C477: Mathematical Introduction to Optimisation

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Outline

- **Topics**
  - Global vs local optimisation
  - Neighbourhoods & Other properties of sets
    - Boundary vs interior points; Closed vs open sets; Compact sets
  - Weierstrass Theorem or *How to assert the existence of an optimum*
  - Min vs Argmin
  - Minimisation vs maximisation
  - Defining types of optimisation problems
  - Formulating a nonlinear optimisation problem
- **Example**
  - Enclosing points
- **Reading**
  - Chap. 6.1 (Introduction), 19.1 (Introduction), & 4.4 (Neighbourhoods) in *An Introduction to Optimization*, Chong & Żak, Third Edition.
- **Acknowledgements**
  - Parts of these slides were originally developed by Benoit Chachuat and Panos Parpas. LaTeX design and proof reading by Miten Mistry. Mistakes by Ruth Misener.

Refresh: Definition: Mathematical Optimisation

Optimisation models (a.k.a. mathematical programs) represent problem choices as decision variables and seek values that minimise (or maximise) objective functions of the decision variables subject to constraints on variable values expressing the limits on possible decision choices

$$
\begin{aligned}
&\min_{\boldsymbol{x}} \; f(\boldsymbol{x}) && \longleftarrow \quad \text{Objective function} \\
&\text{s.t.} \quad \mathbf{h}(\boldsymbol{x}) = \mathbf{0} && \longleftarrow \quad \text{Equality constraints} \\
&\qquad \mathbf{g}(\boldsymbol{x}) \leq \mathbf{0} && \longleftarrow \quad \text{Inequality constraints} \\
&\qquad \boldsymbol{x} \in \left[\boldsymbol{x}^{\mathrm{L}}, \boldsymbol{x}^{\mathrm{U}}\right] = X \subset \mathbb{R}^n && \longleftarrow \quad \text{Variable bounds} \\
&\qquad \boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^m, \; \boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^p &&
\end{aligned}
$$

- **Analytic expressions** of the objective and constraint functions **may or may not be available**
- If we want to **find the absolute best set of admissible decisions**: **Global optimisation**

Defining (Global) Optimality

Feasible Set

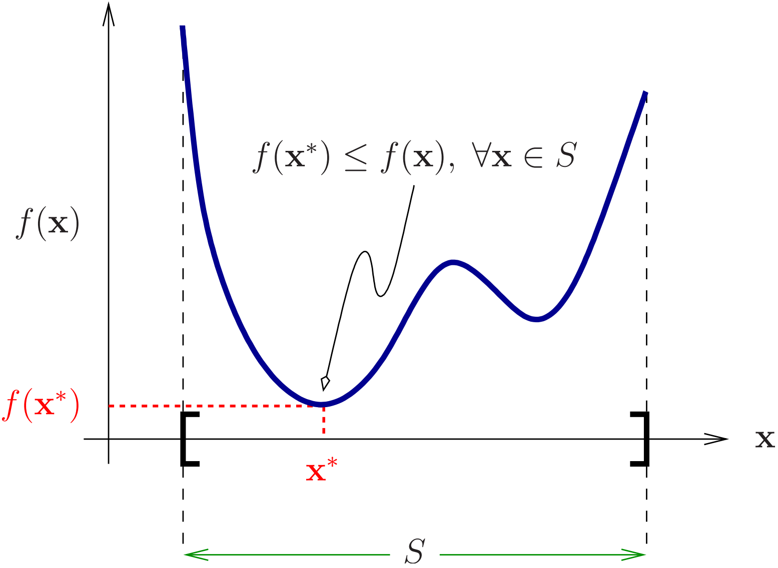
The feasible set S (or feasible region) of an optimisation model is the collection of choices for decision variables satisfying all of the model constraints: $S \triangleq \{\boldsymbol{x} \mid \mathbf{h}(\boldsymbol{x}) = \mathbf{0},\ \mathbf{g}(\boldsymbol{x}) \le \mathbf{0},\ \boldsymbol{x}^{\mathrm{L}} \le \boldsymbol{x} \le \boldsymbol{x}^{\mathrm{U}}\}$

