# Calculus in Infinite Dimensions

Elliott Sullinge-Farrall

University of Surrey

TORUS 2023

# Table of Contents

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

**Infinite Dimensional**

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \ldots$$

**Infinite Dimensional**

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \ldots$$

- Balls

$$B = \{x \in \mathbb{R}^n : |x| < 1\}$$

**Infinite Dimensional**

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \ldots$$

- Balls

$$B = \{x \in \mathbb{R}^n : |x| < 1\}$$

- Cubes

$$Q = [-1, +1]^3$$

**Infinite Dimensional**

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \dots$$

- Balls

$$B = \{x \in \mathbb{R}^n : |x| < 1\}$$

- Cubes

$$Q = [-1, +1]^3$$

**Infinite Dimensional**

- Sequence spaces

$$\mathbb{R}^{\mathbb{N}} = \{(x_i)_{i=1}^{\infty} : x_i \in \mathbb{R}\}$$

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \ldots$$

- Balls

$$B = \{x \in \mathbb{R}^n : |x| < 1\}$$

- Cubes

$$Q = [-1, +1]^3$$

**Infinite Dimensional**

- Sequence spaces

$$\mathbb{R}^{\mathbb{N}} = \{(x_i)_{i=1}^{\infty} : x_i \in \mathbb{R}\}$$

- Function spaces

$$\mathbb{R}^{\mathbb{R}} = \{f : \mathbb{R} \to \mathbb{R}\}$$

# Finite vs Infinite Dimensional Space

**Finite Dimensional**

- Euclidean space

$$\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3, \ldots$$

- Balls

$$B = \{x \in \mathbb{R}^n : |x| < 1\}$$

- Cubes

$$Q = [-1, +1]^3$$

**Infinite Dimensional**

- Sequence spaces

$$\mathbb{R}^{\mathbb{N}} = \{(x_i)_{i=1}^{\infty} : x_i \in \mathbb{R}\}$$

- Function spaces

$$\mathbb{R}^{\mathbb{R}} = \{f : \mathbb{R} \to \mathbb{R}\}$$

- Lebesgue & Sobolev spaces

# Finite Dimensional Calculus

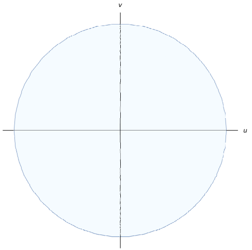
Consider a **function** $f : B \to \mathbb{R}^3$, with $B$ the unit ball in 2D, given by

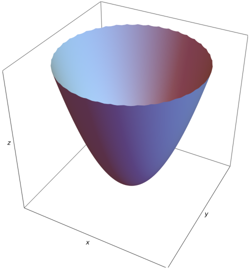
$$f(u,v) = \begin{pmatrix} u+v \\ u-v \\ u^2+v^2 \end{pmatrix}$$

Then the **gradient** is given by

$$\nabla f(u,v) = \begin{pmatrix} +1 & +1 \\ +1 & -1 \\ 2u & 2v \end{pmatrix}$$

We can use this to investigate stationary points, minima, maxima etc.



# Infinite Dimensional Calculus

Now consider a **functional** $f : \mathbb{R}^{\mathbb{N}} \to \mathbb{R}$, given by

$$f(x) = x_1$$

Then the **gradient** is a sequence $\nabla f(x)$ with entries given by

$$(\nabla f(x))_i = \delta_{1,i} = \begin{cases} 1 & i = 1 \\ 0 & i > 1 \end{cases}$$

# Infinite Dimensional Calculus

Now consider a **functional** $f : \mathbb{R}^{\mathbb{N}} \to \mathbb{R}$, given by

$$f(x) = x_1$$

Then the **gradient** is a sequence $\nabla f(x)$ with entries given by

$$(\nabla f(x))_i = \delta_{1,i} = \begin{cases} 1 & i = 1 \\ 0 & i > 1 \end{cases}$$

We shall mainly focus on functionals defined on spaces of functions.

# Local Minima in Finite Dimensions

We often use

$$\nabla f(x) = 0$$

to look for local minima.

# Local Minima in Finite Dimensions

We often use

$$\nabla f(x) = 0$$

to look for local minima. Why does this work?

# Local Minima in Finite Dimensions

We often use

$$\nabla f(x) = 0$$

to look for local minima. Why does this work?
Taylor expand $f$:

$$f(x_0 + \epsilon v) - f(x_0) = \epsilon \nabla f(x_0)[v] + \epsilon^2 \nabla^2 f(x_0)[v, v] + o(\epsilon^2) \geq 0$$

for any vector $v$.

# Local Minima in Finite Dimensions

We often use

$$\nabla f(x) = 0$$

to look for local minima. Why does this work?
Taylor expand $f$:

$$f(x_0 + \epsilon v) - f(x_0) = \epsilon \nabla f(x_0)[v] + \epsilon^2 \nabla^2 f(x_0)[v, v] + o(\epsilon^2) \geq 0$$

for any vector $v$. Then

$$\nabla f(x_0) = 0$$
$$\nabla^2 f(x_0) \geq 0$$

is sufficient. However, only $\nabla^2 f(x_0) \geq 0$ is necessary.

