G-L-5:

# Optimisation

## Advanced Modelling

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- A case study
- The gradient descent method
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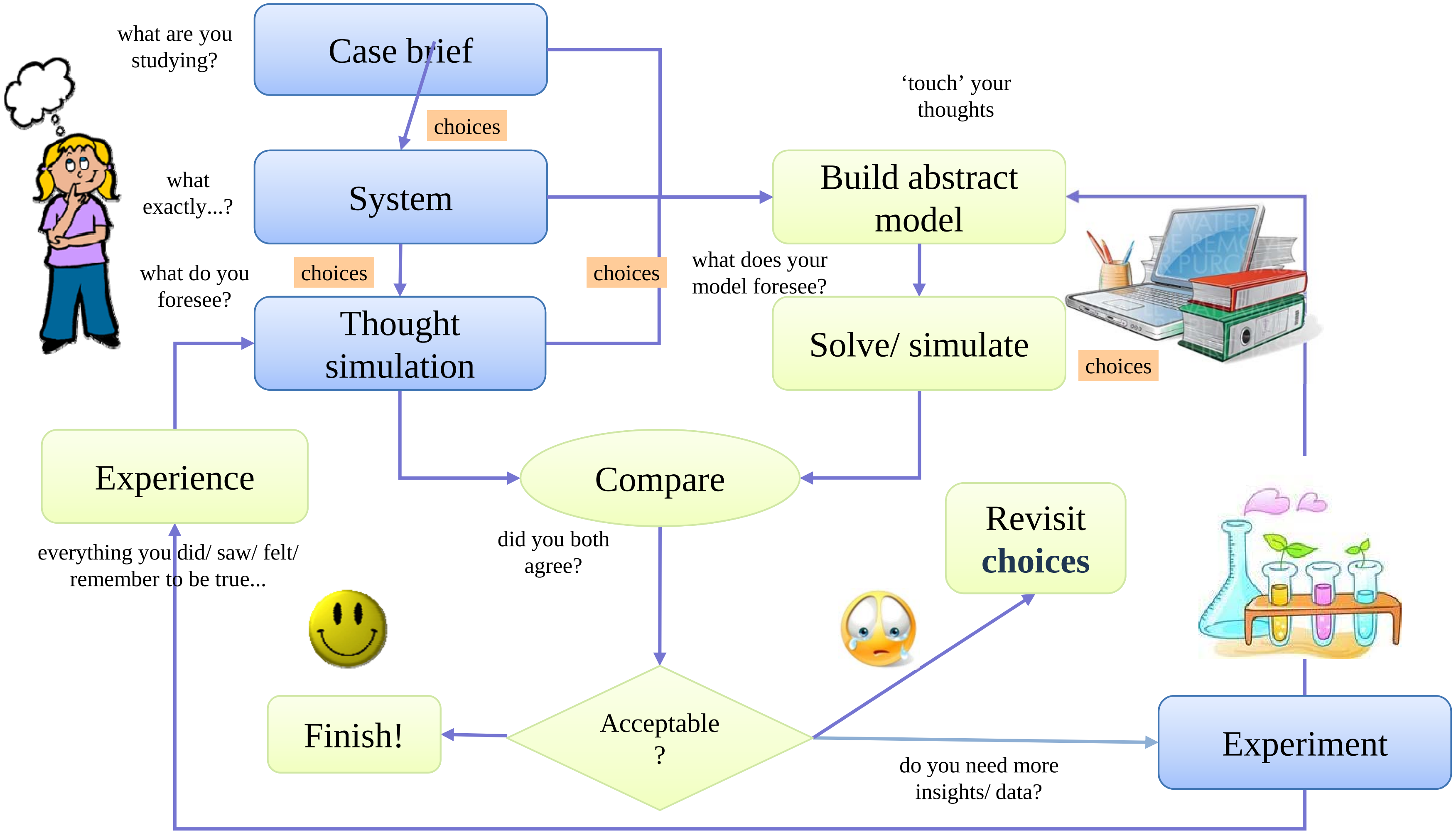
# Optimisation@Modelling