(Global) Optimum

An optimal solution, $\boldsymbol{x}^*$, is a feasible choice for decision variables with objective function value superior to any other feasible point. For a minimisation problem: $f(\boldsymbol{x}^*) \le f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in S$

1. The optimal value f^* in an optimisation model is the objective function value of any optimal solutions: $f^* = f(\boldsymbol{x}^*)$ — It is unique!
2. But, an optimisation model may have:
   - a unique optimal solution
   - several alternative optimal solutions
   - no optimal solutions (unbounded or infeasible models)

Illustration of a (Global) Minimum, x^*



Defining Local Optimality

Neighbourhood

The neighbourhood $N_\delta(\boldsymbol{x})$ of a point $\boldsymbol{x}$ consists of all nearby points; that is, all points within a small distance $\delta > 0$ of $\boldsymbol{x}$:

$$N_\delta(\boldsymbol{x}) \triangleq \{\boldsymbol{y} \mid \|\boldsymbol{y} - \boldsymbol{x}\|_2 < \delta\}$$

Local Optimum

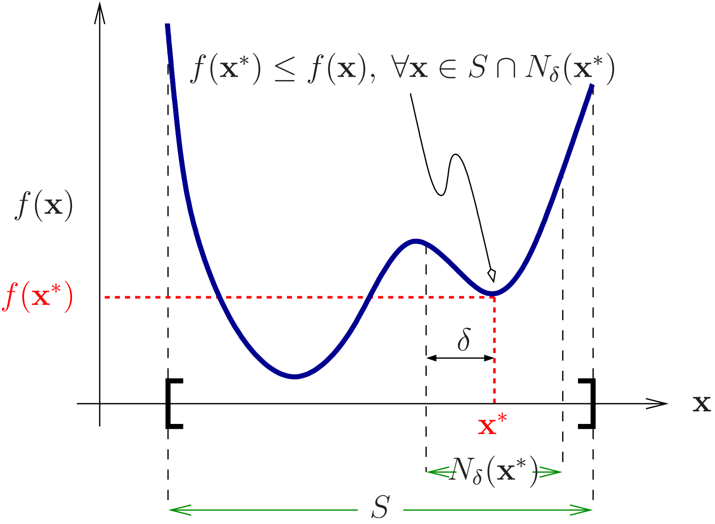
A point $\boldsymbol{x}^*$ is a local optimum for the function $f : \mathbb{R}^n \to \mathbb{R}$ on the set S if it is feasible ($\boldsymbol{x}^* \in S$) and if sufficiently small neighbourhoods surrounding it contain no points that are both feasible and superior in objective value:

$$\exists \delta > 0 : \quad f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in S \cap N_\delta(\boldsymbol{x}^*)$$

Remarks:

1. Global optima are always local optima
2. Local optima may not be global optima

Illustration of a Local Minimum, x^*

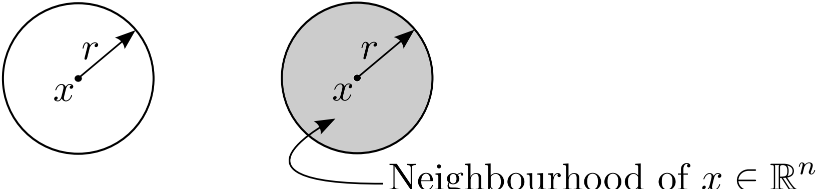


What is a neighbourhood $N_\delta(\boldsymbol{x}^*)$? Backing up for definitions ...

A neighbourhood of a point $\boldsymbol{x} \in \mathbb{R}^n$

Neighbourhood

A **neighbourhood** of a point $\boldsymbol{x} \in \mathbb{R}^n$ is the set, $\{\boldsymbol{y} \mid \|\boldsymbol{x} - \boldsymbol{y}\|_2 < r\}$, for some $r > 0$.



