Differentiable manifolds

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March 10, 2023

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Least squares approximation

Let us consider the problem to find the best approximation for the set of points $\{(x_i, y_i)\}_{i=1}^n$ by the straight line $y = a_1x + a_2$ the problem to find optimal values of (a_1, a_2) . Define the sum of squared residuals:

$$S(k,b) = \sum_{i=1}^{n} (y_i - a_1 x_i - a_2)^2.$$

The minimum of the function with respect to parameters k, b defines the best approximation. The conditions are:

$$\frac{\partial S}{\partial a_1} = 2\sum_{i=1}^n x_i(y_i - a_1x_i - a_2) = 0,$$
$$\frac{\partial S}{\partial a_2} = 2\sum_{i=1}^n (y_i - a_1x_i - a_2) = 0.$$

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Least squares approximation. Example



Consider the set of points (1, 2), (2, 1), (3, 3).

Define the sum of squared residuals:

$$egin{aligned} S(a_1,a_2) &= (a_1+a_2-2)^2 + \ 2a_1+a_2-1)^2 + (3a_1+a_2-3)^2 . \end{aligned}$$

$$\begin{aligned} \frac{\partial S}{\partial a_1} &= 28a_1 + 12a_2 - 26 = 0, \ \frac{\partial S}{\partial a_2} &= 12a_1 + 6a_2 - 12 = 0.\\ &28a_1 + 12a_2 = 26, \quad 12a_1 + 6a_2 = 12.\\ &a_1 &= 1/2, \ a_2 &= 1 \Rightarrow y = \frac{1}{2}x + 1. \end{aligned}$$

Image correction



Figure: Image distortions: barrel and pincushion

The task is to find maps X = X(x, y), Y = Y(x, y) which minimize the sum of residuals:

$$S = \sum_{i=0}^{N} \sum_{j=0}^{M} (X(x_{ij}, y_{ij}) - i)^{2} + (Y(x_{ij}, y_{ij}) - j)^{2} \to \min. \quad (1)$$

Here we use the linear mapping to correct the image

$$X(x, y) = ax + by + c,$$

$$Y(x, y) = ux + vy + w.$$

Problem is find coefficients a, b, c, u, v, w to minimize the sum of squared residuals.

The necessary conditions for the coefficients:

$$2a \sum_{i,j} x_{ij}^{2} + 2b \sum_{i,j} x_{ij}y_{ij} + 2c \sum_{i,j} x_{ij} - 2 \sum_{i,j} ix_{ij} = 0,$$

$$2a \sum_{i,j} x_{ij}y_{ij} + 2b \sum_{i,j} y_{ij}^{2} + 2c \sum_{i,j} y_{ij} - 2 \sum_{i,j} iy_{ij} = 0,$$

$$2a \sum_{i,j} x_{ij} + 2b \sum_{i,j} y_{ij} + 2cMN - M(N-1)N = 0,$$

$$2u \sum_{i,j} x_{ij}^{2} + 2v \sum_{i,j} x_{ij}y_{ij} + 2w \sum_{i,j} x_{ij} - 2 \sum_{i,j} jx_{ij} = 0,$$

$$2u \sum_{i,j} x_{ij}y_{ij} + 2v \sum_{i,j} y_{ij}^{2} + 2w \sum_{i,j} y_{ij} - 2 \sum_{i,j} jy_{ij} = 0,$$

$$2u \sum_{i,j} x_{ij} + 2v \sum_{i,j} y_{ij} + 2wMN - NM(M-1) = 0.$$

Let change the variables:

$$\begin{split} \tilde{X}_3 &= \sum_{i,j} x_{ij}^2, \quad \tilde{X}_2 = \sum_{i,j} i x_{ij}, \quad \tilde{X}_1 = \sum_{i,j} j x_{ij}, \quad \tilde{X}_0 = \sum_{i,j} x_{ij} \\ \tilde{Z} &= \sum_{i,j} x_{ij} y_{ij}, \quad \tilde{Y}_3 = \sum_{i,j} y_{ij}^2, \quad \tilde{Y}_2 = \sum_{i,j} i y_{ij}, \quad \tilde{Y}_1 = \sum_{i,j} j y_{ij}, \\ \tilde{Y}_0 &= \sum_{i,j} y_{ij}. \end{split}$$

Here the letters with tildes are the sums of known expressions of x_{ij} and y_{ij} .

