Supplementary Information

Efficient and robust image registration for two-dimensional mirco-X-ray fluorescence measurements

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A Error estimation for graph registration

We show here that, for Graph Registration with a Moore graph, $\mathrm{Var}[\hat{s}_j]$ tends to 0 as the parameter d of the Moore graph tends to infinity. We assume here a bit more familiarity with graph theory concepts than in the rest of the article. All concepts can be found in a standard textbook.[1]

A Moore graph is a d-regular graph with diameter k, where the number of vertices is $n = 1+d\sum_{i=0}^{k-1}(d-1)^i$. The structure of the Moore graph ensures that the union of paths $P_{i,j}$ that end in j form a balanced tree rooted in j. That is, there are $d(d-1)^{\ell-1}$ vertices at depth ℓ and each of them have $\frac{n-1-d\sum_{m=0}^{\ell-1}(d-1)^m}{d(d-1)^{\ell-1}}$ descendants. As a consequence, if we consider the shortest paths between a fixed vertex j and all other vertices then an edge betwen a vertex at depth ℓ and its parent appears as often as:

$$1 + \frac{n-1-d\sum_{m=0}^{\ell-1}(d-1)^m}{d(d-1)^{\ell-1}} = \frac{n-1-d\sum_{m=0}^{\ell-2}(d-1)^m}{d(d-1)^{\ell-1}}$$

[1] Diestel, R. Graph Theory *(5th edition).* Springer-Verlag, 2017.

With the same assumptions on the errors as before, we compute:

$$\begin{aligned}
\mathrm{Var}\left[\hat{s}_j\right] &= \mathrm{Var}\left[\frac{1}{n}\sum_{i\neq j}\sum_{(u,v)\in E(P_{i,j})}\varepsilon_{u,v}\right] \\
&= \mathrm{Var}\left[\frac{1}{n}\sum_{\ell=1}^{k}\sum_{\substack{\text{vertex } i\\ \text{at depth } \ell}}\left(\frac{n-1-d\sum_{m=0}^{\ell-2}(d-1)^m}{d(d-1)^{\ell-1}}\right)\varepsilon_{i,\mathrm{parent}(i)}\right] \\
&= \frac{1}{n^2}\sum_{\ell=1}^{k}\sum_{\substack{\text{vertex } i\\ \text{at depth } \ell}}\left(\frac{n-1-d\sum_{m=0}^{\ell-2}(d-1)^m}{d(d-1)^{\ell-1}}\right)^2\mathrm{Var}\left[\varepsilon_{i,\mathrm{parent}(i)}\right] \\
&\leq \frac{1}{n^2}\sum_{\ell=1}^{k}d(d-1)^{\ell-1}\left(\frac{n-1-d\sum_{m=0}^{\ell-2}(d-1)^m}{d(d-1)^{\ell-1}}\right)^2\varepsilon \\
&= \frac{1}{n^2}\sum_{\ell=1}^{k}\frac{\left(n-1-d\sum_{m=0}^{\ell-2}(d-1)^m\right)^2}{d(d-1)^{\ell-1}}\varepsilon.
\end{aligned}$$

We continue

$$\mathrm{Var}\left[\hat{s}_j\right] \leq \frac{1}{n^2}\sum_{\ell=1}^{\infty}\frac{n^2}{(d-1)^{\ell}}\varepsilon = \frac{1}{d-2}\varepsilon,$$

where in the last step we have used the identity of a geometric series. Therefore, the variance decreases with d, and thus, with high probability and increasing d, the estimate $\hat{s}_j$ will be close to the true value s_j.

B Expected length of a permutation path

We compute the expected length ℓ of a path of a permutation τ of the positions. The computation involves three expectations: the expectation $\mathbb{E}_{s_1,\ldots,s_n}$ with respect to the random process to draw the shifts s_i, the expectation $\mathbb{E}_{s_{1,2},\ldots,s_{k,k+1}}$ to draw the shifts between consecutive measurements (governed by a 2-dimensional normal distribution with mean 0 and variance σ^2 in each direction), and the expectation $\mathbb{E}_\tau$ with respect to the choice of the random permutation τ. We furthermore use $\mathbb{P}$ to denote a probability.

$$\begin{aligned}
\mathbb{E}_{s_1,\ldots,s_n}\mathbb{E}_\tau\left[\ell\right] &= \mathbb{E}_{s_1,\ldots,s_n}\mathbb{E}_\tau\left[\sum_{i=1}^{n-1}||s_{\tau(i+1)}-s_{\tau(i)}||\right] \\
&= \sum_{i=1}^{n-1}\mathbb{E}_\tau\mathbb{E}_{s_1,\ldots,s_n}\left[||s_{\tau(i+1)}-s_{\tau(i)}||\right] \\
&= \sum_{i=1}^{n-1}\sum_{k=1}^{n-1}\mathbb{P}\left[|\tau(i+1)-\tau(i)|=k\right]\mathbb{E}_{s_{1,2},\ldots,s_{k,k+1}}\left[||\sum_{j=1}^{k}s_{j,j+1}||\right] \\
&= \sum_{i=1}^{n-1}\left[\sum_{k=1}^{n-1}\mathbb{P}\left[|\tau(i+1)-\tau(i)|=k\right]\sqrt{\frac{\pi}{2}}\sqrt{k\sigma^2}\right],
\end{aligned}$$

where the last step uses that $||\sum_{j=1}^{k} s_{j,j+1}||$ is distributed according to a Rayleigh distribution[2] with scale parameter $\sqrt{k\sigma^2}$. We continue

$$\begin{aligned}\mathbb{E}_{s_1,\ldots,s_n}\mathbb{E}_\tau\left[\ell\right] &= (n-1)\sqrt{\frac{\pi}{2}}\sigma \sum_{k=1}^{n-1}\frac{(n-k)}{n(n-1)}\sqrt{k} \\ &= \frac{\sqrt{2\pi}\sigma}{2n}\sum_{k=1}^{n-1}(n-k)\sqrt{k} \\ &= \frac{\sqrt{2\pi}\sigma}{2}\left(\sum_{k=1}^{n-1}\sqrt{k} - \frac{1}{n}\sum_{k=1}^{n-1}k^{\frac{3}{2}}\right)\end{aligned}$$

Using the Euler-Maclaurin formula[3] for both sums, this can be written as:

$$\begin{aligned}\mathbb{E}_{s_1,\ldots,s_n}\mathbb{E}_\tau\left[\ell\right] &= \frac{\sqrt{2\pi}\sigma}{2}\left(\left(\frac{2}{3}n^{\frac{3}{2}} + \frac{1}{2}n^{\frac{1}{2}} + O(1)\right) - \left(\frac{2}{5}n^{\frac{3}{2}} + \frac{1}{2}n^{\frac{1}{2}} + O(1)\right)\right) \\ &= \frac{2\sqrt{2\pi}}{15}\sigma n^{\frac{3}{2}} + \sigma O(1)\end{aligned}$$

(The $O(1)$-notation means: a quantity that is bounded as n grows to infinity.)

[2] Papoulis, A. and Pillai, S. U. Probability, random variables, and stochastic processes. Tata McGraw-Hill Education, 2002.

[3] Apostol, T. M. An elementary view of Euler's summation formula. *The American Mathematical Monthly*, 106(5): 409–418, 1999.