

Mathematics/Statistics Bootcamp

Part II: Calculus

Steven Winter Christine Shen

Department of Statistical Science
Duke University

MSS Orientation, August 2022

Overview

Sequences and Series

Limits and Derivatives

Integrals

Multivariate Calculus

Optimization

Sequences and Series

Limits of Sequences

A **sequence** is an ordered list of numbers. We write $\{a_1, a_2, a_3, \dots\}$, $\{a_n\}$, $\{a_n\}_{n=1}^{\infty}$, (a_n) , etc.

A sequence $\{a_n\}$ has **limit** L ($\lim_{n \rightarrow \infty} a_n = L$, or $a_n \rightarrow L$ as $n \rightarrow \infty$) if

$$\forall \varepsilon > 0, \exists N_{\varepsilon} \in \mathbb{N} \text{ such that } n \geq N_{\varepsilon} \implies |a_n - L| < \varepsilon.$$

If all limits exist, then

1. $\lim_{n \rightarrow \infty} (ca_n) = c(\lim_{n \rightarrow \infty} a_n)$.
2. $\lim_{n \rightarrow \infty} (a_n + b_n) = (\lim_{n \rightarrow \infty} a_n) + (\lim_{n \rightarrow \infty} b_n)$.
3. $\lim_{n \rightarrow \infty} (a_n b_n) = (\lim_{n \rightarrow \infty} a_n)(\lim_{n \rightarrow \infty} b_n)$.
4. $a_n \leq b_n \leq c_n \implies \lim_{n \rightarrow \infty} a_n \leq \lim_{n \rightarrow \infty} b_n \leq \lim_{n \rightarrow \infty} c_n$
(Squeeze theorem).

Sequence Theorems (Optional)

If for every $n \in \mathbb{N}$, $a_n \leq a_{n+1}$ (increasing) or $a_n \geq a_{n+1}$ (decreasing), then the sequence $\{a_n\}$ is **monotonic**.

If there exists a number $M > 0$ such that $|a_n| \leq M$ for every n then the sequence $\{a_n\}$ is **bounded**.

Monotonic Sequence theorem: Every bounded, monotonic sequence is convergent (has a limit).

Bolzano–Weierstrass theorem: Every bounded sequence has a convergent subsequence.

Series Basics

Fix a sequence (a_k) and let

$$s_n = \sum_{k=1}^n a_k$$

be the sequence of partial sums. A **series** is the limit of s_n (written $\sum_{n=1}^{\infty} a_n$).

The series converges if (s_n) has a limit. Same properties as sequence limits (except for products).

Key example is the **geometric series**:

$$\sum_{n=0}^{\infty} x^n = 1 + x + x^2 + \cdots$$

which converges to $1/(1-x)$ if $|x| < 1$ and diverges otherwise.

Series Theorems

The comparison test: Suppose that $\sum a_n$ and $\sum b_n$ are series with positive terms.

- (i) If $\sum b_n$ is convergent and $a_n \leq b_n$ for all n , then $\sum a_n$ is also convergent;
- (ii) If $\sum b_n$ is divergent and $a_n \geq b_n$ for all n , then $\sum a_n$ is also divergent.

Many other tests:

[https://en.wikipedia.org/wiki/Series_\(mathematics\)](https://en.wikipedia.org/wiki/Series_(mathematics))

Discussion

1. Fix $x, p \in \mathbb{R}$. Discuss convergence of the sequences

$$a_n = \frac{1}{n^p}, \quad b_n = \left(1 + \frac{x}{n}\right)^n, \quad c_n = \cos(nx).$$

2. Fix $p \in \mathbb{R}$. Discuss convergence of the series

$$A = \sum_{n=1}^{\infty} \frac{1}{n^p}, \quad B = \sum_{n=1}^{\infty} \frac{\log(n)}{n}.$$

3. Assume

$$\left| \sum_{n=1}^{\infty} a_n \right| < \infty.$$

What, if anything, can we say about the limit of a_n ?