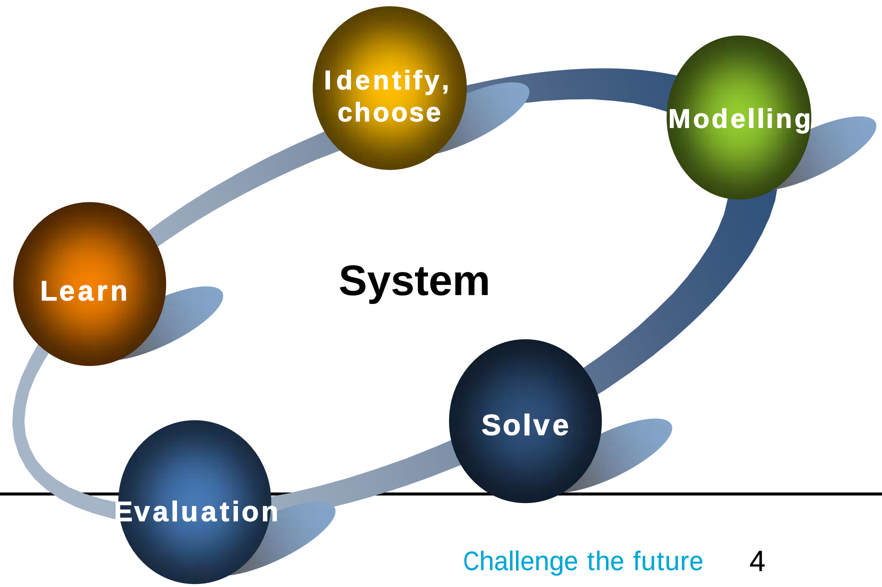

Courtesy of centech.com.pl and http://www.clipsahoy.com/webgraphics4/as5814.htm

# Why Optimisation?

**Product optimisation**

**Product Optimisation** is not just making a product better in some respect (a criterion / metric), but making it the **BEST** (optimal) in this respect.

In mathematics, Optimisation refers to choosing the element from some set of available alternatives that **maximises/minimises** a specified **metric**.



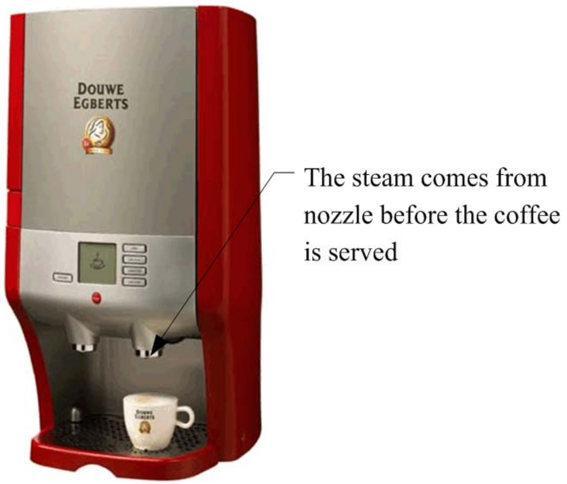
# A case study: The coffee cups

In the new generation of Douwe Egberts® coffee machine, the preheat coffee cup feature is introduced. In the preheating process, water steam from the nozzle preheats the cup to a certain temperature before the coffee is served.

Experiments indicate that:
1. if the cup is preheated to **92°C** , the best coffee can be served;
2. **80% of water steam** is condensed inside the cup, the rest is absorbed by the air.

Besides, Douwe Egberts® also manufactures its own coffee cups with different sizes and materials, for example, the Hollandsche series and the Standard series.

You are asked to find the initial steam temperature and the amount of steam that should be produced in order to **preheat either of the two types of cups as close as possible to 92°C (minimise the deviation)**.





Fictional case study, for education only.
Douwe Egbert® are resisted trademarks.
Courtesy of http://www.douweegbertscoffeesystems.com/dg/OutOfHome/OurProducts/Coffee/Cafitesse/Machines/

