Big)
\end{aligned}$$

Then, at every timestep, $x^{t+1} = x^t + \eta\nabla f(x^t)$, where η is a small stepsize.

Problem 3b. Finding peaks of a density (Newtons Method)

This is a yet another straightforward differentiation exercise.

$$\begin{aligned}
\nabla^2 f(x) &= \nabla\Big(\sum_{i=1}^{n} \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)\Big(-\frac{1}{\sigma^2}(x - x_i)\Big)\Big) \\
&= \sum_{i=1}^{n} \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)\Big(-\frac{1}{\sigma^2}(x - x_i)\Big)(-\frac{1}{\sigma^2}(x - x_i))^\intercal + \exp(-\frac{1}{2\sigma^2}||x - x_i||^2)(-\frac{1}{\sigma^2}I) \\
&= \sum_{i=1}^{n} -\frac{1}{\sigma^2}\exp(-\frac{1}{2\sigma^2}||x - x_i||^2)(I - \frac{1}{\sigma^2}(x - x_i)(x - x_i)^\intercal)
\end{aligned}$$

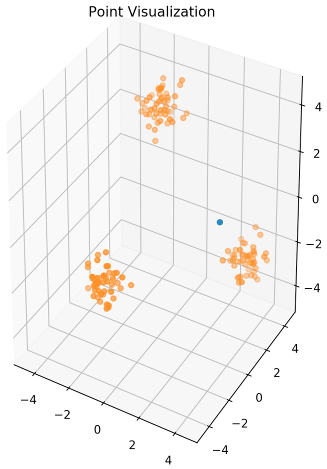

Figure 3: The unit gaussian mixtures are represented by orange points, and x is represented by a single blue point. At convergence, the blue point settles in one of the clusters (intialization dependent).

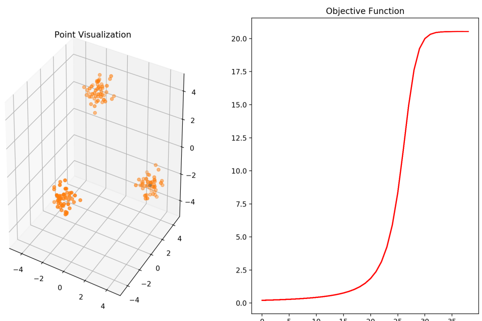

Figure 4: Gradient ascent converges in 30 iterations.

Then, at every timestep, $x^{t+1} = x^t + \nabla^2 f(x)^{-1} \nabla f(x)$.

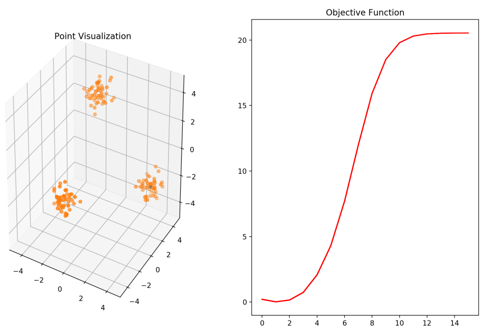

Figure 5: Newtons Method converges in 10 iterations.

Problem 5. If f is convex and L-smooth, show that gradient descent with step size $\frac{1}{L}$ satisfies

$$f(x_t) - f(x^*) \leq \frac{2L||x_o - x^*||^2}{t}$$

First, we will need to take a side path that bounds $f(x)$ and $f(y)$ for every x, y in relation to the difference of the norms.

Lemma 1.2. $f(y) - f(x) - \nabla f(x)^\intercal (y - x) \leq \frac{L}{2}||y - x||^2 \quad \forall x, y.$

