Supplementary Material for the paper: "Non-parametric Regression between manifolds"

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1 Second order approximation of a submanifold in Euclidean space

Given an m-dimensional submanifold M isometrically embedded in $\mathbb{R}^s$, we want to approximate M up to second-order around a given point $p \in M$.

Proposition 1 *Let $x^1, \ldots, x^m$ be the coordinates associated with an orthonormal basis of the tangent space at T_pM. Then in Cartesian coordinates z of $\mathbb{R}^s$, the manifold can be approximated up to second order as*

$$z(x) = (x^1, \ldots, x^m, f^{m+1}(x), \ldots, f^s(x)),$$

where $f^i(x) = \sum_{\alpha,\beta=1}^m \Pi^i_{\alpha\beta} x^\alpha x^\beta$ and $\Pi^i_{\alpha\beta}$ is the second fundamental form of M at p. If M is a hypersurface, then we have $z(x) = (x^1, \ldots, x^{s-1}, f^s(x))$, and f^s is given as

$$f^s(x) = \sum_{i=1}^{s-1} \kappa_i (x^i)^2,$$

if the coordinates x^α are aligned with the principal directions and κ_i are the principal curvatures of M at p.

Proof: Let $\gamma(t)$ be a geodesic on M with $\gamma(0) = p$. Then we can do a Taylor expansion of γ around p with respect to the ambient space $\mathbb{R}^s$,

$$\gamma(t) = \gamma(0) + \gamma'(0)t + \frac{1}{2}\gamma''(0)t^2 + O(t^3).$$

We have $\gamma'(0) \in T_pM$ and, since M is isometrically embedded, $\|\gamma'(0)\|_{T_pM} = \|\gamma'(0)\|_{T_p\mathbb{R}^s} = \|\gamma'(0)\|_{\mathbb{R}^s}$.

That means parametrization by arclength is the same in M and $\mathbb{R}^s$. Now if $\gamma(t)$ is parameterized by arclength which is equivalent to $\|\gamma'(t)\|_{\mathbb{R}^s} = 1$, then we have

$$0 = \frac{\partial}{\partial t} \|\gamma'(t)\|^2_{\mathbb{R}^s} = 2 \langle \gamma''(t), \gamma'(t) \rangle_{\mathbb{R}^s} .$$

However, we even know by the relation between extrinsic and intrinsic derivative, see [1, p. 140], that

$$\gamma'' = D_t\gamma' + \Pi(\gamma', \gamma'),$$

where $\Pi : T_pM \times T_pM \to N_pM$ is the second fundamental form or extrinsic curvature of M, N_pM is the normal space of M (the subspace orthogonal to the tangent space T_pM in $\mathbb{R}^s$) and $D_t\gamma' = {}^M\nabla_{\gamma'}\gamma'$. Since γ is a geodesic, we have $D_t\gamma' = 0$ (the intrinsic acceleration is zero) and get

$$\gamma'' = \Pi(\gamma', \gamma').$$

Note, that $\gamma'' \in N_pM$. Plugging this into the Taylor expansion of the geodesic, we obtain

$$\gamma(t) = \gamma(0) + \gamma'(0)t + \frac{t^2}{2}\Pi(\gamma', \gamma') + O(t^3),$$

where $\gamma'(0) \in T_pM$ and $\Pi(\gamma', \gamma') \in N_pM$. We deduce that, if we introduce orthonormal coordinates x^i for the subspace $p + T_pM$ with origin at $p \in M$ and extend this to a full Cartesian coordinate system of $\mathbb{R}^s$, we get the local second order approximation of M as

$$(x^1, \dots, x^m, f^{m+1}(x), \dots, f^s(x)),$$

where $f^i(x) = \sum_{\alpha,\beta=1}^m \Pi^i_{\alpha\beta} x^\alpha x^\beta$ and $\Pi^i_{\alpha\beta}$ is the second fundamental form described in the local coordinate system (note that $\Pi^i_{\alpha\beta} = 0$ if $i \leq m$ since $\Pi(\frac{\partial}{\partial x^\alpha}, \frac{\partial}{\partial x^\beta}) \in N_pM$).

For a hypersurface M the normal space N_pM is one-dimensional, $\Pi(X, Y) = h(X, Y)N$, where N is the normal vector at p and $h : T_pM \times T_pM \to \mathbb{R}$. Thus in coordinates h is just a $(s-1) \times (s-1)$- symmetric matrix with eigenvalues $\kappa_i,\ i = 1, \dots, s-1$ and thus in the basis formed by the eigenvectors we get

$$h(X, Y) = \sum_{\alpha=1}^{s-1} \kappa_\alpha X^\alpha Y^\alpha,$$

and thus we get the second-order approximation $(x^1, \dots, x^{s-1}, f^s(x))$ with $f^s(x) = \sum_{\alpha=1}^{s-1} \kappa_\alpha x^\alpha\, x^\alpha$. □

2 Representation of the second derivative of Ψ using the second-order approximation of the input manifold

As above, assume that M is an m-dimensional submanifold in $\mathbb{R}^s$.