# System identification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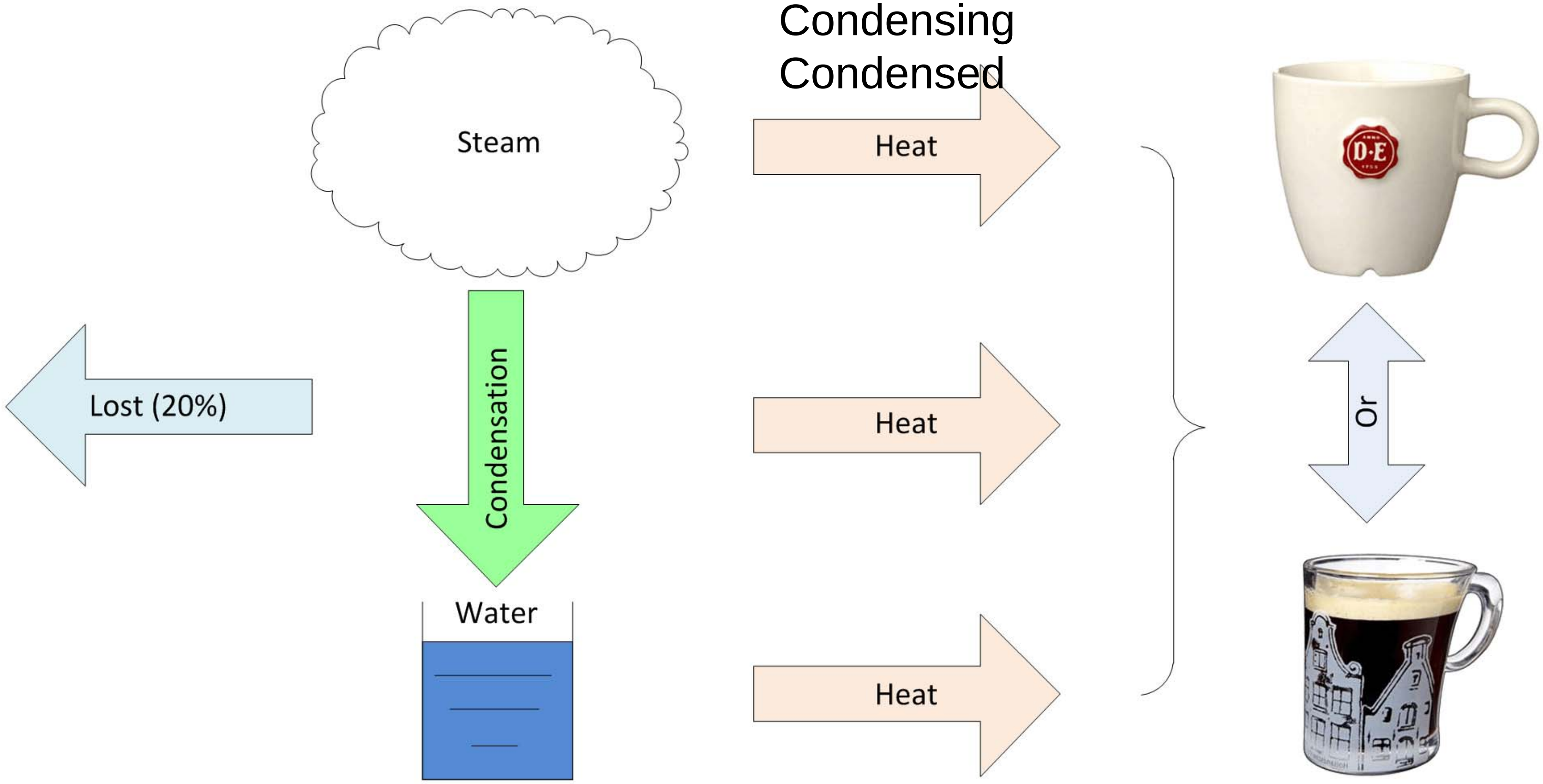
# Cause-effect

Superheated steam
Condensing
Condensed

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# Modelling

## Hollandsche cup

$$\left(m_{steam}c_{steam}(T_{steaminitial}-100)+m_{steam}L_{steam}+m_{steam}c_{water}(100-T_{Hfinal})\right)\cdot 80\% = m_{\text{holland}}c_{\text{holland}}(T_{Hfinal}-T_{initial})$$

Steam cools down

Latent heat

Condensed water cools down

Cup is heated

$$\left(m_{steam}c_{steam}(T_{steaminitial}-100)+m_{steam}L_{steam}+m_{steam}c_{water}(100-T_{Sfinal})\right)\cdot 80\% = m_{\text{standard}}c_{\text{standard}}(T_{Sfinal}-T_{initial})$$

## Standard cup

Courtesy of http://www.douweegbertscoffeesystems.com/dg/OutOfHome/OurProducts/Coffee/Cafitesse/Machines/

# Modelling - Choices

**Hollandsche cup**

$$\left(m_{steam}c_{steam}(T_{steaminitial}-100)+m_{steam}L_{steam}+m_{steam}c_{water}(100-T_{Hfinal})\right)\cdot 80\% = m_{\text{holland}}c_{\text{holland}}(T_{Hfinal}-T_{initial})$$

**Standard cup**

$$\left(m_{steam}c_{steam}(T_{steaminitial}-100)+m_{steam}L_{steam}+m_{steam}c_{water}(100-T_{Sfinal})\right)\cdot 80\% = m_{\text{standard}}c_{\text{standard}}(T_{Sfinal}-T_{initial})$$

## We choose

- The density of water is 1000 kg/m3;
- The latent heat of water vaporization is 2,260,000 J/kg;
- The specific heat of water steam is 2080 J/(kg·K);
- The specific heat of water is 4181 J/(kg·K);
- The initial temperatures of both cups are 20 °C;
- The weight of the Hollandsche cup is 0.20 kg, the specific heat is 750 J/(kg·K);
- The weight of the Standard cup is 0.13 kg, the specific heat is 1070 J/(kg·K);
- The steam temperature doesn’t change before it reaches the cup;
- The complete process happens in a very short time;

# Solving/Simulation

**Hollandsche cup final temperature**

$$T_{Hfinal}(m_{steam}, T_{\text{steaminitial}}) = \frac{8320 m_{steam} T_{\text{steaminitial}} + 9.8804 \cdot 10^6 m_{steam} + 15000}{16724 m_{steam} + 750}$$

Design parameters $(m_{steam}, T_{\text{steaminitial}})$

$$T_{Sfinal}(m_{steam}, T_{\text{steaminitial}}) = \frac{8320 m_{steam} T_{\text{steaminitial}} + 9.8804 \cdot 10^6 m_{steam} + 13910}{16724 m_{steam} + 695.5}$$

**Standard cup final temperature**

# Our wishes

## Design brief

In the new generation of Douwe Egberts® coffee machine, the preheat coffee cup feature is introduced. In the preheating process, water steam from the nozzle preheats the cup to a certain temperature before the coffee is served.