Limits and Derivatives

Pointwise Limits

A function $f : \mathbb{R} \rightarrow \mathbb{R}$ has **limit** L at a (written $\lim_{x \rightarrow a} f(x) = L$) if

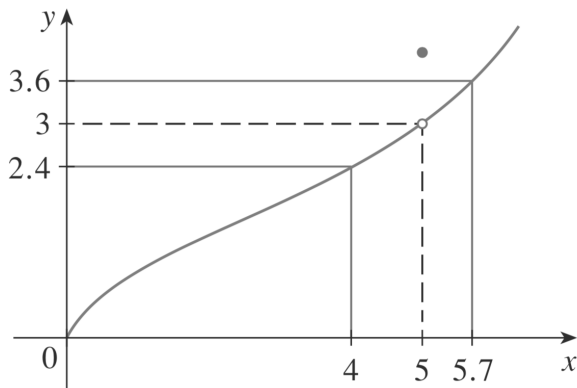
$$\forall \varepsilon > 0, \exists \delta_\varepsilon > 0 \text{ such that } |x - a| < \delta_\varepsilon \implies |f(x) - L| < \varepsilon.$$

Equivalently, if the sequence $(f(x_1), f(x_2), \dots)$ converges to L for any sequence x_n converging to a . Same properties as sequences.

Left-hand limit: $\lim_{x \rightarrow a^-} f(x) = L$ if for any $\epsilon > 0$, there exists $\delta > 0$ such that $|f(x) - L| < \epsilon$ whenever $a - \delta < x < a$.

Right-hand limit: $\lim_{x \rightarrow a^+} f(x) = L$ if for any $\epsilon > 0$, there exists $\delta > 0$ such that $|f(x) - L| < \epsilon$ whenever $a < x < a + \delta$.

Example



► What is $\lim_{x \rightarrow 5^-} f(x)$?

► What is $\lim_{x \rightarrow 5^+} f(x)$?

► What is $\lim_{x \rightarrow 5} f(x)$?

► What is $\lim_{x \rightarrow 4} f(x)$?

Continuity Basics

A function f is continuous at a if

$$\lim_{x \rightarrow a} f(x) = f(a).$$

Right continuous at a if $\lim_{x \rightarrow a^-} f(x) = f(a)$; **left continuous** at a if $\lim_{x \rightarrow a^+} f(x) = f(a)$.

You should know:

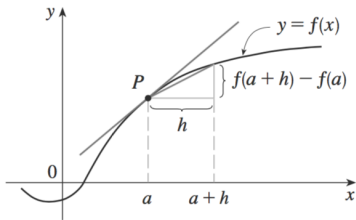
- ▶ Continuous functions form a vector space!
- ▶ Composition of continuous functions is continuous.
- ▶ Results like the intermediate value theorem.

Derivative Basics

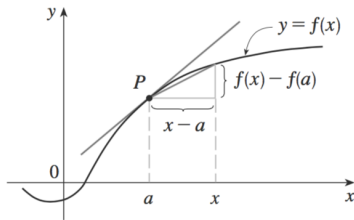
The derivative of function f at $a \in X$, denoted by $f'(a)$, is

$$f'(a) = \lim_{h \rightarrow 0} \frac{f(a+h) - f(a)}{h}$$

if this limit exists. Differentiable implies continuous.



$$\begin{aligned} \text{(a) } f'(a) &= \lim_{h \rightarrow 0} \frac{f(a+h) - f(a)}{h} \\ &= \text{slope of tangent at } P \\ &= \text{slope of curve at } P \end{aligned}$$



$$\begin{aligned} \text{(b) } f'(a) &= \lim_{x \rightarrow a} \frac{f(x) - f(a)}{x - a} \\ &= \text{slope of tangent at } P \\ &= \text{slope of curve at } P \end{aligned}$$

Derivative Rules

Derivatives of some common functions:

- ▶ $f(x) = \text{const}$, then $f'(x) = 0$;
- ▶ $f(x) = x^\alpha$, $\alpha \neq 0$, then $f'(x) = \alpha x^{\alpha-1}$;
- ▶ $(e^x)' = e^x$, $(\ln x)' = 1/x$ ($x > 0$);
- ▶ $(\sin x)' = \cos x$, $(\cos x)' = -\sin x$, $(\tan x)' = 1/\cos^2 x$;