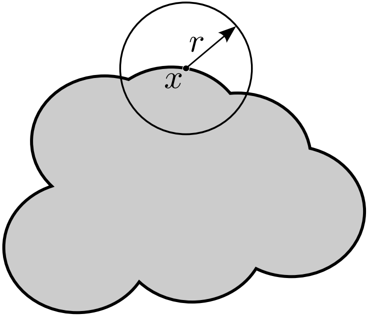
Formal definition

A **neighbourhood** of p in metric space X is a set $N_r(p)$ consisting of all q such that $d(p, q) < r$ for distance metric d and some $r > 0$. The number r is called the **radius** of $N_r(p)$.

Boundary points

Boundary point

A point x is called a **boundary point** if **every** neighbourhood of x contains a point in the set and a point outside the set.



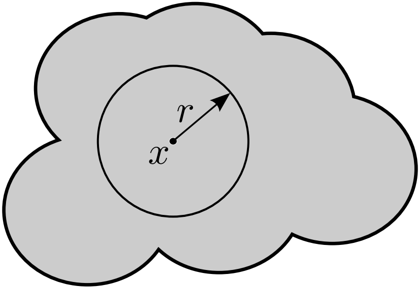
Sanity Check

Give an example of a boundary point?

Interior points

Interior point

A point x is called an **interior point** if all points within **some** neighbourhood of x are contained in the set.



Sanity Check

Give an example of an interior point?

Interior points

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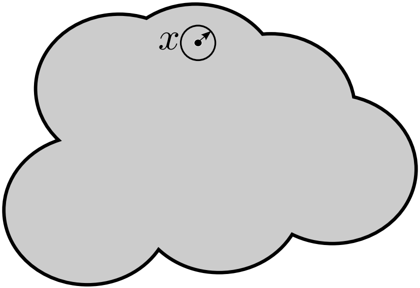


Sanity Check

Give an example of an interior point?

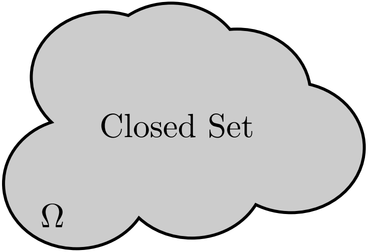
Closed/Open Sets

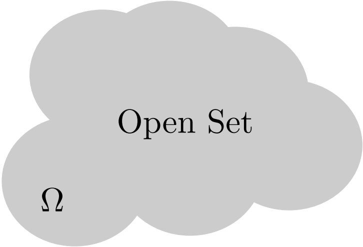
Closed set

A set is **closed** if it contains its boundary.

Open set

A set is **open** if it contains no boundary points.





Sanity Check

Examples of closed and open sets?

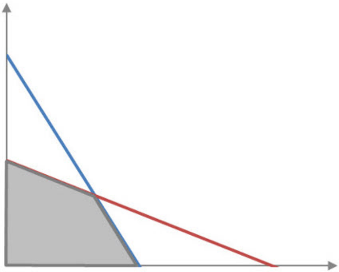
Bounded & Compact Sets

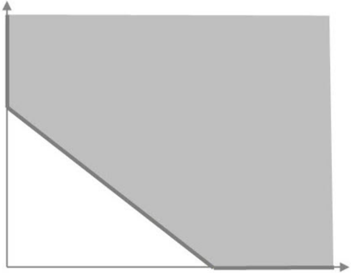
Bounded Set

A set that is contained in a ball of finite radius is **bounded**.

Compact set

A **compact** set is both **closed** and **bounded**.





Sanity Check

Which set is bounded?

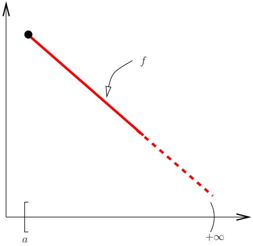
Asserting Existence of Optima

How do we know an optimal solution exists?

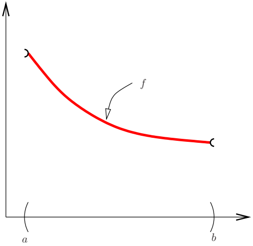
Weierstrass Theorem

Let $S \subset \mathbb{R}^n$ be a nonempty, compact set, and let $f : S \to \mathbb{R}$ be continuous on S. Then, the problems $\min / \max_{\boldsymbol{x} \in S} f(\boldsymbol{x})$ attain their optimal values; that is, there exist optimal solution points for either problems.