# Local Minima in Infinite Dimensions

Consider a functional

$$F[x] = \int_0^1 f(t, x(t), x'(t))\,\mathrm{d}t \qquad x \in C^2((0,1), \mathbb{R}^d)$$

For now, assume $f \in C^1$.

# Local Minima in Infinite Dimensions

Consider a functional

$$F[x] = \int_0^1 f(t, x(t), x'(t))\,\mathrm{d}t \qquad x \in C^2((0,1), \mathbb{R}^d)$$

For now, assume $f \in C^1$. Again, use a Taylor expansion:

$$F(x_0 + \epsilon\varphi) - F(x_0) = \int_0^1 f(t, x_0 + \epsilon\varphi, x_0' + \epsilon\varphi') - f(t, x_0, x_0')\,\mathrm{d}t$$

# Local Minima in Infinite Dimensions

Consider a functional

$$F[x] = \int_0^1 f(t, x(t), x'(t))\,\mathrm{d}t \qquad x \in C^2((0,1), \mathbb{R}^d)$$

For now, assume $f \in C^1$. Again, use a Taylor expansion:

$$\begin{aligned} F(x_0 + \epsilon\varphi) - F(x_0) &= \int_0^1 f(t, x_0 + \epsilon\varphi, x_0' + \epsilon\varphi') - f(t, x_0, x_0')\,\mathrm{d}t \\ &= \epsilon \int_0^1 f_x(t, x_0, x_0')\varphi + f_{x'}(t, x_0, x_0')\varphi'\,\mathrm{d}t + o(\epsilon) \end{aligned}$$

## Local Minima in Infinite Dimensions

Consider a functional

$$F[x] = \int_0^1 f(t, x(t), x'(t))\,\mathrm{d}t \qquad x \in C^2((0,1), \mathbb{R}^d)$$

For now, assume $f \in C^1$. Again, use a Taylor expansion:

$$\begin{aligned} F(x_0 + \epsilon\varphi) - F(x_0) &= \int_0^1 f(t, x_0 + \epsilon\varphi, x_0' + \epsilon\varphi') - f(t, x_0, x_0')\,\mathrm{d}t \\ &= \epsilon \int_0^1 f_x(t, x_0, x_0')\varphi + f_{x'}(t, x_0, x_0')\varphi'\,\mathrm{d}t + o(\epsilon) \\ &= \epsilon \int_0^1 \left(f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')'\right)\varphi\,\mathrm{d}t + o(\epsilon) \end{aligned}$$

# Local Minima in Infinite Dimensions

Consider a functional

$$F[x] = \int_0^1 f(t, x(t), x'(t))\,\mathrm{d}t \qquad x \in C^2((0,1), \mathbb{R}^d)$$

For now, assume $f \in C^1$. Again, use a Taylor expansion:

$$\begin{aligned} F(x_0 + \epsilon\varphi) - F(x_0) &= \int_0^1 f(t, x_0 + \epsilon\varphi, x_0' + \epsilon\varphi') - f(t, x_0, x_0')\,\mathrm{d}t \\ &= \epsilon \int_0^1 f_x(t, x_0, x_0')\varphi + f_{x'}(t, x_0, x_0')\varphi'\,\mathrm{d}t + o(\epsilon) \\ &= \epsilon \int_0^1 \left(f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')'\right)\varphi\,\mathrm{d}t + o(\epsilon) \end{aligned}$$

We want this to be positive for all $\varphi \in C_c^\infty(0,1)$ and small $\epsilon$.

# Local Minima in Infinite Dimensions

If we want

$$\int_0^1 \left(f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')'\right) \varphi \,\mathrm{d}t = 0 \qquad \forall \varphi \in C_c^\infty(0,1)$$

we must have

$$\frac{\delta F}{\delta x} := f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')' = 0 \qquad \forall t \in [0,1]$$

# Local Minima in Infinite Dimensions

If we want

$$\int_0^1 \left( f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')' \right) \varphi \, \mathrm{d}t = 0 \qquad \forall \varphi \in C_c^\infty(0,1)$$

we must have

$$\frac{\delta F}{\delta x} := f_x(t, x_0, x_0') - f_{x'}(t, x_0, x_0')' = 0 \qquad \forall t \in [0,1]$$

This is known as the **Euler-Lagrange** equation. It is a second order differential equation to be solved for $x_0(t)$, provided we specify initial/boundary conditions.

# Table of Contents

# Arc Length

Consider two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$.
What is the shortest path connecting them?