If both $f(x)$ and $g(x)$ are differentiable:

- ▶ $(cf(x))' = cf'(x)$, $(f(x) + g(x))' = f'(x) + g'(x)$;
- ▶ $(f(x)g(x))' = f'(x)g(x) + f(x)g'(x)$;
- ▶ $\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) - f(x)g'(x)}{g^2(x)}$ (assume $g(x) \neq 0$);
- ▶ The **chain rule**: if $F = f \circ g$, then $F'(x) = f'(g(x))g'(x)$.

Taylor Series

If f is infinitely differentiable at a , then it can be expressed as a power series:

$$\begin{aligned} f(x) &= f(a) + f'(a)(x - a) + \frac{f''(a)}{2}(x - a)^2 + \dots \\ &= \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x - a)^n \end{aligned}$$

This is called the **Taylor series** of f at a .

Intuition: we can approximate nice functions arbitrarily well with polynomials.

Very useful in statistics: CLT, delta method, optimization algorithms, etc.

Exercises

1. Differentiate

$$f(x) = xe^{-x}, \quad g(x) = 1 - \cos^2(x), \quad h(x) = \frac{\log(x)}{x}.$$

2. Fix $\mu, x \in \mathbb{R}$ and $\gamma > 0$. Let

$$f(x) = \frac{1}{\sqrt{\gamma}} \exp\left(-\frac{(x - \mu)^2}{\gamma}\right)$$

Find $x_0 \in \mathbb{R}$ such that the tangent line of $f(x)$ at x_0 is horizontal.

3. Find the Taylor series of $f(x) = e^x$ around 0.

4. Find $\lim_{x \rightarrow 0} (1 + x)^{1/x}$.

Solutions

1. Skipped.
2. Skipped.
3. Combining $f' = f$ and $f(0) = 1$ gives

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}.$$

Solutions

4. **Solution 1:** Work on the log scale. Let $f(x) = \ln x$ and note

$$\begin{aligned}\lim_{x \rightarrow 0} \ln((1+x)^{1/x}) &= \lim_{x \rightarrow 0} \frac{\ln(1+x)}{x} \\ &= \lim_{x \rightarrow 0} \frac{\ln(1+x) - \ln(1)}{x} \\ &= f'(1)\end{aligned}$$

Since $f'(1) = 1$, $\lim_{x \rightarrow 0} (1+x)^{1/x} = e^1 = e$.

Solution 2: Reparameterize:

$$\lim_{x \rightarrow 0} (1+x)^{1/x} = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^n = e.$$

Integrals

The Fundamental Theorem of Calculus

If f is continuous on $[a, b]$, then the function

$$g(x) = \int_a^x f(s)ds$$

is continuous on $[a, b]$, differentiable on (a, b) , and $g'(x) = f(x)$.

If F is any anti-derivative of f ($F' = f$), then

$$\int_a^b f(x)dx = F(b) - F(a).$$

Definite Integral Rules

Let $a \leq d \leq b \in \mathbb{R}$:

- ▶ If $c \in \mathbb{R}$ is a constant, then $\int_a^b c dx = c(b - a)$;
- ▶ $\int_a^b cf(x) dx = c \int_a^b f(x) dx$;
- ▶ $\int_a^b [f(x) + g(x)] dx = \int_a^b f(x) dx + \int_a^b g(x) dx$;
- ▶ $\int_a^d f(x) dx + \int_d^b f(x) dx = \int_a^b f(x) dx$;
- ▶ If $f(x) \geq g(x)$ for $a \leq x \leq b$, then $\int_a^b f(x) dx \geq \int_a^b g(x) dx$;
- ▶ If $m \leq f(x) \leq M$ for $a \leq x \leq b$, then $m(b - a) \leq \int_a^b f(x) dx \leq M(b - a)$.