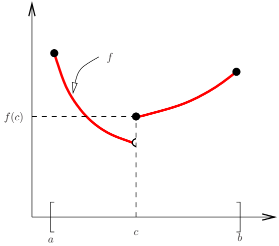
Why boundedness of S?



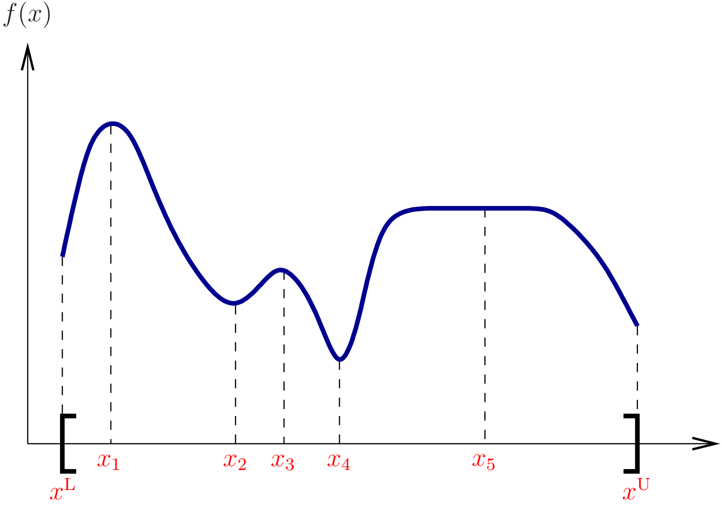
Why closedness of S?



Why continuity of f?



Global vs Local Optima



Sanity Check

Identify the minima & maxima types for f on $S := [x^{\mathrm{L}}, x^{\mathrm{U}}]$

Min vs Argmin

Terminology

If $\boldsymbol{x}^*$ is a global minimiser we write

$$f^* = \min_{\boldsymbol{x} \in \Omega} \; f(\boldsymbol{x})$$

$$\boldsymbol{x}^* = \arg\min_{\boldsymbol{x} \in \Omega} \; f(\boldsymbol{x})$$

Examples Assume $x \in \mathbb{R}$. What is $\arg\min f(x)$? What is $\min f(x)$?

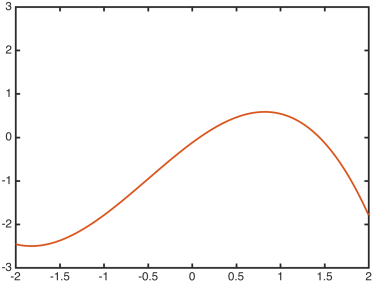
- $f(x) = (x+1)^2 + 3$
  - $\arg\min f(x) = -1$; $\min f(x) = 3$
- $f(x) = (x+1)^2\,(x-1)^2 + 3$
  - $\arg\min f(x) = \{-1, 1\}$; $\min f(x) = 3$

Sanity Check

What is $\arg\min_{\boldsymbol{x} \in \Omega} \; f(\boldsymbol{x})$ on the previous slide.

Minimisation & Maximisation are Equivalent

$$\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) = -\max_{\boldsymbol{x}\in\Omega} -f(\boldsymbol{x}).$$



$$\min \quad f(x) = -\frac{1}{2}(x+0.5)^2 + 2x - \frac{1}{3}x^3$$

$$x \in [-2,\, 2]$$

$$\Rightarrow \quad x^* \approx -1.823$$

$$f^* \approx -2.502$$

$$-\max -f(x) = \frac{1}{2}(x+0.5)^2 - 2x + \frac{1}{3}x^3$$

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Most optimisation problems in this class will be **minimisation** problems.