# Arc Length

Consider two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$.
What is the shortest path connecting them?
The arc length of a path $\mathbf{r}(t)$ is

$$L[\mathbf{r}] = \int_0^1 \left|\mathbf{r}'(t)\right|_2 \,\mathrm{d}t$$

# Arc Length

Consider two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$.
What is the shortest path connecting them?
The arc length of a path $\mathbf{r}(t)$ is

$$L[\mathbf{r}] = \int_0^1 \left|\mathbf{r}'(t)\right|_2 \, \mathrm{d}t$$

so

$$\frac{\delta L}{\delta \mathbf{r}} = 0 - \frac{d}{dt} \frac{\mathbf{r}'(t)}{|\mathbf{r}'(t)|_2}$$

# Arc Length

Consider two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$.
What is the shortest path connecting them?
The arc length of a path $\mathbf{r}(t)$ is

$$L[\mathbf{r}] = \int_0^1 \left|\mathbf{r}'(t)\right|_2 \,\mathrm{d}t$$

so

$$\frac{\delta L}{\delta \mathbf{r}} = 0 - \frac{d}{dt}\frac{\mathbf{r}'(t)}{|\mathbf{r}'(t)|_2} = -\frac{\mathbf{r}''(t)\,|\mathbf{r}'(t)|_2 - \mathbf{r}'(t)\frac{\mathbf{r}'(t)}{|\mathbf{r}'(\mathbf{t})|_2}\cdot \mathbf{r}''(t)}{|\mathbf{r}'(t)|_2^2}$$

$$= \left(\mathbf{r}'(t) \otimes \mathbf{r}'(t) - \left|\mathbf{r}'(t)\right|_2^2 I\right) \frac{\mathbf{r}''(t)}{|\mathbf{r}'(t)|_2^3}$$

# Arc Length

When $d > 1$

$$\mathbf{r}'(t) \otimes \mathbf{r}'(t) - \left|\mathbf{r}'(t)\right|_2^2 I \neq 0$$

Hence we solve

$$\mathbf{r}''(t) = 0 \qquad \mathbf{r}(0) = \mathbf{a}, \quad \mathbf{r}(1) = \mathbf{b}$$

# Arc Length

When $d > 1$

$$\mathbf{r}'(t) \otimes \mathbf{r}'(t) - \left|\mathbf{r}'(t)\right|_2^2 I \neq 0$$

Hence we solve

$$\mathbf{r}''(t) = 0 \qquad \mathbf{r}(0) = \mathbf{a}, \quad \mathbf{r}(1) = \mathbf{b}$$

This gives

$$\mathbf{r}(t) = (\mathbf{b} - \mathbf{a})t + \mathbf{a}$$

## Projectiles

The action of a particle of mass $m$ travelling along a path $\mathbf{r}(t)$, under the influence of gravity, is

$$S[\mathbf{r}] = \int_0^1 \frac{m}{2} \left|\mathbf{r}'(t)\right|_2^2 + m\mathbf{g} \cdot \mathbf{r}(t) \, \mathrm{d}t \qquad \mathbf{g} = (0, -g)$$

# Projectiles

The action of a particle of mass $m$ travelling along a path $\mathbf{r}(t)$, under the influence of gravity, is

$$S[\mathbf{r}] = \int_0^1 \frac{m}{2} \left|\mathbf{r}'(t)\right|_2^2 + m\mathbf{g} \cdot \mathbf{r}(t)\,\mathrm{d}t \qquad \mathbf{g} = (0, -g)$$

so

$$\frac{\delta S}{\delta \mathbf{r}} = m\mathbf{g} - \frac{d}{dt} m\mathbf{r}'(t)$$

# Projectiles

The action of a particle of mass $m$ travelling along a path $\mathbf{r}(t)$, under the influence of gravity, is

$$S[\mathbf{r}] = \int_0^1 \frac{m}{2} \left|\mathbf{r}'(t)\right|_2^2 + m\mathbf{g} \cdot \mathbf{r}(t)\,\mathrm{d}t \qquad \mathbf{g} = (0, -g)$$

so

$$\frac{\delta S}{\delta \mathbf{r}} = m\mathbf{g} - \frac{d}{dt} m\mathbf{r}'(t) = -m(\mathbf{r}''(t) - \mathbf{g})$$

# Projectiles

The action of a particle of mass $m$ travelling along a path $\mathbf{r}(t)$, under the influence of gravity, is

$$S[\mathbf{r}] = \int_0^1 \frac{m}{2} \left|\mathbf{r}'(t)\right|_2^2 + m\mathbf{g} \cdot \mathbf{r}(t) \, \mathrm{d}t \qquad \mathbf{g} = (0, -g)$$

so

$$\frac{\delta S}{\delta \mathbf{r}} = m\mathbf{g} - \frac{d}{dt} m\mathbf{r}'(t) = -m(\mathbf{r}''(t) - \mathbf{g})$$

If we launch a particle from a cannon at the origin and it lands at $(1, 0)$. The trajectory must solve

$$\mathbf{r}''(t) = \mathbf{g} \qquad \mathbf{r}(0) = (0, 0), \quad \mathbf{r}(1) = (1, 0)$$

# Brachistochrone

Consider a smooth light ball travelling along a path $\mathbf{r}(t)$ from the origin to $(+1, -1)$.