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Then we can rewrte the equations for a, b, c

$$2a\tilde{X}_3 + 2b\tilde{Z} + 2c\tilde{X} - 2\tilde{X}_2 = 0,$$

$$2a\tilde{Z} + 2b\tilde{Y}_3 + 2c\tilde{Y} - 2K\tilde{Y}_2 = 0,$$

$$2a\tilde{X} + 2b\tilde{Y} + 2cMN - MN(N - 1) = 0$$

and for u, v, w.

$$\begin{aligned} & 2u\tilde{X}_3 + 2v\tilde{Z} + 2w\tilde{X} - 2\tilde{X}_1 = 0, \\ & 2u\tilde{Z} + 2v\tilde{Y}_2 + 2w\tilde{Y} - 2\tilde{Y}_1 = 0, \\ & 2u\tilde{X} + 2v\tilde{Y} + 2wMN - NM(M-1) = 0. \end{aligned}$$

These solutions define the linear maps X(x, y) and Y(x, y).

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Linear image correction $S \sim 8.5 \rightarrow S = 4.23$



Figure: Linear correction of barrel distorsion.

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Cubic image correction

Consider a cubic map:

$$\begin{aligned} X(x,y) &= a_0 + a_1 x + a_2 y + b_{20} x^2 + b_{11} x y + b_{02} y^2 + \\ &\quad c_{30} x^3 + c_{21} x^2 y + c_{12} x y^2 + c_{03} y^3, \\ Y(x,y) &= u_0 + u_1 x + u_2 y + v_{20} x^2 + v_{11} x y + v_{20} y^2 + \\ &\quad w_{30} x^3 + w_{21} x^2 y + w_{12} x y^2 + w_{03} y^3. \end{aligned}$$

The necessary conditions are

$$\frac{\partial S}{\partial a_i} = 0, \quad i = 0, 1, 2; \quad \frac{\partial S}{\partial u_i} = 0, \quad i = 0, 1, 2;$$
$$\frac{\partial S}{\partial b_{ij}} = 0 \quad 0 \ge i, j, \quad i + j = 2; \quad \frac{\partial S}{\partial v_{ij}} = 0 \quad 0 \ge i, j, \quad i + j = 2;$$
$$\frac{\partial S}{\partial c_{ij}} = 0 \quad 0 \ge i, j, \quad i + j = 3; \quad \frac{\partial S}{\partial b_{ij}} = 0 \quad 0 \ge i, j, \quad i + j = 3.$$

Cubic image correction $S \sim 8.5 \rightarrow S \sim 0.08$



Figure: Cubic correction of barrel distorsion.

The cubic map leads to the sum of residuals from $S \sim 8.5$ to $S \sim 0.08$ which better wthat the linear correction: S = 4.23.

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A gradient-wise descent

Seeking of a local minima looks like a descent to the lowest point in a neighborhood. The best direction to the descent opposites to the gradient.

Example

Define the gradient of the function

$$f(\vec{x}) = x_1^2 - 3x_1x_2 + x_2^4,$$

in the point (1, 2). The partial derivatives are:

$$\frac{\partial f}{\partial x_1} = 2x_1 - 3x_2, \quad \frac{\partial f}{\partial x_2} = -3x_1 + 4x_2^3.$$
$$\vec{\nabla} f|_{(1,2)} = (-4, 29).$$

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Typical steps of the gradient descent

Consider an algorithm of the gradient descent. Let Δ be a length of the step in opposite of the gradient.

- Let a current point x_1, \ldots, x_n .
- ► Calculate the gradient *F* at the current point.
- A step in direction opposite to the gradient $\vec{X} = \vec{x} \Delta \text{grad}(F)$.
- Check $F(\vec{X}) < F(\vec{x})$.
- If the condition fulfills then new position $\vec{x} = \vec{X}$.
- Another case a local minimum in the distance less than Δ .

Calculation of the partial derivatives using the Lagrange theorem



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Change the gradient descent method for the opposite gradient direction as function of the variable Δ :

$$\Phi(\Delta) = F(\vec{x} - \vec{\nabla}F(\vec{x}) \cdot \Delta), \quad \{x_1, \dots, x_N\} = \text{const.}$$

So we seek the minimum of the one dimension function $\Phi(\Delta)$ on the given direction.