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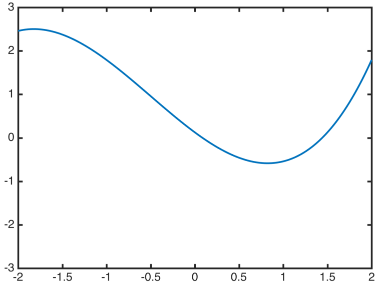

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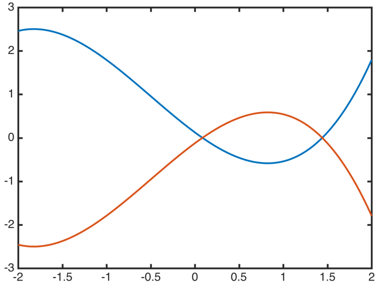

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$$x^* \approx -1.823$$

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Most optimisation problems in this class will be **minimisation** problems.

Minimisation & Maximisation are Equivalent (proof)

Assume that both the minimum and maximum of f are attained within set Ω and show that:
$$\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) = -\max_{\boldsymbol{x}\in\Omega} -f(\boldsymbol{x}).$$

Proof.

- The minimum of f satisfies:
$$\min \quad f(\boldsymbol{x}) = f^* \leq \quad f(\boldsymbol{x}), \ \ \forall \boldsymbol{x} \in \Omega$$
- The maximum of $-f$ satisfies:
$$\max -f(\boldsymbol{x}) = F^* \geq -f(\boldsymbol{x}), \ \ \forall \boldsymbol{x} \in \Omega$$
- If $-F^* < f^*$ then there exists an $\bar{\boldsymbol{x}} \in \Omega$ such that $f(\bar{\boldsymbol{x}}) < f^*$ contradicting the optimality of f^*.
- If $-f^* > F^*$ then there exists an $\bar{\boldsymbol{x}} \in \Omega$ such that $-f(\bar{\boldsymbol{x}}) > F^*$ contradicting the optimality of F^*.

Therefore $f^* = -F^*$. □

Definitions: Types of Optimisation Models (1/4)

Unconstrained Optimisation

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} \ f(\boldsymbol{x})$$

Example Soft-margin Support Vector Machine

$$\min_{\boldsymbol{w},\, b} f(\boldsymbol{w},\, b) = \left[\frac{1}{n} \sum_{i=1}^{n} \max \Big(0,\, 1 - y_i (\boldsymbol{w}^\top \boldsymbol{x_i} + b) \Big) \right] + \lambda \left\| \boldsymbol{w} \right\|_2^2$$

Constrained Optimisation

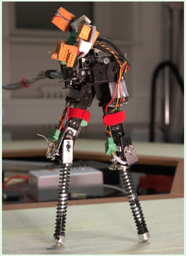
$$\min_{x \in \Omega} \ f(x)$$

Definitions: Types of Optimisation Models (2/4)

Box-Constrained Optimisation

$$\min_{\boldsymbol{x} \in [\boldsymbol{x}^{\mathrm{L}}, \boldsymbol{x}^{\mathrm{U}}]} \quad f(\boldsymbol{x})$$

Example Make a robot walk



Objective: optimise performance, e.g., as measured by velocity, within the range of reasonable gait parameters. But there is no closed-form mathematical formulation for the velocity as a function of the input parameters. To solve this problem, the authors use a type of **black-box optimisation** called **Bayesian optimisation**.

`http://wp.doc.ic.ac.uk/sml/project/bayesian-optimization/`

Definitions: Types of Optimisation Models (3/4)

Linear Programming (LP)

$$
\begin{aligned}
\min\ & \boldsymbol{c}^\top \boldsymbol{x} \\
& \mathbf{A}\,\boldsymbol{x} \le \boldsymbol{b} \\
& \boldsymbol{x} \in \mathbb{R}^n
\end{aligned}
$$

Quadratic Programming (QP)

$$
\begin{aligned}
\min\ & \frac{1}{2}\boldsymbol{x}^\top \mathbf{Q}\,\boldsymbol{x} + \boldsymbol{c}^\top \boldsymbol{x} \\
& \mathbf{A}\,\boldsymbol{x} \le \boldsymbol{b} \\
& \boldsymbol{x} \in \mathbb{R}^n
\end{aligned}
$$

Portfolio optimisation is often formulated as a QP

Balance expected value of the portfolio's return versus financial risk measures.