Useful Formulas for Integration

- ▶ **Substitution:** If $u = g(x)$ is continuously differentiable on $[a, b]$ and f is continuous on the range of u , then

$$\int_a^b f(g(x))g'(x)dx = \int_{g(a)}^{g(b)} f(u)du.$$

Proof: chain rule.

- ▶ **Integration by parts:** If functions u and v are both continuously differentiable on $[a, b]$, then

$$\int_a^b u(x)v'(x)dx = [u(x)v(x)]|_a^b - \int_a^b v(x)u'(x)dx.$$

Proof: product rule.

Improper Integrals

Assume $\int_a^b f(x)dx$ exists for every $b \geq a$ and define

$$\int_a^\infty f(x)dx = \lim_{b \rightarrow \infty} \int_a^b f(x)dx.$$

if the limit exists. Likewise for $\int_{-\infty}^b f(x)dx$.

Extend these to define

$$\int_{-\infty}^\infty f(x)dx = \lim_{b \rightarrow -\infty} \lim_{a \rightarrow \infty} \int_a^b f(x)dx.$$

if all limits exist.

Intuition: solve integral on a “safe” domain, take limits.

Discontinuous Integrand

If f is continuous on $[a, b)$ and is discontinuous at b , then

$$\int_a^b f(x)dx = \lim_{t \rightarrow b^-} \int_a^t f(x)dx$$

if this limit exists. Likewise if f is continuous on $(a, b]$.

Same intuition: solve integral on a “safe” domain, take limits.

Exercises

1. Calculate $\int_1^e \frac{\ln(x)}{x} dx$.
2. Calculate $\int_0^\pi x \cos(x) dx$.
3. Fix $p \in \mathbb{R}$. Calculate $I_1 = \int_0^1 \frac{1}{x^p} dx$ and $I_2 = \int_1^\infty \frac{1}{x^p} dx$.

Solutions

1. Let $u = \log(x)$ so $du = dx/x$. Then

$$\int_1^e \frac{\ln(x)}{x} dx = \int_0^1 u du = \left[\frac{u^2}{2} \right]_0^1 = \frac{1}{2} - 0 = \frac{1}{2}$$

2. Let $u = x$ and $dv = \cos(x)$ so $v = \sin(x)$. Then

$$\begin{aligned} \int_0^\pi x \cos(x) dx &= \left[x \sin(x) \right]_0^\pi - \int_0^\pi \sin(x) dx \\ &= \left[x \sin(x) \right]_0^\pi - \left[\cos(x) \right]_0^\pi \\ &= 0 - 0 - (1 - (-1)) \\ &= -2 \end{aligned}$$

Solutions

3. Divide into $p = 1$ and $p \neq 1$:

$$\int \frac{1}{x} dx = \log(x), \quad \int \frac{1}{x^p} dx = \frac{x^{1-p}}{1-p}.$$

The first equation shows they both diverge with $p = 1$. The second shows I_1 is finite if and only if $p < 1$, in which case

$$I_1 = \int_0^1 \frac{1}{x^p} dx = \frac{1}{1-p}.$$

Conversely, I_2 is finite if and only if $p > 1$, in which case

$$I_2 = \int_1^\infty \frac{1}{x^p} dx = \frac{1}{p-1}.$$

Multivariate Calculus

Partial Derivatives

Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}$. The **partial derivative** with respect to the i th variable x_i is

$$\frac{\partial f}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{h}.$$

Strategy: treat other variables as constants.

If $\frac{\partial^2 f}{\partial x_i \partial x_j}$ and $\frac{\partial^2 f}{\partial x_j \partial x_i}$ are both continuous on \mathbb{R}^n , then $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$.

Gradients and Hessians

Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}$. If all first-order partial derivatives exist, then the **gradient**¹ is

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right)^T.$$

Intuition: points uphill.

If all second-order partial derivatives exist, then the **Hessian** is

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}.$$

Intuition: local curvature. When is this symmetric?

¹Technically $\nabla f(\mathbf{x})$ is a map $T_{\mathbf{x}}\mathbb{R}^n \rightarrow T_{f(\mathbf{x})}\mathbb{R}$.