Experiments indicate that:
1. if the cup is preheated to **92°C** , the best coffee can be served;
2. **80% of water steam** i condensed inside the cup, the rest is absorbed by the a

Besides, Douwe Egbert also manufactures its own coffee cups with differen izes and materials, for example, the Hollandsch series and the Standard series.

You are asked to find the itial temperature and the amount of steam that sh ld be produced in order to **preheat either of the two types of cups as close as possible to 92°C (minimize the deviation)**.

Wishes

Make the deviation

$$T_{Hfinal}(m_{steam}, T_{\text{steaminitial}}) - 92$$

as small as possible

AND

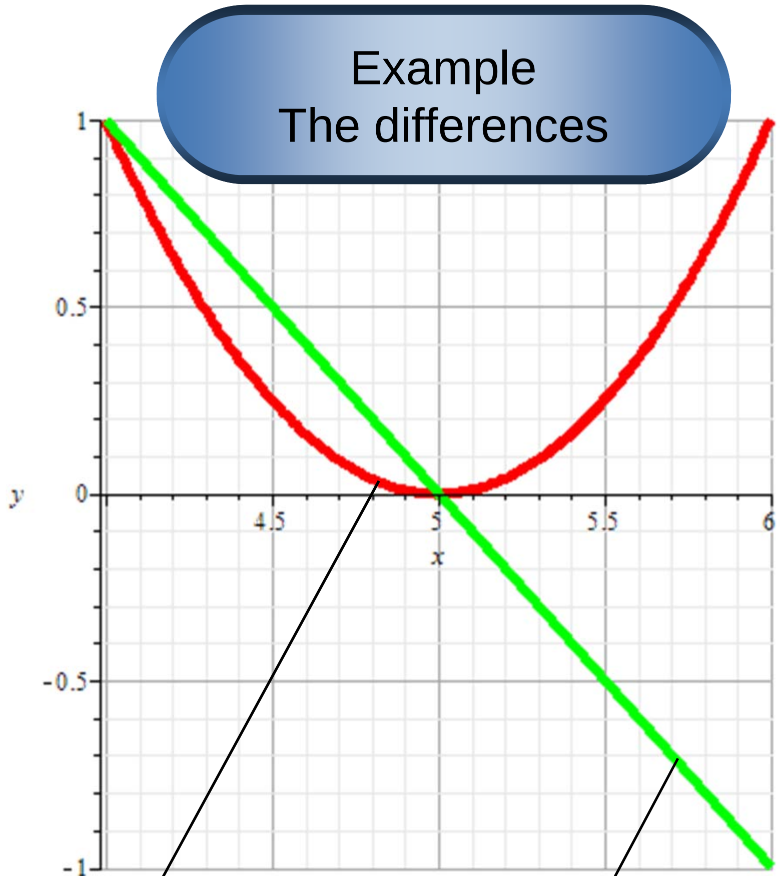
Make the deviation

$$T_{Sfinal}(m_{steam}, T_{\text{steaminitial}}) - 92$$

as small as possible

# The metrics

$$M_1 = (T_{Hfinal}(m_{steam}, T_{\mathrm{steaminitial}}) - 92)^2$$




$$M_2 = (T_{Sfinal}(m_{steam}, T_{\mathrm{steaminitial}}) - 92)^2$$

$y(x) = (-x+5)^2$ $\quad$ $y(x) = -x+5$

# Formulate the objective function based on metrics

$$f(m_{steam}, T_{\text{steaminitial}}) = \sum_{i=1}^{2} W_i M_i$$

The objective function

Non-dimensional

We want to minimise

$$\min\ f(m_{steam}, T_{\text{steaminitial}}) \quad \text{where} \quad f(m_{steam}, T_{\text{steaminitial}}) = \sum_{i=1}^{2} W_i M_i$$