# Brachistochrone

Consider a smooth light ball travelling along a path $\mathbf{r}(t)$ from the origin to $(+1, -1)$.
The time taken for the ball to reach its destination is

$$T[\mathbf{r}] = \int_0^1 \frac{|\mathbf{r}'(t)|_2}{\sqrt{2\mathbf{g}\cdot\mathbf{r}(t)}}\,\mathrm{d}t = \int_0^{-1} \frac{\sqrt{1+y'(x)^2}}{\sqrt{-2gy(x)}}\,\mathrm{d}x$$

# Brachistochrone

Consider a smooth light ball travelling along a path $\mathbf{r}(t)$ from the origin to $(+1, -1)$.
The time taken for the ball to reach its destination is

$$T[\mathbf{r}] = \int_0^1 \frac{|\mathbf{r}'(t)|_2}{\sqrt{2\mathbf{g}\cdot\mathbf{r}(t)}}\,\mathrm{d}t = \int_0^{-1} \frac{\sqrt{1+y'(x)^2}}{\sqrt{-2gy(x)}}\,\mathrm{d}x$$

so

$$\frac{\delta T}{\delta \mathbf{r}} = \frac{\sqrt{1+y'(x)^2}}{\sqrt{8g(-y(x))^3}} - \frac{d}{dx}\frac{y'(x)}{\sqrt{1+y'(x)^2}\sqrt{-2gy(x)}}$$

# Brachistochrone

Consider a smooth light ball travelling along a path $\mathbf{r}(t)$ from the origin to $(+1, -1)$.
The time taken for the ball to reach its destination is

$$T[\mathbf{r}] = \int_0^1 \frac{|\mathbf{r}'(t)|_2}{\sqrt{2\mathbf{g}\cdot\mathbf{r}(t)}}\,\mathrm{d}t = \int_0^{-1} \frac{\sqrt{1+y'(x)^2}}{\sqrt{-2gy(x)}}\,\mathrm{d}x$$

so

$$\begin{aligned}\frac{\delta T}{\delta \mathbf{r}} &= \frac{\sqrt{1+y'(x)^2}}{\sqrt{8g(-y(x))^3}} - \frac{d}{dx}\frac{y'(x)}{\sqrt{1+y'(x)^2}\sqrt{-2gy(x)}} \\ &= \frac{1+y'(x)^2+2y(x)y''(x)}{\sqrt{-8gy(x)^3(1+y'(x))^3}}\end{aligned}$$

# Brachistochrone

Thus we need to solve

$$1 + y'(x)^2 + 2y(x)y''(x) = 0 \qquad y(0) = 0, \quad y(1) = -1$$

# Brachistochrone

Thus we need to solve

$$1 + y'(x)^2 + 2y(x)y''(x) = 0 \qquad y(0) = 0, \quad y(1) = -1$$

The solution to this is an example of a **cycloid** and can be written as

$$x(\omega\theta) = \alpha(\theta - \sin(\theta))$$
$$y(\omega\theta) = \alpha(1 - \cos(\theta))$$

for an appropriate choice of $\alpha > 0$ and $\omega$.

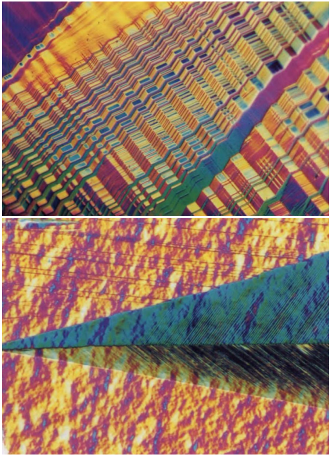
# Elasticity & SME

Deformations of materials $\Omega$ are often investigated by studying functionals:

$$E[u] = \int_{\Omega} \varphi(\nabla u, \theta) \, \mathrm{d}V$$

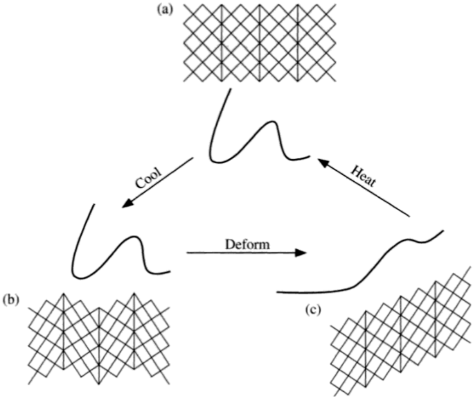
where

- $E$ is the total energy of the material.
- $\varphi$ is the stored energy density.
- $u$ is an admissible deformation.
- $\theta$ is the temperature.



# Shape Memory Effect

Changing the temperature changes the functional and thus changes the minimisers (what we observe).



# Table of Contents

# Dirichlet Energy Functional

The Dirichlet energy functional $\mathbb{D}(u)$ can be used to describe the strain energy density under a deformation $u$.

$$\mathbb{D}(u) = \int_B |\nabla u|_F^2 \, \mathrm{d}x \qquad u \in u_0 + W_0^{1,2}(B;\mathbb{R}^2)$$

with $B$ the unit ball and $u_0$ is the **double-covering map** [1].

# Dirichlet Energy Functional

The Dirichlet energy functional $\mathbb{D}(u)$ can be used to describe the strain energy density under a deformation $u$.

$$\mathbb{D}(u) = \int_B |\nabla u|_F^2 \, \mathrm{d}x \qquad u \in u_0 + W_0^{1,2}(B; \mathbb{R}^2)$$

with $B$ the unit ball and $u_0$ is the **double-covering map** [1].

