Optimal Voronoi Tessellations with Hessian-based Anisotropy
Supplemental Material

Max Budninskiy, Caltech

Beibei Liu, Caltech

Fernando de Goes, Pixar

Yiying Tong, MSU

Pierre Alliez, Inria

Mathieu Desbrun, Caltech/Inria

In this additional document, we provide a detailed proof of the bound on L^p kissing approximations stated for $p=1$ in our main submission (Eq. (22)), and give expressions for the gradient and Hessian of the approximation error $\mathcal{E}_{\text{OVT}}$ for completeness.

1 Proof of approximation error bound

Assume that function $f:\Omega\mapsto\mathbb{R}$ is in $C^2(\Omega)$ and is convex in a convex region $D\subset\mathbb{R}^n$ containing Ω. Suppose that the kissing approximation approach applied to f leads to an OVT tessellation $\mathcal{V}=\{V_i\}_{i=1}^N$ of Ω satisfying conditions (1-4) in Sec 3.3 of the paper.

We use the following shorthand notations:

$$H_p(x)=(\det \text{Hess}[f]\,(x))^{-\frac{1}{2p+n}}\,\text{Hess}[f]\,(x),\quad H_{V_i}=\frac{1}{|V_i|}\int_{V_i}\text{Hess}[f]\,(x)dx,\quad H_{V_i,p}=(\det H_{V_i})^{-\frac{1}{2p+n}}H_{V_i},$$

$$|V_i|_{H_{V_i}}=(\det H_{V_i})^{\frac{1}{2}}|V_i|,\quad |V_i|_{H_{V_i,p}}=(\det H_{V_i,p})^{\frac{1}{2}}|V_i|=(\det H_{V_i})^{\frac{p}{2p+n}}|V_i|,$$

$$\text{Vol}\,(\Omega;\rho;H_{V_i,p})=\sum_i\rho_{V_i}^{\frac{n}{2p+n}}|V_i|_{H_{V_i,p}},\quad \text{Vol}\,(\Omega;\rho;H_p)=\int_\Omega(\det H_p(x))^{\frac{1}{2}}\rho(x)^{\frac{n}{2p+n}}dx=\int_\Omega(\det \text{Hess}[f]\,(x))^{\frac{p}{2p+n}}\rho(x)^{\frac{n}{2p+n}}dx. \tag{1}$$

Condition 3 can be rewritten as: $\exists\,\beta_0>0$, such that

$$\forall V_i\in\mathcal{V},\ \frac{\text{diam}_{H_{V_i,p}}V_i}{|V_i|_{H_{V_i,p}}^{\frac{1}{n}}}=\frac{\text{diam}_{H_{V_i}}V_i}{|V_i|_{H_{V_i}}^{\frac{1}{n}}}\le\beta_0. \tag{2}$$

Similarly, Condition 4 (with density modulation) is equivalent to: $\exists\,\beta_1>0$, such that

$$\frac{\max_i\rho_{V_i}^{\frac{n}{2p+n}}|V_i|_{H_{V_i,p}}}{\min_i\rho_{V_i}^{\frac{n}{2p+n}}|V_i|_{H_{V_i,p}}}\le\beta_1.$$

First case: $1\le p<\infty$

In star-shaped cell $V_i\in\mathcal{V}$ (Condition 1) we can reexpress $f-T_i$ using Taylor expansion at x_i for any $x\in V_i$ with the Lagrange remainder:

$$f(x)-T_i(x)=\frac{1}{2}(x-x_i)^t\ \ \text{Hess}[f]\,(x_i+\theta(x-x_i))\ \ (x-x_i).$$

where $\theta\in[0,1]$. From the second inequality of Condition 2, it follows that:

$$f(x)-T_i(x)\le\frac{1}{2}\alpha_1(x-x_i)^t\ H_{V_i}\ (x-x_i). \tag{3}$$

The star shape assumption of V_i and Eqs. (3) and (2) lead to

$$f(x)-T_i(x)\le\frac{1}{2}\alpha_1\beta_0^2|V_i|_{H_{V_i}}^{\frac{2}{n}}. \tag{4}$$