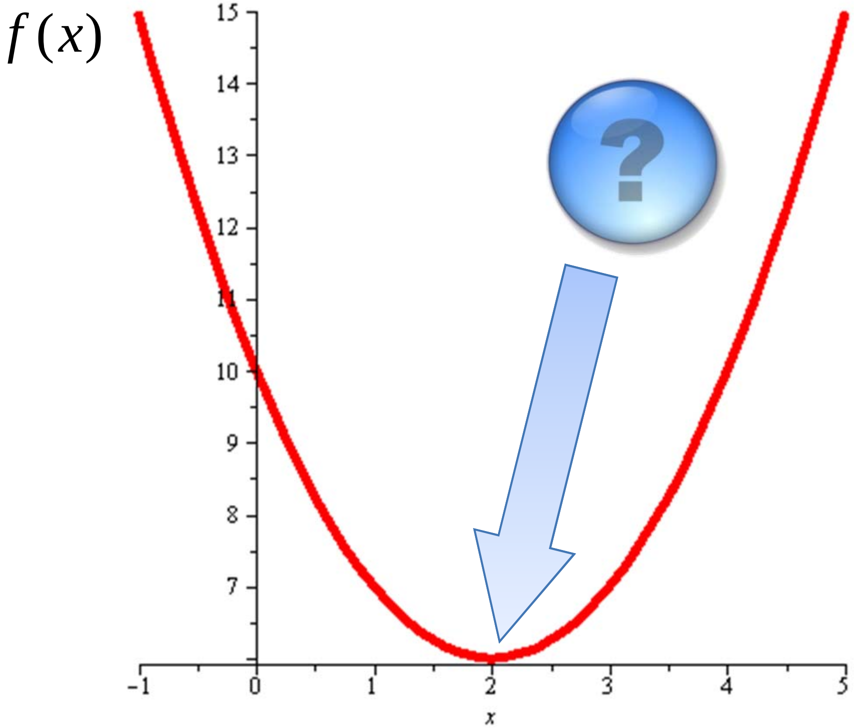
# Formulate the objective function based on metrics

In our case study, we choose

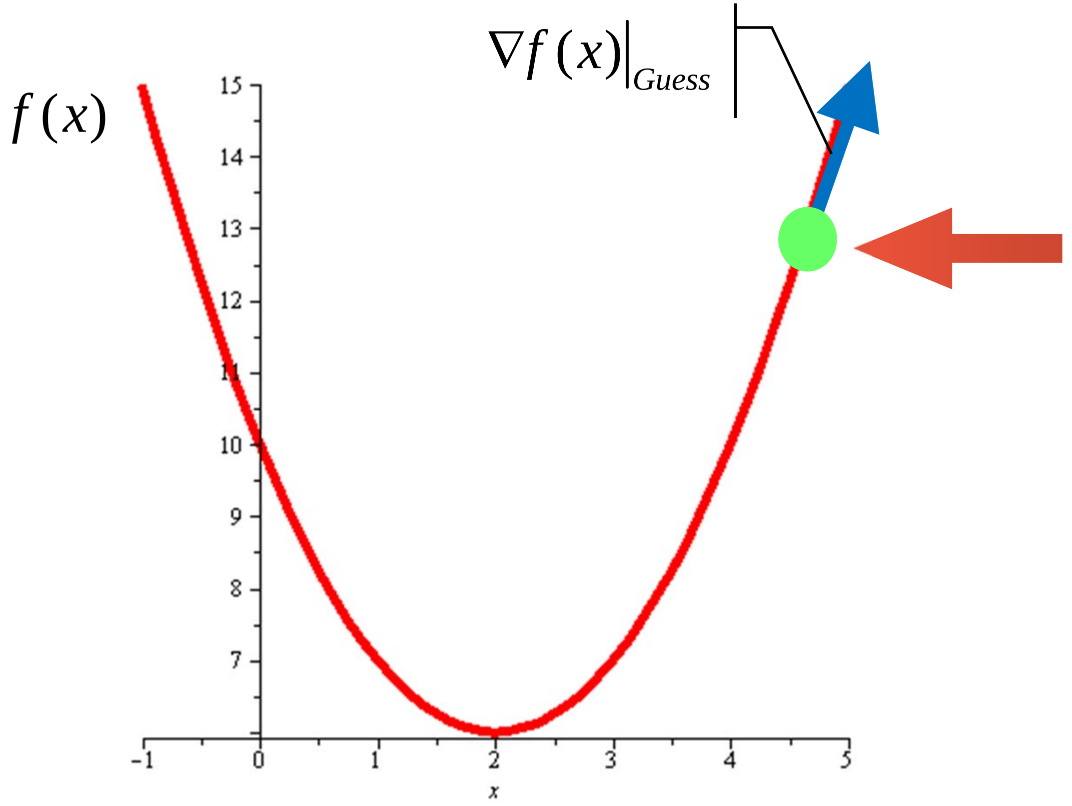
$$W_i = 0.5$$

$$\min\ f(m_{steam}, T_{\text{steaminitial}}) = 0.5(T_{\text{Hfinal}}(m_{steam}, T_{\text{steaminitial}}) - 92)^2 + 0.5(T_{\text{Sfinal}}(m_{steam}, T_{\text{steaminitial}}) - 92)^2$$