Jacobians

Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$. If all first-order partial derivatives exist, then the **Jacobian** is

$$J = \begin{pmatrix} \nabla^T f_1 \\ \vdots \\ \nabla^T f_m \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

Intuition: locally approximates f as a linear transformation (stretching, rotating, permuting, etc).

When $n = m$, $|J|$ describes how f locally distorts volume.

Change of Variables (Optional)

Consider integrating a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ over a set $U \subseteq \mathbb{R}^n$. Let $\varphi : U \rightarrow \mathbb{R}^n$ denote a change of coordinates with Jacobian J . Then under some conditions,

$$\int_U f(\mathbf{x}) d\mathbf{x} = \int_{\varphi(U)} f(\varphi(\mathbf{u})) |J(\mathbf{u})| d\mathbf{u}.$$

Extremely useful for finding probability density functions.

Note: need Fubini's theorem to freely change order of integrals.

Matrix Calculus

We sometimes need to differentiate with respect to a matrix.

E.g., if we model data $\mathbf{x}_1, \dots, \mathbf{x}_n \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and want the MLE of $\boldsymbol{\Sigma}$, then we differentiate

$$\ell(\boldsymbol{\Sigma}) = -\frac{n}{2} \log |2\pi\boldsymbol{\Sigma}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu})$$

with respect to $\boldsymbol{\Sigma}$.

Rely on

- ▶ The Matrix Cookbook
- ▶ https://en.wikipedia.org/wiki/Matrix_calculus
- ▶ Matrix Algebra From a Statistician's Perspective by Harville.

Optimization

Extrema

Derivative condition: If f has a local minimum or maximum at c and $f'(c)$ exists, then $f'(c) = 0$. Converse is false.

Second derivative test: If $f'(c) = 0$ and f has second derivative on $(c - \epsilon_0, c + \epsilon_0)$ for some $\epsilon_0 > 0$, then

- ▶ $f''(c) > 0$ implies c is a local minimum,
- ▶ $f''(c) < 0$ implies c is a local maximum.

Why? Draw pictures.

Multivariate analogue: local optima satisfy $\nabla f(\mathbf{c}) = 0$. Minimum if Hessian is positive definite; maximum if negative definite.

Useful for minimizing error, finding MLEs, etc.

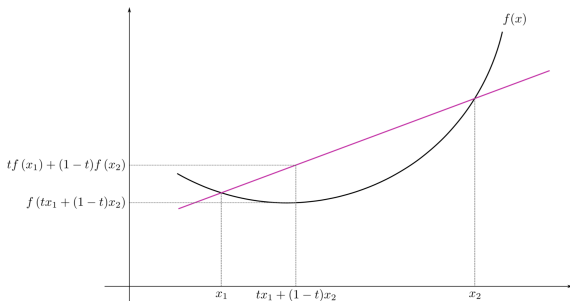
Convexity Basics

A subset X of \mathbb{R}^n is **convex** if for any $x, y \in X$ and $t \in [0, 1]$.

$$tx + (1 - t)y \in X.$$

A function $f : X \rightarrow \mathbb{R}$ is **convex** if for any $x, y \in X$ and $t \in [0, 1]$,

$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y).$$



Convexity Theorems

Suppose a function $f : \mathbb{R} \rightarrow \mathbb{R}$ is twice differentiable on an open set. The following are equivalent

- ▶ f is convex.
- ▶ $f(x) \geq f(y) + f'(y)(x - y)$; the graph is above all tangents.
- ▶ $f''(x) \geq 0$.

Similar tests for multivariate functions.

Any local minimum of a convex function is also a global minimum.

Lagrange Multipliers

Let $f, g : \mathbb{R}^n \rightarrow \mathbb{R}$ be differentiable. **Lagrange multipliers** are a method of optimizing f subject to $g = 0$.

Procedure:

1. Solve the following system of equations:

$$\begin{aligned}\nabla f(\mathbf{x}) &= \lambda \nabla g(\mathbf{x}) \\ g(\mathbf{x}) &= 0\end{aligned}$$

2. Plug all solutions into f to find the global optima.

Often introduce the Lagrangian,

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda g(\mathbf{x}).$$

Example

Consider rolling a k -sided die n times. Let p_j denote the true probability of face j and X_j count the number of times we see face j . Mathematically, $(X_1 \dots X_k) \sim \text{Multinomial}(n, p_1 \dots p_k)$.