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Together with the relations among cell volumes in different metrics, i.e.,

$$|V_i| = (\det H_{V_i})^{-\frac{1}{2}} |V_i|_{H_{V_i}} \quad \text{and} \quad (\det H_{V_i})^{-\frac{1}{2}} |V_i|_{H_{V_i}}^{\frac{2p+n}{n}} = |V_i|_{H_{V_i,p}}^{\frac{2p+n}{n}},$$

we then have

$$\int_{V_i} |f(x) - T_i(x)|^p \rho(x) dx \leq |V_i| \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \rho_{V_i} |V_i|_{H_{V_i}}^{\frac{2p}{n}} = \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \rho_{V_i} |V_i|_{H_{V_i,p}}^{\frac{2p+n}{n}} = \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \left(\rho_{V_i}^{\frac{n}{2p+n}} |V_i|_{H_{V_i,p}}\right)^{\frac{2p+n}{n}}.$$

Condition 4 implies that for every $V_i \in \mathcal{V}$,

$$\rho_{V_i}^{\frac{n}{2p+n}} |V_i|_{H_{V_i,p}} \leq \beta_1 N^{-1} \operatorname{Vol}(\Omega; \rho; H_{V_i,p}),$$

where N is the number of cells in $\mathcal{V}$. Therefore,

$$||f - f_d||_{L^p}^p = \sum_{i=1}^N \int_{V_i} [f(x) - T_i(x)]^p \rho(x) dx \leq \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \sum_{i=1}^N \left(\rho_{V_i}^{\frac{n}{2p+n}} |V_i|_{H_{V_i,p}}\right)^{\frac{2p+n}{n}}$$
$$\leq \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p N \left[\beta_1 N^{-1} \operatorname{Vol}(\Omega; \rho; H_{V,p})\right]^{\frac{2p+n}{n}} = \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \beta_1^{\frac{2p+n}{n}} N^{-\frac{2p}{n}} \operatorname{Vol}(\Omega; \rho; H_{V,p})^{\frac{2p+n}{n}}.$$

Finally, using the first inequality of Condition 2, the strict positivity of ρ and the fact that for two matrices $M_1 \preceq M_2$ we have $\det M_1 \leq \det M_2$, we get:

$$||f - f_d||_{L^p}^p \leq \left(\frac{1}{2}\alpha_1\beta_0^2\right)^p \beta_1^{\frac{2p+n}{n}} \alpha_0^{-p} N^{-\frac{2p}{n}} \operatorname{Vol}(\Omega; \rho; H_p)^{\frac{2p+n}{n}}.$$

Taking p-th root of the above and using Eq. (1), we arrive at

$$||f - f_d||_{L^p} \leq C(\alpha_0, \alpha_1, \beta_0, \beta_1, n) N^{-\frac{2}{n}} \left|\left|(\det \operatorname{Hess}[f])^{\frac{1}{n}} (\rho)^{\frac{1}{p}}\right|\right|_{L^{\frac{pn}{2p+n}}(\Omega)}.$$

Second case: $p = \infty$

Denote the limits of $\operatorname{Vol}(\Omega; \rho; H_{V,p})$ and $\operatorname{Vol}(\Omega; \rho; H_p)$ as $p \to \infty$, respectively, by

$$|\Omega|_{H_V} = \sum_{i=1}^N |V_i|_{H_{V_i}} = \sum_{i=1}^N (\det H_{V_i})^{\frac{1}{2}} |V_i|,$$

and

$$|\Omega|_H = \int_\Omega (\det \operatorname{Hess}[f](x))^{\frac{1}{2}} dx.$$

Assume the difference $(f - f_d)$ attains its maximum at point x^* in a cell V^*. Then, analogously to the previous case, we use the bound inside the cell V^* demonstrated earlier and Conditions 1-4 to obtain

$$||f - f_d||_{L^\infty} \leq \frac{1}{2}\alpha_1\beta_0^2 |V^*|_{H_{V^*}}^{\frac{2}{n}} \leq \frac{1}{2}\alpha_1\beta_0^2\beta_1^{\frac{2}{n}} N^{-\frac{2}{n}} |\Omega|_{H_V}^{\frac{2}{n}} \leq \frac{1}{2}\alpha_1\beta_0^2\beta_1^{\frac{2}{n}} \alpha_0^{-1} N^{-\frac{2}{n}} |\Omega|_H^{\frac{2}{n}}.$$