# Start from a 1D problem:
# Finding the minimum of a function



# The gradient descent method

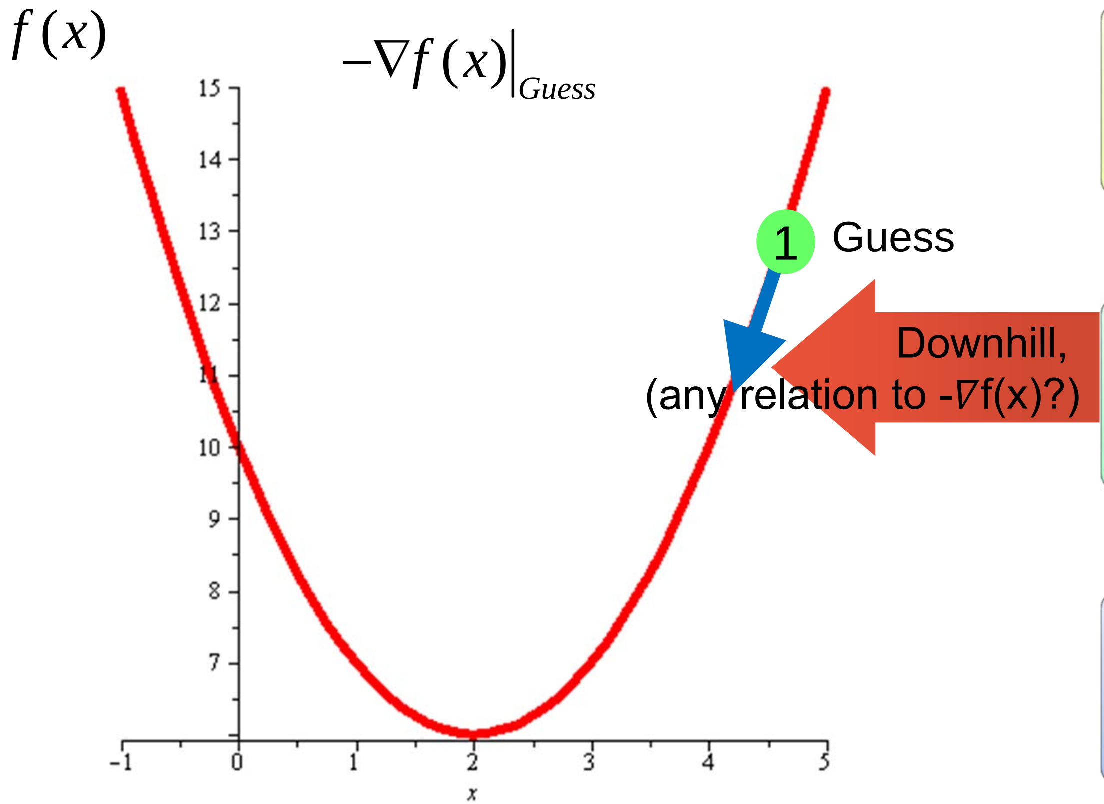



Start with a point (guess)

Repeat
- Determine a decent direction
- Choose a step
- Update

Until stopping criterion is satisfied

# The gradient descent method




Start with a point (guess)

Repeat
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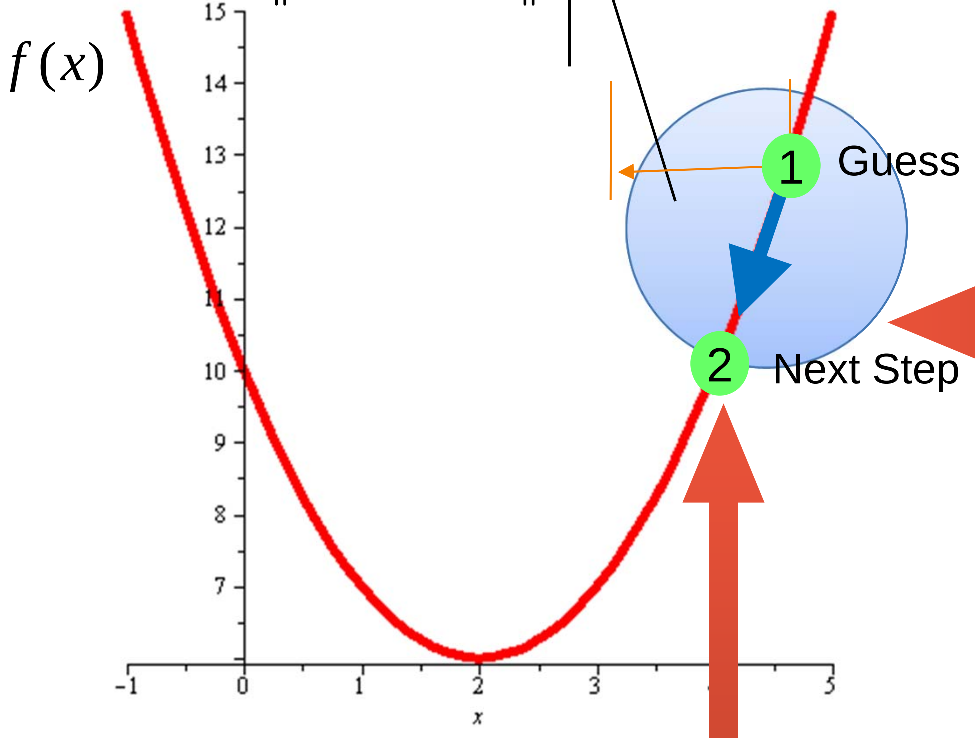
Until stopping criterion is satisfied