Proposition 2 *Using a second-order approximation of M centered at $p \in M$, we get in Cartesian coordinates $z = (x^1, \ldots, x^m, f^{m+1}(x), \ldots, f^s(x))$ that*

$$g_{\alpha\beta}(0) = \delta_{\alpha\beta}, \qquad {}^M\Gamma^{\alpha}_{\beta\gamma}(0) = 0.$$

Furthermore, we have at $p \in M$,

$$\Big[\frac{\partial^2 \Psi^\mu}{\partial x^\beta \partial x^\alpha} - \frac{\partial \Psi^\mu}{\partial x^\gamma} {}^M\Gamma^{\gamma}_{\beta\alpha}\Big] = \Big[\frac{\partial^2 \Psi^\mu}{\partial z^\beta \partial z^\alpha} + \sum_{r=m+1}^{s} \frac{\partial \Psi^\mu}{\partial z^r} \Pi^r_{\beta\alpha}\Big].$$

Proof: The function $i : \mathbb{R}^m \to \mathbb{R}^s$ defined as

$$(x^1, \ldots, x^m) \quad \mapsto \quad i(x) = (x^1, \ldots, x^m, f^{m+1}(x), \ldots, f^s(x)),$$

can be seen as the embedding of the second order approximation of M into $\mathbb{R}^s$. The induced metric is given as

$$g_{\alpha\beta} = \sum_{r=1}^{s} \frac{\partial i^r}{\partial x^\alpha} \frac{\partial i^r}{\partial x^\beta} = \begin{cases} 1 + \sum_{k=m+1}^{s} \left(\frac{\partial f^k}{\partial x^\alpha}\right)^2, & \text{if } \alpha = \beta, \\ \sum_{k=m+1}^{s} \frac{\partial f^k}{\partial x^\alpha} \frac{\partial f^k}{\partial x^\beta}, & \text{if } \alpha \neq \beta. \end{cases}$$

Since the functions f^k are all quadratic in the coordinates x^α, we immediately see that $g_{\alpha\beta}(0) = \delta_{\alpha\beta}$. Moreover, we have

$$\frac{\partial g_{\alpha\beta}}{\partial x^\gamma} = \begin{cases} 2 \sum_{k=m+1}^{s} \frac{\partial^2 f^k}{\partial x^\gamma \partial x^\alpha} \frac{\partial f^k}{\partial x^\alpha}, & \text{if } \alpha = \beta, \\ \sum_{k=m+1}^{s} \left(\frac{\partial^2 f^k}{\partial x^\gamma \partial x^\alpha} \frac{\partial f^k}{\partial x^\beta} + \frac{\partial f^k}{\partial x^\alpha} \frac{\partial^2 f^k}{\partial x^\gamma \partial x^\beta} \right), & \text{if } \alpha \neq \beta. \end{cases}$$

Again, since f^i are quadratic functions in x^α we have $\frac{\partial g_{\alpha\beta}}{\partial x^\gamma} = 0$ at the origin. Now, the Christoffel symbols in local coordinates x^α are given as [1, p. 70]

$$\Gamma^\gamma_{\alpha\beta} = \frac{1}{2} g^{\gamma\rho} (\partial_\alpha g_{\beta\rho} + \partial_\beta g_{\alpha\rho} - \partial_\rho g_{\alpha\beta}),$$

and with the previous result, we also obtain $\Gamma^\gamma_{\alpha\beta} = 0$ at the origin. Moreover, we have

$$\frac{\partial^2 \Psi^\mu}{\partial x^\beta \partial x^\alpha} = \frac{\partial^2 \Psi^\mu}{\partial z^r \partial z^u} \frac{\partial z^r}{\partial x^\alpha} \frac{\partial z^u}{\partial x^\beta} + \frac{\partial \Psi^\mu}{\partial z^r} \frac{\partial^2 z^r}{\partial x^\alpha \partial x^\beta},$$

and

$$\frac{\partial z^r}{\partial x^\alpha} = \begin{cases} 1, & \text{if } r = \alpha, \\ 0, & \text{if } r \leq m \text{ and } r \neq \alpha, \\ \frac{\partial f^r}{\partial x^\alpha}, & \text{if } r > m, \end{cases}$$

$$\frac{\partial^2 z^r}{\partial x^\beta \partial x^\alpha} = \begin{cases} 0, & \text{if } r \leq m, \\ \Pi^r_{\alpha\beta}, & \text{if } r > m, \end{cases}$$

and thus, we obtain at $x = 0$,

$$\frac{\partial^2 \Psi^\mu}{\partial x^\beta \partial x^\alpha} = \frac{\partial^2 \Psi^\mu}{\partial z^r \partial z^u} \frac{\partial z^r}{\partial x^\alpha} \frac{\partial z^u}{\partial x^\beta} + \frac{\partial \Psi^\mu}{\partial z^r} \frac{\partial^2 z^r}{\partial x^\alpha \partial x^\beta}$$
$$= \frac{\partial^2 \Psi^\mu}{\partial z^\beta \partial z^\alpha} + \sum_{r=m+1}^{s} \frac{\partial \Psi^\mu}{\partial z^r} \Pi^r_{\beta\alpha}.$$

For a hypersurface M we have $\Pi^r_{\beta\alpha} = N^r h_{\beta\alpha}$, where h is the so called shape operator. If the coordinates x^α are aligned with the principal directions (the eigenvectors of $h_{\beta\alpha}$), we get $\Pi^r_{\beta\alpha} = 0$ if $r < s$ and $\Pi^s_{\beta\alpha} = \kappa_\alpha \delta_{\alpha\beta}$. □

References

[1] J. M. Lee. *Riemannian Manifolds - An introduction to curvature*. Springer, New York, 1997.