In showing that $u_0$ is a stationary point of this functional, we introduce an 'excess' functional $E$:

$$\mathbb{D}(u) = \mathbb{D}(u_0) + E(u - u_0)$$

# Dirichlet Energy Functional

The Dirichlet energy functional $\mathbb{D}(u)$ can be used to describe the strain energy density under a deformation $u$.

$$\mathbb{D}(u) = \int_B |\nabla u|_F^2 \, \mathrm{d}x \qquad u \in u_0 + W_0^{1,2}(B; \mathbb{R}^2)$$

with $B$ the unit ball and $u_0$ is the **double-covering map** [1].

In showing that $u_0$ is a stationary point of this functional, we introduce an 'excess' functional $E$:

$$\mathbb{D}(u) = \mathbb{D}(u_0) + E(u - u_0)$$

where, in particular, we have

$$E(u) = E_f(u) := \int_B |\nabla u|_F^2 + f(x) \det \nabla u \, \mathrm{d}x$$

with $f(u) = 3 \log |x|_2$ (often called a 'pressure' function) [1].

# A 1D Family of Polyconvex Functions

The functional

$$E_f(u) = \int_B |\nabla u|_F^2 + f(x) \det \nabla u \,\mathrm{d}x \qquad u \in W_0^{1,2}(B; \mathbb{R}^2)$$

is **polyconvex** for any choice of $f \in \mathrm{Lip}(B)$.

# A 1D Family of Polyconvex Functions

The functional

$$E_f(u) = \int_B |\nabla u|_F^2 + f(x) \det \nabla u \, \mathrm{d}x \qquad u \in W_0^{1,2}(B; \mathbb{R}^2)$$

is **polyconvex** for any choice of $f \in \mathrm{Lip}(B)$.

We will focus on the case of $f(x) = \lambda |x|_2$ for a parameter $\lambda \in \mathbb{R}^+$ and denote $E_\lambda := E_f$.

# A 1D Family of Polyconvex Functions

The functional

$$E_f(u) = \int_B |\nabla u|_F^2 + f(x) \det \nabla u \, \mathrm{d}x \qquad u \in W_0^{1,2}(B; \mathbb{R}^2)$$

is **polyconvex** for any choice of $f \in \mathrm{Lip}(B)$.

We will focus on the case of $f(x) = \lambda |x|_2$ for a parameter $\lambda \in \mathbb{R}^+$ and denote $E_\lambda := E_f$.

We observe that:

- $E_\lambda(0) = 0$.
- $E_\lambda$ is either unbounded below or bounded below by zero.

# A 1D Family of Polyconvex Functions

The functional

$$E_f(u) = \int_B |\nabla u|_F^2 + f(x) \det \nabla u \, \mathrm{d}x \qquad u \in W_0^{1,2}(B; \mathbb{R}^2)$$

is **polyconvex** for any choice of $f \in \mathrm{Lip}(B)$.

We will focus on the case of $f(x) = \lambda |x|_2$ for a parameter $\lambda \in \mathbb{R}^+$ and denote $E_\lambda := E_f$.

We observe that:

- $E_\lambda(0) = 0$.
- $E_\lambda$ is either unbounded below or bounded below by zero.

Hence $E_\lambda$ has a global minimum iff $E_\lambda \geq 0$.

# Pointwise Hadamard

We can use of the following theorem

## Hadamard's Inequality [3]

For any matrix $A \in \mathbb{R}^{2\times 2}$, we have $|A|_F^2 \geq 2\,|\det A|$.

# Pointwise Hadamard

We can use of the following theorem

**Hadamard's Inequality [3]**

For any matrix $A \in \mathbb{R}^{2\times 2}$, we have $|A|_F^2 \geq 2\,|\det A|$.

to show

$$\begin{aligned} E_\lambda(u) &\geq \int_B |\nabla u(x)|_F^2 - \frac{\lambda}{2}\,|x|_2\,|\nabla u(x)|_F^2 \,\mathrm{d}x \\ &= \int_B \left(1 - \frac{\lambda}{2}\,|x|_2\right) |\nabla u(x)|_F^2 \,\mathrm{d}x \geq 0 \end{aligned}$$

for $\lambda \leq 2$.

# Pointwise Hadamard

We can use of the following theorem

**Hadamard's Inequality [3]**

For any matrix $A \in \mathbb{R}^{2\times 2}$, we have $|A|_F^2 \geq 2\,|\det A|$.

to show

$$\begin{aligned} E_\lambda(u) &\geq \int_B |\nabla u(x)|_F^2 - \frac{\lambda}{2}\,|x|_2\,|\nabla u(x)|_F^2 \,\mathrm{d}x \\ &= \int_B \left(1 - \frac{\lambda}{2}\,|x|_2\right)|\nabla u(x)|_F^2 \,\mathrm{d}x \geq 0 \end{aligned}$$

for $\lambda \leq 2$. Can we do better?