# The gradient descent method

$$Step \cdot \left\| \nabla f(x)\big|_{Guess} \right\|$$




Start with a point (guess)

Repeat
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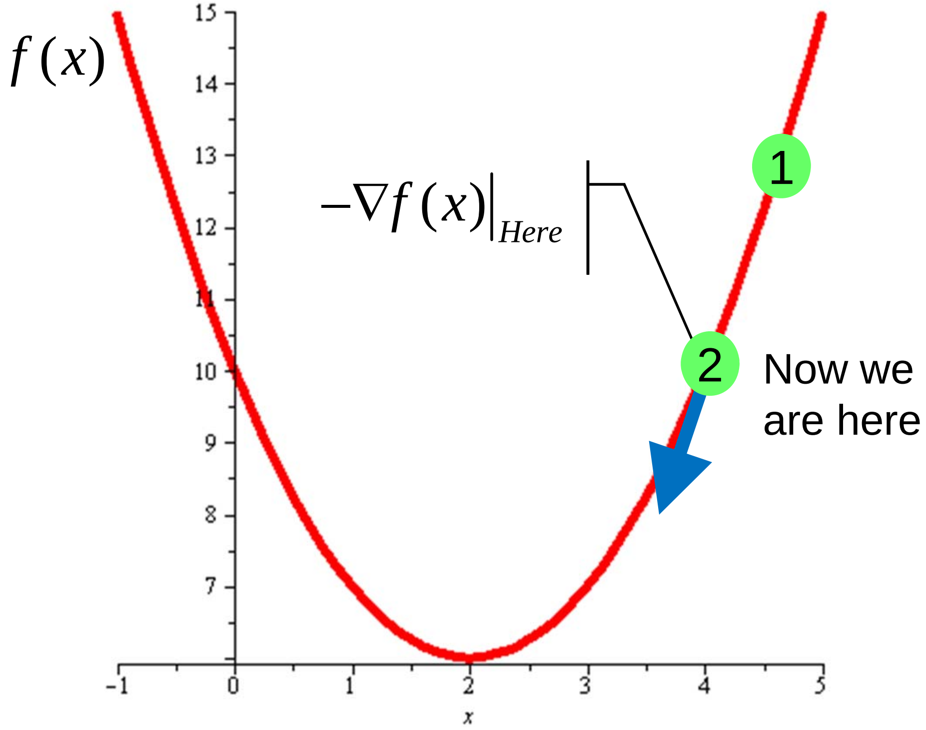
$$x_{NextSep} = x_{Guess} + Step \cdot \left( -\nabla f(x)\big|_{Guess} \right)$$

# The gradient descent method




Start with a point (guess)

Repeat

- Determine a decent direction
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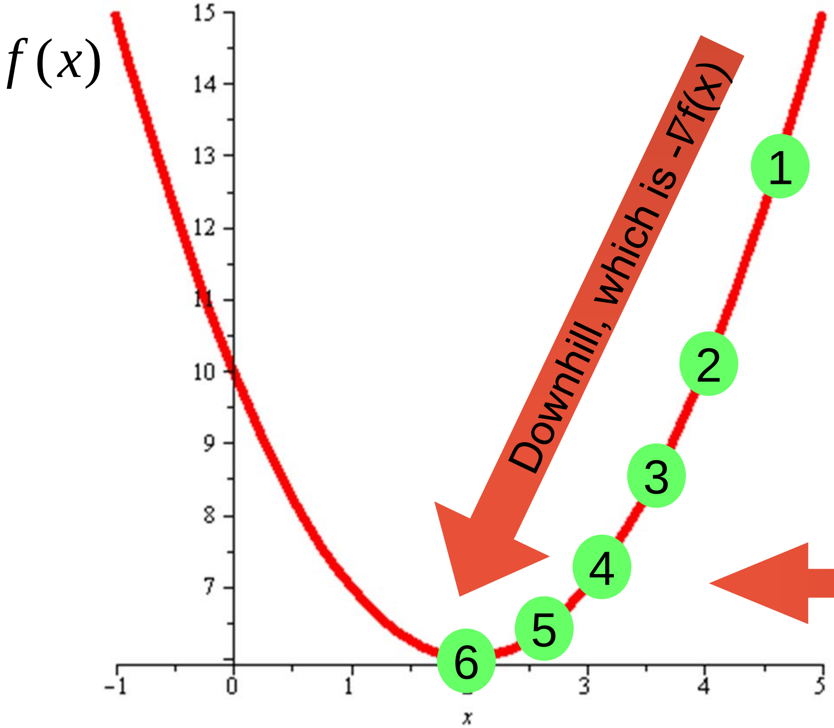
Until stopping criterion is satisfied