We want to infer $\mathbf{p} = (p_1, \dots, p_k)$ from the data, e.g. with the MLE. Requires maximizing the log-likelihood subject to $\sum_{i=1}^k p_i = 1$.

The Lagrangian is

$$\begin{aligned}\mathcal{L}(\mathbf{p}, \lambda) &= \ell(\mathbf{p}; X_1, \dots, X_k) + \lambda \left(1 - \sum_{i=1}^k p_i \right) \\ &= \log(n!) - \sum_{i=1}^k \log(x_i!) + \sum_{i=1}^k x_i \log(p_i) + \lambda \left(1 - \sum_{i=1}^k p_i \right)\end{aligned}$$

Example

First solve $\nabla \mathcal{L}(\mathbf{p}, \lambda) = 0$. The partial derivatives are

$$\frac{\partial \mathcal{L}}{\partial p_j} = \frac{x_j}{p_j} - \lambda.$$

Setting to zero gives $\hat{p}_j = x_j / \lambda$.

Now plug this into $g(\mathbf{p}) = 0$ to find λ .

$$1 = \sum_{i=1}^k \hat{p}_i = \sum_{i=1}^k \frac{x_i}{\lambda} = \frac{1}{\lambda} \sum_{i=1}^k x_i.$$

Solving for λ gives $\lambda = \sum_{i=1}^k x_i$, hence the MLE is
 $\hat{p}_j = x_j / \sum_{i=1}^k x_i$

Exercises

1. Let $f : \mathbb{R}_+ \times [0, 2\pi] \rightarrow \mathbb{R}^2$ transform polar coordinates to Cartesian coordinates:

$$(r, \theta) \mapsto (r \cos(\theta), r \sin(\theta)).$$

Find the Jacobian and its determinant.

2. Prove/disprove convexity for the following functions:

$$f(x) = |x|, \quad g(x) = \log(x^2 + 1), \quad h(x) = e^{-x}.$$

3. Fix $\alpha, \beta > 0$. Find the global maximum of

$$f(x) = x^{\alpha-1} e^{-\beta x} \mathbf{1}(x > 0).$$

Justify all claims.

Solutions

1. Using the definition:

$$J = \begin{pmatrix} \partial_r f_1 & \partial_\theta f_1 \\ \partial_r f_2 & \partial_\theta f_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -r \sin(\theta) \\ \sin(\theta) & r \cos(\theta) \end{pmatrix}.$$

The determinant formula gives $|J| = r \cos^2(\theta) + r \sin^2(\theta) = r$.

2. Only f and h are convex. Use the triangle inequality for f and the second derivative test for g , h .

Solutions

3. Let $\ell(x) = \log(f(x)) = (\alpha - 1)\log(x) - \beta x$. Compute

$$\ell'(x) = \frac{\alpha - 1}{x} - \beta$$

$$\ell''(x) = -\frac{(\alpha - 1)}{x^2}$$

Set ℓ' equal to zero and solve: $\hat{x} = (\alpha - 1)/\beta$.

Case 1: If $\alpha > 1$, then $\hat{x} > 0$ and $\ell''(\hat{x}) < 0$, so this is a local max. Plug it in and double check that $f(\hat{x}) > f(0)$, or argue concavity.

Case 2: If $\alpha = 1$, then $f(x)$ is strictly increasing to $e^{-\beta}$ as $x \rightarrow 0^+$. There is no global max.

Case 3: If $\alpha < 1$, then $f(x) \rightarrow \infty$ as $x \rightarrow 0^+$. There is no global max.

Acknowledgements

Past contributors:

- ▶ Jordan Bryan, PhD student
- ▶ Brian Cozzi, MSS alumni
- ▶ Michael Valancius, MSS alumni
- ▶ Graham Tierney, PhD student
- ▶ Becky Tang, PhD student