# Fourier Series & Poincaré Inequality

Consider a Fourier expansion of $u$ as

$$u = \sum_{j\geq 0} u^{(j)} = \frac{1}{2}\mathbf{A}_0(r) + \sum_{j>0} \mathbf{A}_j(r)\cos(j\theta) + \mathbf{B}_j(r)\sin(j\theta)$$

with $\mathbf{A}_j(1) = \mathbf{B}_j(1) = 0$ for each $j \geq 0$ [1].

# Fourier Series & Poincaré Inequality

Consider a Fourier expansion of $u$ as

$$u = \sum_{j \geq 0} u^{(j)} = \frac{1}{2}\mathbf{A}_0(r) + \sum_{j>0} \mathbf{A}_j(r)\cos(j\theta) + \mathbf{B}_j(r)\sin(j\theta)$$

with $\mathbf{A}_j(1) = \mathbf{B}_j(1) = 0$ for each $j \geq 0$ [1].

Then we make use of a Poincaré inequality for the Fourier modes:

## Poincaré Inequality for Fourier Modes

Let $j \geq 1$. Then

$$\int_B \left| u^{(j)} \right|_2^2 \mathrm{d}x \leq \frac{1}{j_0^2} \int_B \left| u_{,r}^{(j)} \right|_2^2 \mathrm{d}x$$

where $j_0$ is the first zero of a Bessel function.

# Applying the Inequality

Applying this inequality, we find

$$\begin{aligned} E_\lambda(u) &= \sum_{j\geq 0} \int_B \left| u_{,r}^{(j)} \right|_2^2 + \left| u_{,\tau}^{(j)} \right|_2^2 + \frac{\lambda}{2} \left\langle u^{(j)}, J u_{,\tau}^{(j)} \right\rangle_2 \, \mathrm{d}x \\ &\geq \sum_{j\geq 0} \int_B j_0^2 \left| u^{(j)} \right|_2^2 + \left| u_{,\tau}^{(j)} \right|_2^2 - \frac{\lambda}{2} \left| u^{(j)} \right|_2 \left| u_{,\tau}^{(j)} \right|_2 \, \mathrm{d}x \end{aligned}$$

# Applying the Inequality

Applying this inequality, we find

$$
\begin{aligned}
E_\lambda(u) &= \sum_{j\geq 0} \int_B \left| u_{,r}^{(j)} \right|_2^2 + \left| u_{,\tau}^{(j)} \right|_2^2 + \frac{\lambda}{2} \left\langle u^{(j)}, J u_{,\tau}^{(j)} \right\rangle_2 \, \mathrm{d}x \\
&\geq \sum_{j\geq 0} \int_B j_0^2 \left| u^{(j)} \right|_2^2 + \left| u_{,\tau}^{(j)} \right|_2^2 - \frac{\lambda}{2} \left| u^{(j)} \right|_2 \left| u_{,\tau}^{(j)} \right|_2 \, \mathrm{d}x \\
&= \sum_{j\geq 0} \int_B \mathbf{U}_j^\mathsf{T} M_\lambda \mathbf{U}_j \, \mathrm{d}x \qquad \mathbf{U}_j = \begin{pmatrix} \left| u^{(j)} \right|_2 \\ \left| u_{,\tau}^{(j)} \right|_2 \end{pmatrix} \quad M_\lambda = \begin{pmatrix} j_0^2 & -\frac{\lambda}{4} \\ -\frac{\lambda}{4} & 1 \end{pmatrix}
\end{aligned}
$$

# Applying the Inequality

Applying this inequality, we find

$$
\begin{aligned}
E_\lambda(u) &= \sum_{j\geq 0} \int_B \left|u_{,r}^{(j)}\right|_2^2 + \left|u_{,\tau}^{(j)}\right|_2^2 + \frac{\lambda}{2}\left\langle u^{(j)}, Ju_{,\tau}^{(j)}\right\rangle_2 \,\mathrm{d}x \\
&\geq \sum_{j\geq 0} \int_B j_0^2 \left|u^{(j)}\right|_2^2 + \left|u_{,\tau}^{(j)}\right|_2^2 - \frac{\lambda}{2}\left|u^{(j)}\right|_2 \left|u_{,\tau}^{(j)}\right|_2 \,\mathrm{d}x \\
&= \sum_{j\geq 0} \int_B \mathbf{U}_j^\mathsf{T} M_\lambda \mathbf{U}_j \,\mathrm{d}x \qquad \mathbf{U}_j = \begin{pmatrix} \left|u^{(j)}\right|_2 \\ \left|u_{,\tau}^{(j)}\right|_2 \end{pmatrix} \quad M_\lambda = \begin{pmatrix} j_0^2 & -\frac{\lambda}{4} \\ -\frac{\lambda}{4} & 1 \end{pmatrix}
\end{aligned}
$$

Then we have that $\lambda \leq 4 j_0 \Rightarrow M_\lambda \geq 0 \Rightarrow E_\lambda \geq 0$.