- 1. Define an interval $\Delta \in [0, b]$ such that $\Phi(\Delta) \leq \Phi(0)$.
- Find a minimum Φ(Δ*) on Δ ∈ [0, b] using for example a bisection method.
- 3. The point $\vec{X} = \vec{x} \vec{\nabla}F(\vec{x}) \cdot \Delta^*$ is considered as next position for the next step.
- 4. If $||\vec{X} \vec{x}|| > \delta$, then this process repeats.



Consider the fastest gradient descent for the function

 $f(x_1, x_2) = (x_1 + x_2)^2 + 3(x_1 - x_2)^2.$

The level curves are ellipses with big semi axis along the straight line $x_1 = x_2$ and the minimum is (0, 0).

The fastest descent

Let the initial point is (2,3) then f(2,3) = 28. Find the derivatives and the gradient:

$$\frac{\partial f}{\partial x_1} = 8x_1 - 4x_2, \ \frac{\partial f}{\partial x_2} = -4x_1 + 8x_2, \ \vec{\nabla}f|_{(2,3)} = (4,16);$$

Then the descent direction starting the point (2,3): $x_1 = 2 - 4t$, $x_2 = 3 - 16t$, t > 0. The minimized one-dimensional function is:

$$f(x_1(t), x_2(t)) = 832t^2 - 272t + 28 = 832\left(t - \frac{272}{2 \cdot 832}\right)^2 + \frac{75}{13}.$$

$$t_1 = \frac{272}{2 \cdot 832} \sim 0.16346, \ x_1 = 2 - 4t_1 \sim 2 - 4 \cdot 0.16346 \sim 1.35,$$

$$x_2 = 3 - 16t_1 \sim 3 - 16 \cdot 0.16346 \sim 0.38, \ f = \frac{75}{13} \sim 5.77.$$



The track of minimizing for the function $f = (x_1 + x_2)^2 + 3(x_1 - x_2)^2$ is shown of the picture. All

turning points lie on tangent line for the level curves.

A global minimum

A global and local minima



Figure: The example of the surface with two minima which are a global and local ones. If one starts the gradient descent near the local minimum, then one does not reach the global minimum.

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Primary concepts for definition of a differentiable manifold

- ▶ $a_1x_1 + a_2x_2 + c = 0$, is a one function of one variable: $x_1(x_2) = -\frac{1}{a_1}(a_2x_2 + c)$ or $x_2(x_1) = -\frac{1}{a_2}(a_1x_1 + c)$. Both forms are appropriated if $a_{1,2} \neq 0$.
- $a_1x_1 + a_2x_2 + a_3x_3 + c = 0$ is a a function of two variables: $x_k = -\frac{1}{a_k} \left(\sum_{n \neq k} a_n x_n + c \right).$
- ► The following two equals define one dimensional function.

 $a_1x_1 + a_2x_2 + a_3x_3 + c = 0, \ b_1x_1 + b_2x_2 + b_3x_3 + d = 0.$

In a general case the *m* equalities of *N* variables define *N* - *m* dimensional implicit function:

$$f_k(x_1,\ldots,x_N)=0,\ k=1,\ldots,m.$$

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Primary concepts for definition of differentiable manifolds

► Does the formula $\sum_{k=1}^{3} x_k^2 - R^2 = 0$ define a two-dimensional function?

$$x_i = +\sqrt{R^2 - \sum_{k=1, k \neq i}^3 x_k^2}, \ x_i = -\sqrt{R^2 - \sum_{k=1, k \neq i}^3 x_k^2}.$$

The answer looks like NO! because one obtains two different values for x_i for the same set of coordinates $\{x_k\}_{i \neq k}$.

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Primary concepts for definition of differentiable manifolds

Another point of view for the spherical coordinates:

 $x_1 = R\sin(\theta)\cos(\phi), x_2 = R\sin(\theta)\sin(\phi), x_3 = R\cos(\theta).$

So we can see that in the spherical coordinate system one obtain one-to-one map $[0, \pi] \times [0, 2\pi) \rightarrow$ a set of x_1, x_2, x_3 .

We need a generalization for the function definition.

Consider

$$x^2 + y^2 + z^2 - 1 = 0,$$

A normal vector \vec{N} at a point $A = (x_0, y_0, z_0)$ looks like $\vec{N} = (2x_0, 2y_0, 2z_0)$. The tangent plain at the point A is follows: $2x_0(x - x_0) + 2y_0(y - y_0) + 2z_0(z - z_0) = 0$. Without loss of a generality let's assume $x_0 \neq 0$. Define $\vec{e_1}$:

$$(\vec{N}, \vec{\eta}) = 0, \ \vec{\eta} = (-z_0, 0, x_0),$$

$$\vec{\zeta} : \ \vec{\zeta} = \vec{\eta} \times \vec{N} = (-x_0 y_0, x_0^2 + z_0^2, -y_0 z_0),$$

$$(\vec{\eta}, \vec{\zeta}) = z_0 x_0 y_0 - x_0 y_0 z_0 = 0.$$

The $\vec{\eta}$ and $\vec{\zeta}$ define an orthogonal basis in the tangent plain.