$$\begin{aligned}
f(y) - f(x) - \nabla f(x)^\intercal (y - x) &= \int_0^1 \frac{df}{dt} dt - \nabla f(x)^\intercal (y - x) \\
&= \int_0^1 \nabla f(g(t))^\intercal \frac{dg}{dt} dt - \nabla f(x)^\intercal (y - x) \\
&= \int_0^1 \nabla f(x + t(y - x))^\intercal (y - x) - \nabla f(x)^\intercal (y - x) \frac{dg}{dt} dt \\
&= \int_0^1 \Big(\nabla f(x + t(y - x)) - \nabla f(x)\Big)^\intercal (y - x) \frac{dg}{dt} dt \\
&\leq \int_0^1 ||\nabla f(x + t(y - x)) - \nabla f(x)|| \; ||y - x|| \frac{dg}{dt} dt && \text{By Cauchy Shwartz} \\
&\leq \int_0^1 L||t(y - x)|| \; ||y - x|| \frac{dg}{dt} dt && \text{By convexity} \\
&= \int_0^1 Lt||y - x||^2 \frac{dg}{dt} dt \\
&= \frac{L}{2}||y - x||^2
\end{aligned}$$

□

Using this lemma, we can bound the gap $f(x_{t+1}) - f(x_t)$.

$$\begin{aligned}
f(x_{t+1}) - f(x_t) &\leq \nabla f(x_t)^\intercal (x_{t+1} - x_t) + \frac{L}{2}||x_{t+1} - x_t||^2 && \text{By lemma} \\
&= \nabla f(x_t)^\intercal (-\frac{1}{L}\nabla f(x_t)) + \frac{L}{2}||x_{t+1} - x_t||^2 \\
&= -\frac{1}{L}||\nabla f(x_t)||^2 + \frac{1}{2L}||\nabla f(x_t)||^2 \\
&= -\frac{1}{2L}||\nabla f(x_t)||^2 && (\star)
\end{aligned}$$

With a bit more algebraic manipulation -

$$\begin{aligned}
f(x_{t+1}) &\leq f(x_t) - \frac{1}{2L}||\nabla f(x_t)||^2 \\
&\leq f(x^*) + \nabla f(x_t)^\intercal (x_t - x^*) - \frac{1}{2L}||\nabla f(x_t)||^2 && \text{By convexity}
\end{aligned}$$

To simplifify this term we need another algebraic trick.

$$\begin{aligned}
||x_{t+1} - x^*||^2 &= ||x_t - \frac{1}{L}\nabla f(x_t) - x^*||^2 && \text{By gradient step} \\
&= || - \frac{1}{L}\nabla f(x_t) + (x_t - x^*)||^2 \\
&= \frac{1}{L^2}||\nabla f(x_t)||^2 - \frac{2}{L}\nabla f(x_t)^\intercal (x_t - x^*) + ||x_t - x^*||^2
\end{aligned}$$

So clearly,

$$-\frac{L}{2}\Big(||x_{t+1}-x^*||^2-||x_t-x^*||^2\Big)=-\frac{1}{2L}||\nabla f(x_t)||^2+\nabla f(x_t)^\intercal(x_t-x^*) \qquad (\star\star)$$

With this, we have that

$$\begin{aligned}
f(x_{t+1}) &\leq f(x^*)+\nabla f(x_t)^\intercal(x_t-x^*)-\frac{1}{2L}||\nabla f(x_t)||^2 \\
&= f(x^*)-\frac{L}{2}\Big(||x_{t+1}-x^*||^2-||x_t-x^*||^2\Big) && \text{By } (\star\star)
\end{aligned}$$

From this, we have a closed form for $\sum_{i=1}^{t} f(x_i) \leq tf(x^*)-\frac{L}{2}||x_t-x^*||^2+\frac{L}{2}||x_0-x^*||^2$ as all the alternating terms cancel out.

Finally, we are ready to show the initial claim.

$$\begin{aligned}
f(x_t)-f(x^*) &\leq \frac{1}{t}\sum_{i=1}^{t}(f(x_i)-f(x^*)) && \text{Since the gap is decreasing} \\
&\leq -\frac{L}{2t}||x_t-x^*||^2+\frac{L}{2t}||x_0-x^*||^2 && \text{From above sum with algebra} \\
&\leq \frac{L}{2t}||x_0-x^*||^2 && \text{Since the left term is negative} \\
&\leq \frac{2L}{t}||x_0-x^*||^2
\end{aligned}$$

□