# Applying the Inequality

Applying this inequality, we find

$$\begin{aligned} E_\lambda(u) &= \sum_{j\geq 0} \int_B \left|u^{(j)}_{,r}\right|_2^2 + \left|u^{(j)}_{,\tau}\right|_2^2 + \frac{\lambda}{2}\left\langle u^{(j)}, Ju^{(j)}_{,\tau}\right\rangle_2 \,\mathrm{d}x \\ &\geq \sum_{j\geq 0} \int_B j_0^2 \left|u^{(j)}\right|_2^2 + \left|u^{(j)}_{,\tau}\right|_2^2 - \frac{\lambda}{2}\left|u^{(j)}\right|_2 \left|u^{(j)}_{,\tau}\right|_2 \,\mathrm{d}x \\ &= \sum_{j\geq 0} \int_B \mathbf{U}_j^{\mathsf{T}} M_\lambda \mathbf{U}_j \,\mathrm{d}x \qquad \mathbf{U}_j = \begin{pmatrix} \left|u^{(j)}\right|_2 \\ \left|u^{(j)}_{,\tau}\right|_2 \end{pmatrix} \quad M_\lambda = \begin{pmatrix} j_0^2 & -\frac{\lambda}{4} \\ -\frac{\lambda}{4} & 1 \end{pmatrix} \end{aligned}$$

Then we have that $\lambda \leq 4j_0 \Rightarrow M_\lambda \geq 0 \Rightarrow E_\lambda \geq 0$.

Here $4j_0 \approx 9.619$ is a significant improvement on the previous bound of $\lambda \leq 2$.

# The Approach

We shall first construct a solution $u^* \in W_0^{1,2}$ to

$$\nabla u^*(x) \in \mathrm{O}(2) \qquad \text{a.e. } x \in Q := [-2, +2]^2$$

# The Approach

We shall first construct a solution $u^* \in W_0^{1,2}$ to

$$\nabla u^*(x) \in \mathrm{O}(2) \qquad \text{a.e. } x \in Q := [-2, +2]^2$$

We will then shift/scale this solution on part of the ball to construct a map $u$.

# The Approach

We shall first construct a solution $u^* \in W_0^{1,2}$ to

$$\nabla u^*(x) \in \mathrm{O}(2) \qquad \text{a.e. } x \in Q := [-2, +2]^2$$

We will then shift/scale this solution on part of the ball to construct a map $u$.

On the remainder of the ball (which we shall denote by $K$), we will take $u = 0$.

# The Approach

We shall first construct a solution $u^* \in W_0^{1,2}$ to

$$\nabla u^*(x) \in \mathrm{O}(2) \qquad \text{a.e. } x \in Q := [-2,+2]^2$$

We will then shift/scale this solution on part of the ball to construct a map $u$.

On the remainder of the ball (which we shall denote by $K$), we will take $u = 0$.

A necessary condition can then be derived:

$$\lambda \leq \frac{2(\pi - |K|)}{|\mathcal{I}_0|}$$

# Partial Differential Inclusions

The PDI

$$\nabla u \in \mathrm{O}(2)$$

is an example of the **probelm of potential wells**:

**The Problem of Potential Wells [2, 4, 5]**

$$\nabla u \in \bigcup_i \mathrm{SO}(d) A_i \qquad A_i \in \mathbb{R}^{d \times d}$$

# Partial Differential Inclusions

The PDI

$$\nabla u \in O(2)$$

is an example of the **probelm of potential wells**:

**The Problem of Potential Wells [2, 4, 5]**

$$\nabla u \in \bigcup_i SO(d)A_i \qquad A_i \in \mathbb{R}^{d\times d}$$

The following is known for this PDI:

**Theorem (Dacorogna and Marcellini) [3]**

There exists a dense set of solutions in $W^{1,\infty}(Q;\mathbb{R}^2)$.

**Theorem (Liouville) [4]**

All solutions are piecewise affine.

# Constructed Solution

A solution has been constructed for the 3D equivalent of this PDI [2].

# Constructed Solution

A solution has been constructed for the 3D equivalent of this PDI [2]. We can adapt this for our needs.

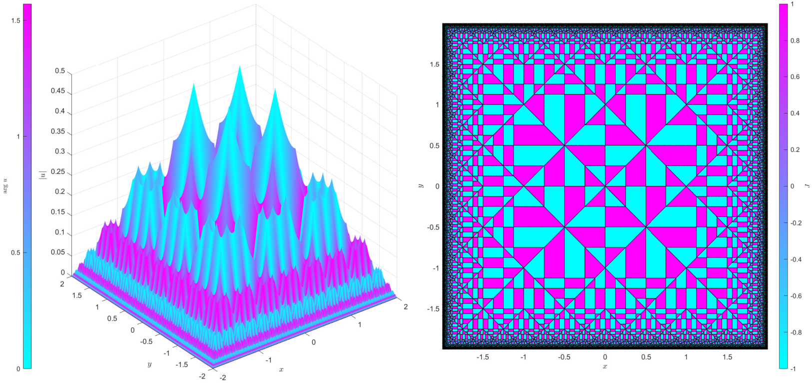



Figure: Constructed solution $u^*$ and its Jacobian $\det \nabla u^*$

# Tiling the Solution

We can then tile the ball with this solution.

# Tiling the Solution

We can then tile the ball with this solution.

