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Local approximation in many variables

12.1 Higher-order partial derivatives

Just as in the single variable case, the higher-order partial derivatives of f convey nuances about the local shape of the function about the point of interest that are missed by the local affine approximation, suggesting that a better approximation could be attained if only we could incorporate also the information conveyed by the second partial derivatives of f.

We say that a function $f : \mathbb{R}^n \to \mathbb{R}$ is *continuously differentiable* at a if it is differentiable and its partial derivatives are continuous in a neighborhood of a. Analogously, we say that f is 2 *times continuously differentiable* at a if all of its partial derivatives are continuously differentiable at a.

Theorem 6 (Schwarz)**.** *If f is 2 times continuously differen-*

tiable, then its second order partial derivatives are symmetric, i.e.

$$\frac{\partial^2 f}{\partial x_i \partial x_j}(a) = \frac{\partial^2 f}{\partial x_j \partial x_i}(a)$$

for all $1 \leq i, j \leq n$.

We omit the proof of this theorem, although the interested reader might be able to find it in any standard multivariable differential calculus resource.

12.2 Quadratic approximation

Since using affine functions we have no more room left to carry more information about the local shape of f at a, we must think of another type of function. Just as we did in the single variable case, we will look into candidate functions that are homogeneous polynomials of degree 2, namely, a function of the form:

$$Q(x) = q_0 + L(x - a) + \frac{1}{2}(x - a)^t H(x - a)$$

where $L \in \mathbb{R}^{1\times n}$ and $H \in \mathbb{R}^{n\times n}$ is a symmetrix matrix, which must satisfy the following requirements:

1. $Q(a) = f(a)$
2. $\frac{\partial Q}{\partial x_i}(a) = \frac{\partial f}{\partial x_i}(a)$ for all $1 \leq i \leq n$
3. $\frac{\partial^2 Q}{\partial x_i \partial x_j}(a) = \frac{\partial^2 f}{\partial x_i \partial x_j}(a)$ for all $1 \leq i, j \leq n$

The requirements imply that $L = Jf(a)$, the Jacobian matrix, whilst $H = [\frac{\partial^2 f}{\partial x_i \partial x_j}(a)]$ is the matrix whose entries are the second-order partial derivatives, also known as the *Hessian matrix* of f at a. For the time being, we will denote the Hessian matrix as $Hf(a)$.

Proposition 38 (Multivariable quadratic approximation)**.** *If f is 2 times continuously differentiable at a, then*

$$Q(x) = f(a) + Jf(a)(x-a) + \frac{1}{2}(x-a)^t Hf(a)(x-a)$$

is a local quadratic approximation of f at a satisfying

$$f(x) = Q(x) + \mathfrak{o}(\|x-a\|^2).$$

Note that if a is critical point of f, i.e. $Jf(a) = [0 \ldots 0]$, locally at a the function f can be approximated by

$$f(a) + \frac{1}{2}(x-a)^t Hf(a)(x-a).$$

The second term corresponds to a class of polynomials known as a *quadratic forms*. If we are able to classify the different quadratic forms that can arise, we will be able to classify a as a critical point.

12.3 Affine change of coordinates

Informally, we can think of using different coordinate systems to represent the same points of $\mathbb{R}^n$ in the hope that the new representation can lead to an easier-to-understand representation of e.g. some function or geometric shape.

We say that a function $\psi : \mathbb{R}^n \to \mathbb{R}^n$ is an *affine change of coordinates* of $\mathbb{R}^n$ if it can be expressed as

$$\psi(x) = A^{-1}(x-a),$$

for some invertible matrix $A \in \mathbb{R}^{n \times n}$ and $a \in \mathbb{R}^n$. What does such a coordinate change achieve? It is easy to see that such a change takes the point a to the origin. But not just this. For example, suppose that $\psi : \mathbb{R}^2 \to \mathbb{R}^2$ is the affine change of coordinates

$$\psi(x) = A^{-1}(x - a),$$

with A being the rotation of $\pi/4$ radians about the origin. There are two ways of thinking about the change of perspective the change of coordinates ψ represents:

1. **Move the coordinate axes**. The new coordinates of a point P will correspond to new coordinate axes obtained by first shifting the original coordinate until the origin overlaps a, then rotating the axes $\pi/4$ radians about the new origin.

2. **Move the space**. The new coordinates of a point P will be as if we obtained a new point P' obtained by first getting the vector aP', then rotating it $-\pi/4$ radians about the origin.

An affine change of coordinates $\psi(x) = A^{-1}(x - a)$ has always an inverse affine change of coordinates ψ^{-1} that can be expressed as

$$\psi^{-1}(y) = Ay + a.$$

12.4 Change of variables

Given some function $f : \mathbb{R}^n \to \mathbb{R}$ which has some expression in the original coordinate system, i.e. a way to compute the output using a representation of the input in the original coordinate system, we now want to study how the expression of the function changes if we provide the a representation of the input in a new coordinate system. More specifically, suppose that P is some point in $\mathbb{R}^n$ which in the original coordinate system has coordinates x, furthermore we know how to compute the value of f at P using x as an input, e.g. evaluating some expression $F(x)$. What would be the way to compute f if we provide P represented in a new coordinate system?