Definitions: Types of Optimisation Models (4/4)

Nonlinear Optimisation (NLP)

$$
\begin{aligned}
&\min_{\boldsymbol{x} \in X} \; f(\boldsymbol{x}) && \leftarrow \quad \text{Objective function} \\
&\text{s.t.} \quad \mathbf{h}(\boldsymbol{x}) = \mathbf{0} && \leftarrow \quad \text{Equality constraints} \\
&\qquad\;\; \mathbf{g}(\boldsymbol{x}) \leq \mathbf{0} && \leftarrow \quad \text{Inequality constraints} \\
&\qquad\;\; \boldsymbol{x} \in \left[\boldsymbol{x}^{\mathrm{L}}, \boldsymbol{x}^{\mathrm{U}}\right] = X \subset \mathbb{R}^n && \leftarrow \quad \text{Continuous variable bounds}
\end{aligned}
$$

$f : \mathbb{R}^n \to \mathbb{R}$, $\boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^m$, $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^p$

Historical Note

I keep saying *program* when I mean *optimisation problem* because the first well-defined optimisation problems solved *training and logistics schedules*. George Dantzig referred to the solution, or proposed plan, as a *program*.

Mixed-Integer Nonlinear Optimisation (C343 covers mixed-integer optimisation)

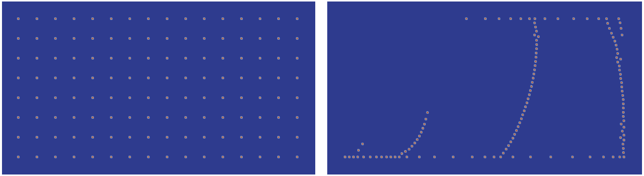
Mixed-Integer Nonlinear Optimisation (MINLP)

$$
\begin{aligned}
\min_{\boldsymbol{x}\in X,\,\boldsymbol{y}\in Y} \quad & f(\boldsymbol{x},\,\boldsymbol{y}) && \leftarrow \text{Objective function} \\
\text{s.t.} \quad & \mathbf{h}(\boldsymbol{x},\,\boldsymbol{y}) = \mathbf{0} && \leftarrow \text{Equality constraints} \\
& \mathbf{g}(\boldsymbol{x},\,\boldsymbol{y}) \leq \mathbf{0} && \leftarrow \text{Inequality constraints} \\
& \boldsymbol{x} \in \left[\boldsymbol{x}^{\mathrm{L}},\,\boldsymbol{x}^{\mathrm{U}}\right] = X \subset \mathbb{R}^n && \leftarrow \text{Continuous variable bounds} \\
& y \in \{0,\,1\}^{n_y} && \leftarrow \text{Binary variables}
\end{aligned}
$$

- Widely used in industry — MIP
- Commercial [IBM CPLEX, 2014] — MIQP
  - Passed academic codes from Imperial & CMU in 2015 [ISMP]
- Strong commercial goal — MIQCQP
- Wait-&-See — MINLP

Other types of optimisation

- Dynamic optimisation is useful for optimisation-based control;
- Partial differential equation-constrained optimisation has loads of engineering applications, e.g. in the *Grantham Institute for Climate Change* at Imperial: `http://arxiv.org/pdf/1304.1768.pdf`
  - Oceanic tide stream generators could harvest renewable energy;
  - *Optimisation objective:* How to place the turbines within the site and individually tune them for maximal power output?
  - *Optimisation constraints:* Need to accurately consider tidal flow, turbine wakes, and the resulting power output.



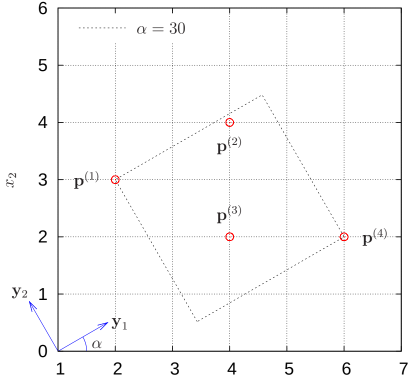
(a) Initial turbine positions (128 turbines) (b) Optimised turbine positions (128 turbines)