The result follows from the expression for $|\Omega|_H$:

$$||f - f_d||_{L^\infty} \leq C(\alpha_0, \alpha_1, \beta_0, \beta_1, n) N^{-\frac{2}{n}} ||(\det \operatorname{Hess}[f])^{\frac{1}{n}}||_{L^{\frac{n}{2}}(\Omega)}.$$

2 Derivatives of OVT Energy

Our derivation of the gradient and Hessian of the objective function $\mathcal{E}_{\text{OVT}}$ is based on *Reynold's transport theorem*, which states that for a function $f(\mathbf{x}, \mathbf{p})$, a parameter $\mathbf{p}$, and a domain D, one has

$$\frac{\partial}{\partial \mathbf{p}} \int_D f d\mathbf{x} = \int_D \frac{\partial f}{\partial \mathbf{p}} d\mathbf{x} + \int_{\partial D} f \left(\frac{\partial \mathbf{x}}{\partial \mathbf{p}} \cdot \mathbf{n}\right) d\mathbf{A},$$

where $\mathbf{n}$ is the outward unit normal field of the boundary ∂D.

Gradient. As site location $\mathbf{x}_i$ is a parameter of the objective function $\mathcal{E}$, we have

$$\nabla_{\mathbf{x}_i} \mathcal{E}_{\text{OVT}}(f, X) = \int_\Omega \nabla_{\mathbf{x}_i} (f - f_d)\, d\mathbf{x} + \int_{\partial\Omega} (f - f_d)\, \frac{\partial \mathbf{x}}{\partial \mathbf{x}_i} \cdot \mathbf{n}\, d\mathbf{A}.$$

The second term is zero since the boundary of the domain does not depend on the site location, while the first integral reduces to $-\int_{V_i} \nabla_{\mathbf{x}_i} T_i(\mathbf{x}) d\mathbf{x}$, since f does not depend on $\mathbf{x}_i$ and the continuous function f_d depends on $\mathbf{x}_i$ only within V_i.

Analogously, $\nabla_{\mathbf{x}_i} \mathcal{E}_{\rho\text{-OVT}}(f, X) = -\int_{V_i} \rho(\mathbf{x}) \nabla_{\mathbf{x}_i} T_i(\mathbf{x})\, d\mathbf{x}$.

Hessian. Applying Reynold's theorem to the general case of non-uniform density again and denoting $H_i = \text{Hess}[f]\,(\mathbf{x}_i)$, we obtain:

$$\nabla_{\mathbf{x}_i}\nabla_{\mathbf{x}_i}\mathcal{E}_{\rho\text{-OVT}} = H_i|V_i|_\rho \,\text{Id} - |V_i|_\rho \nabla^3 f(\mathbf{x}_i)\cdot(\mathbf{b}_i - \mathbf{x}_i) \\ - \sum_{j\in N(i)} \frac{1}{2l_{ij}} \int_{A_{ij}} \rho(\mathbf{x})\ [H_i(\mathbf{x}-\mathbf{x}_i)] \otimes [H_i(\mathbf{x}-\mathbf{x}_i)]\, d\mathbf{A},$$

where $N(i)$ is the set of one-ring neighbors of site i and A_{ij} is the boundary facet between the two adjacent cells V_i and V_j, while l_{ij} is the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$. Here, the boundary term cannot be omitted as the integral is associated with (over) V_i, which (whose) boundary depends on $\mathbf{x}_i$. Taking into account the influence of $\mathbf{x}_j$ on the boundary of V_i, we also have

$$\nabla_{\mathbf{x}_j}\nabla_{\mathbf{x}_i}\mathcal{E}_{\rho\text{-OVT}} = \frac{1}{2l_{ij}} \int_{A_{ij}} \rho(\mathbf{x})\ [H_i(\mathbf{x}-\mathbf{x}_i)] \otimes [H_j(\mathbf{x}-\mathbf{x}_j)]\ d\mathbf{A}.$$

Since we assume $f \in \mathcal{C}^2$, the expressions above imply that $\mathcal{E}_{\rho\text{-OVT}}$ is twice continuously differentiable as a function of sites.