Suppose that the coordinates of P in the new coordinate system are

$$y = \psi(x) = A^{-1}(x - a),$$

for some invertible matrix A and $a \in \mathbb{R}^n$. We know how to compute the output of P using the coordinates x as $F(x)$. But we can provide, using y as an input, the coordinates in the original coordinate system as

$$x = \psi^{-1}(y) = Ay + a.$$

The expression of f if we represent the input in coordinates of the new coordinate system is

$$G(y) = F(\psi^{-1}(y)) = F(Ay + a).$$

We say to have obtained G from F doing a *change of variables.*

12.5 Symmetric quadratic forms

Symmetric quadratic forms are (multivariable) polynomials that can be expressed as

$$Q(x) = (x - a)^t H(x - a),$$

where H is a symmetric matrix and $a \in \mathbb{R}^n$. In this section we will examine whether there is a change of variables that can render a simple expression for computing and understanding Q.

Since H is a symmetric matrix, there is an orthonormal basis of eigenvectors of H. If U is the orthogonal matrix that has such vectors as columns, then there is an orthgonal matrix U such that

$$U^t H U = \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n).$$

Can we use this observation to our advantage and find a better representation of the quadratic form via change of variables? If we use the following change of coordinates

$$y = U^t(x - a),$$

we can express the old coordinates using the new ones

$$x = Uy + a,$$

thereby obtaining the following expression:

$$\widetilde{Q}(y) = Q(Uy + a) = (Uy)^t H(Uy) =$$

$$= y^t U^t H U y = y^t \Lambda y = \sum_{i=1}^{n} \lambda_i y_i^2.$$

Proposition 39. *Given a symmetric quadratic form in n variables*

$$Q(x) = (x - a)^t H(x - a)$$

there is an affine change of coordinates where the quadratic form has the following expression:

$$\widetilde{Q}(y) = \sum_{i=1}^{n} \lambda_i y_i^2,$$

with λ_i the eigenvalues of H.

The quadratic form $\widetilde{Q}(y)$ in the proposition is said to be in *canonical form.*

12.6 Classification of critical points

Given a (2 times continuously differentiable) function $f : \mathbb{R}^n \to \mathbb{R}$ and a critical point a of f, the eigenvalues of the Hessian matrix $Hf(a)$ give us a very valuable piece of information to study the local shape of f about the point a, as f can be approximated as

$$f(x) = f(a) + \frac{1}{2} \sum_{i=1}^{n} \lambda_i x_i^2 + \mathfrak{o}(\|x\|^2)$$

with λ_i being the eigenvalues of $Hf(a)$, taking an appropriate coordinate system. Using this expression alone we can already derive a practical rule to classify the critical points of f.

Theorem 7 (Classification of critical points). *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a 2 times continuously differentiable function, a be a critical point of f and $\lambda_1, \dots, \lambda_n$ be the eigenvalues of $Hf(a)$, the Hessian matrix of f at a. Then the following rule holds:*

1. *If $\lambda_i > 0$ for all $1 \leq i \leq n$, then a is a local minimum.*

2. *If $\lambda_i < 0$ for all $1 \leq i \leq n$, then a is a local maximum.*

3. *If $\lambda_i \lambda_j < 0$ for some $i \neq j$, then a is a saddle point.*

4. *Otherwise, we cannot conclude anything.*

Let's see how we can prove the claims of the theorem. Using the multivariable quadratic approximation within an appropriate coordinate system, about the critical point a, f takes the form:

$$f(x) = f(a) + \frac{1}{2} \sum_{i=1}^{n} \lambda_i x_i^2 + \mathfrak{o}(\|x\|^2)$$

If $\lambda_i > 0$ for all $1 \leq i \leq n$, we should prove that justify that there is an neighborhood about a where $f(a)$ is the minimum value that $f(x)$ can take. This would mean that $f(x) - f(a) > 0$ for $x \neq a$ in the said neighborhood. Since

$$\psi(x) = f(x) - f(a) = \frac{1}{2} \sum_{i=1}^{n} \lambda_i x_i^2 + \mathfrak{o}(\|x\|^2),$$

dividing by $\|x\|^2$ would not change the sign:

$$\frac{\psi(x)}{\|x\|^2} = \frac{1}{2\|x\|^2} \sum_{i=1}^{n} \lambda_i x_i^2 + \frac{\mathfrak{o}(\|x\|^2)}{\|x\|^2}$$

But we know that the second term converges towards zero as $x \to \vec{0}$, while the first term remains positive for any x, since

$$\frac{1}{\|x\|^2} \sum_{i=1}^{n} \lambda_i x_i^2 \geq \min(\lambda_1, \ldots, \lambda_n) > 0.$$

This means that for values x close enough to $\vec{0}$,

$$\frac{\psi(x)}{\|x\|^2} > 0.$$

Since the sign of $\psi(x)/\|x\|^2$ is equal to the sign of $\psi(x) = f(x) - f(a)$ the conclusion follows. The other cases of the theorem can be justified in exactly the same way.

12.7 TL;DR

The higher-order derivatives of f at a help us understanding the local behaviour of f about a. If the functions are smooth enough, we can provide a quadratic approximation that encapsulates all the information up to the second-order partial derivatives. At the critical points of f this polynomial takes a very gentle form to work with, a symmetric quadratic form, that allows us to find a new coordinate system in which the interpretation of the critical points is very intuitive. Looking at f with appropriate coordinates, we can then go about classifying the critical points of f into three main categories: local maxima, local minima, saddle points. However convenient, our classification theorem is not complete, in that there may be situations where we would not be able to classify the critical points. Addressing this would involve studying higher-order multivariable Taylor expansions, just as we did for single variable functions. But this, it will be another story.