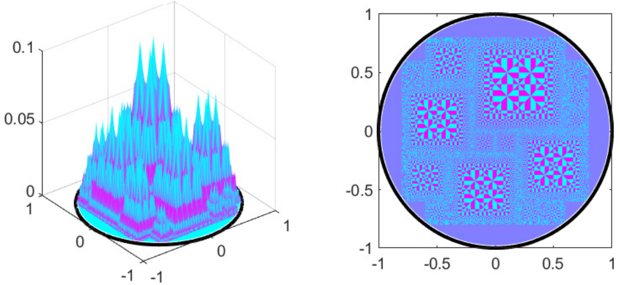



Figure: Tiled Solution with 15 Squares

# Numerical Results

We will make use of a simple tiling of 2 squares with

$$c_1 = \begin{pmatrix} +0.1 \\ +0.3 \end{pmatrix} \quad w_1 = 1.0 \qquad c_2 = \begin{pmatrix} -0.3 \\ -0.5 \end{pmatrix} \quad w_1 = 0.6$$

# Numerical Results

We will make use of a simple tiling of 2 squares with

$$c_1 = \begin{pmatrix} +0.1 \\ +0.3 \end{pmatrix} \quad w_1 = 1.0 \qquad c_2 = \begin{pmatrix} -0.3 \\ -0.5 \end{pmatrix} \quad w_1 = 0.6$$

We then find that

$$|K| = \pi - 1.36 \approx 1.78159$$
$$|\mathcal{I}_0| = 1.83384 \times 10^{-2} \pm 2 \times 7.62939 \times 10^{-6}$$

# Numerical Results

We will make use of a simple tiling of 2 squares with

$$c_1 = \begin{pmatrix} +0.1 \\ +0.3 \end{pmatrix} \quad w_1 = 1.0 \qquad c_2 = \begin{pmatrix} -0.3 \\ -0.5 \end{pmatrix} \quad w_1 = 0.6$$

We then find that

$$|K| = \pi - 1.36 \approx 1.78159$$
$$|\mathcal{I}_0| = 1.83384 \times 10^{-2} \pm 2 \times 7.62939 \times 10^{-6}$$

where the integral was approximated by calculating symbolically on the region $|x|_\infty \leq \sum_{k=0}^{21} \frac{1}{2^k}$ and bounding on the remaining square annulus.

# Numerical Results

We will make use of a simple tiling of 2 squares with

$$c_1 = \begin{pmatrix} +0.1 \\ +0.3 \end{pmatrix} \quad w_1 = 1.0 \qquad c_2 = \begin{pmatrix} -0.3 \\ -0.5 \end{pmatrix} \quad w_1 = 0.6$$

We then find that

$$|K| = \pi - 1.36 \approx 1.78159$$
$$|\mathcal{I}_0| = 1.83384 \times 10^{-2} \pm 2 \times 7.62939 \times 10^{-6}$$

where the integral was approximated by calculating symbolically on the region $|x|_\infty \leq \sum_{k=0}^{21} \frac{1}{2^k}$ and bounding on the remaining square annulus.

This leads to a bound of $\lambda \leq 148.446$.

# Summary

To summarise we have found that:

# Summary

To summarise we have found that:

- $\lambda \leq 9.619$ is sufficient for $E_\lambda \geq 0$.

# Summary

To summarise we have found that:

- $\lambda \leq 9.619$ is sufficient for $E_\lambda \geq 0$.
- $\lambda \leq 148.446$ is necessary for $E_\lambda \geq 0$.

# Summary

To summarise we have found that:

- $\lambda \leq 9.619$ is sufficient for $E_\lambda \geq 0$.
- $\lambda \leq 148.446$ is necessary for $E_\lambda \geq 0$.

With further optimisations, we could try to refine these bounds.

# Summary

To summarise we have found that:

- $\lambda \leq 9.619$ is sufficient for $E_\lambda \geq 0$.
- $\lambda \leq 148.446$ is necessary for $E_\lambda \geq 0$.

With further optimisations, we could try to refine these bounds.

We could try to find $\lambda_{\text{crit}}$ such that $E_\lambda \geq 0$ iff $\lambda \leq \lambda_{\text{crit}}$.

# References I


- Jonathan Bevan, *On double-covering stationary points of a constrained Dirichlet energy*, Annales de l'Institut Henri Poincaré C, Analyse non linéaire **31** (2014), no. 2, 391–411, doi.
- Arrigo Cellina and Stefania Perrotta, *On a problem of potential wells*, J. Convex Anal **2** (1995), no. 1-2, 103–115.
- Bernard Dacorogna and Paolo Marcellini, *Implicit partial differential equations*, Progress in Nonlinear Partial Differential Equations and Their Applications, no. v. 37, Birkhäuser, Boston, 1999.
- Stefan Müller, *Variational models for microstructure and phase transitions*, vol. 1713, pp. 85–210, Springer Berlin Heidelberg, Berlin, Heidelberg, 1999, doi.

# References II


Vladimír Šverák, *On the Problem of Two Wells*, Microstructure and Phase Transition (Avner Friedman, Willard Miller, David Kinderlehrer, Richard James, Mitchell Luskin, and Jerry L. Ericksen, eds.), vol. 54, Springer New York, New York, NY, 1993, pp. 183–189, doi.