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New coordinates (ξ, η, ζ) :

$$\begin{pmatrix} 2x_0 & 2y_0 & 2z_0 \\ -z_0 & 0 & x_0 \\ -x_0y_0 & x_0^2 + z_0^2 & -y_0z_0 \end{pmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \\ z - z_0 \end{pmatrix} = \begin{pmatrix} \xi \\ \eta \\ \zeta \end{pmatrix}$$

A determinant of the matrix $y_0^2 - 1$. The inverse transform:

$$\begin{pmatrix} x_0 & \frac{z_0}{y_0^2 - 1} & \frac{x_0 y_0}{y_0^2 - 1} \\ y_0 & 0 & 1 \\ z_0 & \frac{x_0}{1 - y_0^2} & \frac{y_0 z_0}{y_0^2 - 1} \end{pmatrix} \begin{pmatrix} \xi \\ \eta \\ \zeta \end{pmatrix} = \begin{pmatrix} x - x_0 \\ y - y_0 \\ z - z_0 \end{pmatrix}$$

For any point A of the implicit function

$$x^2 + y^2 + z^2 - 1 = 0$$

one can define a new coordinate system and rewrite the implicit function in the explicit one in new coordinates.

Theorem about explicit form of the function

Let's consider

$$f_k(x_1,...,x_n) = 0, k \in \{1,...,M\}, n \in \{1,...,N\},$$

where all f_k are continuously differentiable functions at the origin.

If a rank of the matrix

$$S = \left(\frac{\partial f_k}{\partial x_n}\right), \ s_{k,n} = \frac{\partial f_k}{\partial x_n}$$

is equal M at the origin then exists a neighborhood of the origin, where the implicit function can be rewritten in an explicit form as a function of N - M independent variables.

Sketch of proof

Let's change the variables:

 $\xi_k = f(x_1, \dots, x_N), \ k \in \{1, \dots, M\},$ Consider the matrix $M \times M$

$$\tilde{S} = \left(\frac{\partial f_k}{\partial x_n}\right), \quad \text{Rank}(\tilde{S}) = M.$$

Then $\exists \epsilon >, x_k = \phi_k(\vec{\xi}, x_{M+1}, \dots, N), \forall \vec{\xi} : ||\vec{\xi}|| < \epsilon.$

$$d\xi_k \equiv \sum_{n=1}^M \frac{\partial f_k}{\partial x_n} dx_n,$$

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Sketch of proof

Then one can rewrite

$$x_k = \sum_{n=1}^M rac{\partial \phi_k}{\partial \xi_n} \xi_k + o(||\xi||).$$

Hence one can rewrite:

$$x_k = F_k(x_{M+1},\ldots,x_N), k \in \{1,2,\ldots,M\}.$$

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A definition of differentiable manifold

The set in *N* dimensional space is called N - M dimensional differentiable manifold if for any point *A* of the set exists neighborhood of the *A* such that $\exists \epsilon > 0$ and the manifold can be defined by

$$x_k = F_k(x_1,\ldots,x_{N-M}) = 0, \ k \in \{M,\ldots,N\}, \ \forall x : ||x|| < \epsilon.$$

The set of maps covered all range of the variables is called an atlas.

Definition for a Jacobian

Let's consider the changing of variables:

 $y_k = f_k(x).$

the matrix

($\frac{\partial f_1}{\partial x_1}$	•••	$\frac{\partial f_1}{\partial x_n}$ \	١
		• • •		
	$\frac{\partial f_k}{\partial x_1}$		$\frac{\partial f_k}{\partial x_n}$	/

is called Jacobian.

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$$y_1 = x_1^4 + x_1^2 x_2 + x_3, y_2 = x_2, y_3 = x_3.$$

$$\frac{\partial(y_1, y_2, y_3)}{\partial(x_1, x_2, x_3)} = \begin{pmatrix} 4x_1^3 + 2x_1x_2 & x_1^2 & 1\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix}$$

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