Figure: `http://arxiv.org/pdf/1304.1768.pdf`

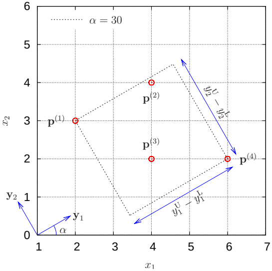
A First Example Problem – Statement

Workshop. Find a rectangle with minimum area enclosing the set of points $\{\mathbf{p}^{(1)} := (2,3), \mathbf{p}^{(2)} := (4,4), \mathbf{p}^{(3)} := (4,2), \mathbf{p}^{(4)} := (6,2)\}$

➥ Formulate this problem as an NLP
Hint: Consider the coordinate system (y_1, y_2) aligned with the axis of the rectangle, as obtained by rotating (x_1, x_2) by the angle α



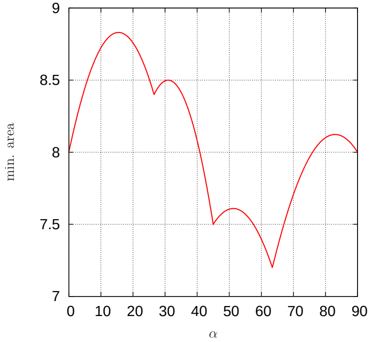
A First Example Problem – NLP Formulation

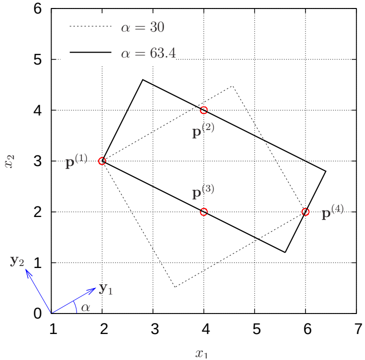


- Formulation using Projections

$$
\begin{aligned}
\min_{\boldsymbol{y}_1, \boldsymbol{y}_2, y_1^U, y_1^L, y_2^U, y_2^L} \quad & (y_1^U - y_1^L)(y_2^U - y_2^L) \\
\text{s.t.} \quad & y_1^U := \max\{\boldsymbol{y}_1^\top \mathbf{p}^{(k)}, k = 1, \ldots, 4\} \\
& y_1^L := \min\{\boldsymbol{y}_1^\top \mathbf{p}^{(k)}, k = 1, \ldots, 4\} \\
& y_2^U := \max\{\boldsymbol{y}_2^\top \mathbf{p}^{(k)}, k = 1, \ldots, 4\} \\
& y_2^L := \min\{\boldsymbol{y}_2^\top \mathbf{p}^{(k)}, k = 1, \ldots, 4\} \\
& \boldsymbol{y}_1^\top \boldsymbol{y}_2 = 0 \\
& \|\boldsymbol{y}_1\|_2 = 1; \ \|\boldsymbol{y}_2\|_2 = 1
\end{aligned}
$$

A First Example Problem – Results

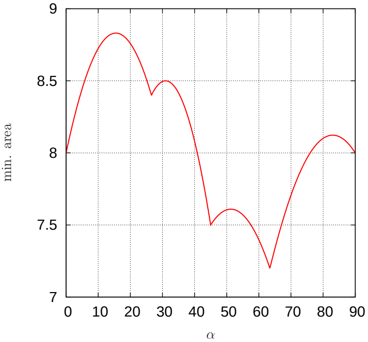




- Multi-Start Gradient Descent: 20,000 Random Initial points

Freq	Area	α	y_1^U	y_1^L	y_2^U	y_2^L
32.6%	8.00	0.0	6.000	2.000	4.000	2.000
30.5%	**7.20**	**63.4**	**5.367**	**3.578**	**-0.447**	**-4.472**
15.2%	8.00	90.0	4.000	2.000	-2.000	-6.000
12.1%	7.50	45.0	5.657	3.536	0.707	-2.828
9.7%	8.40	26.6	6.261	3.130	1.789	-0.894

Motivation for next time



What is going on? We are getting different answers depending on where we initialise the algorithm. When is a local optimum also the global solution?

Key concept: **convexity**. If a problem is convex, then a local optimum solution must be a global solution. (More on this Wednesday!!)