# The gradient descent method




$$\|\nabla f\| < \varepsilon$$

Start with a point (guess)

Repeat
- Determine a decent direction
- Choose a step
- Update

Until stopping criterion is satisfied

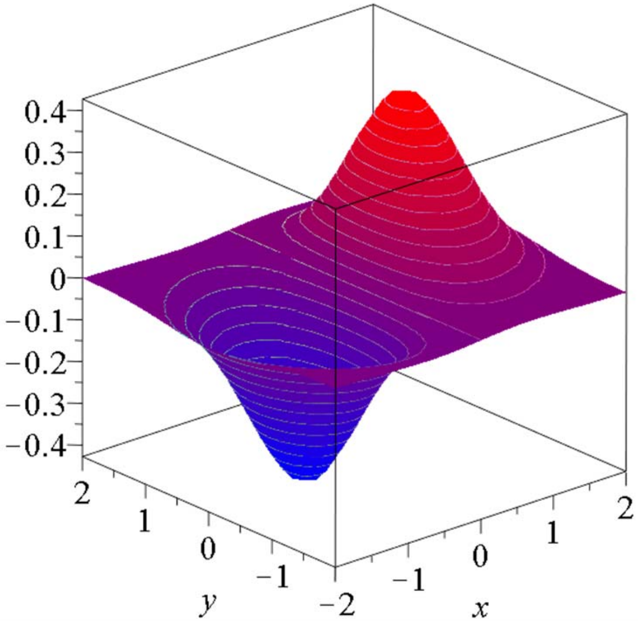
# 2D gradient descent method

x

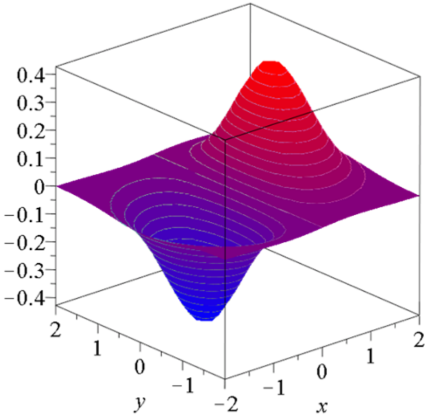
y

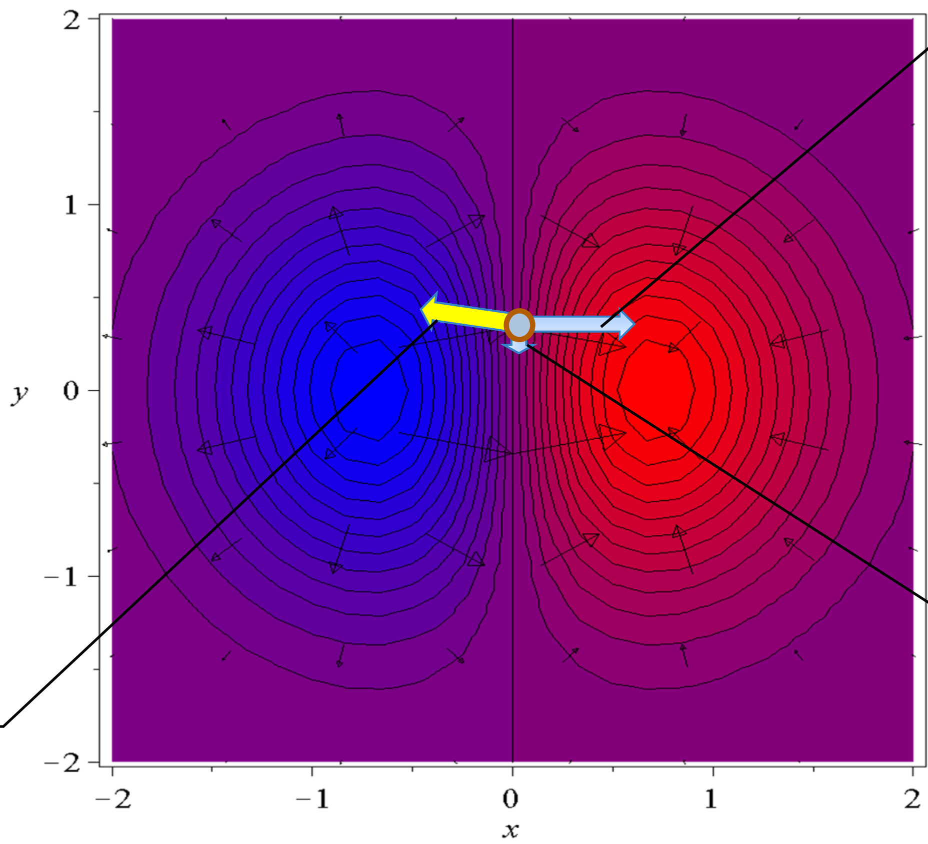
$$f(x,y) = xe^{-x^2-y^2}$$

$f(x,y)$



# 2D gradient descent method



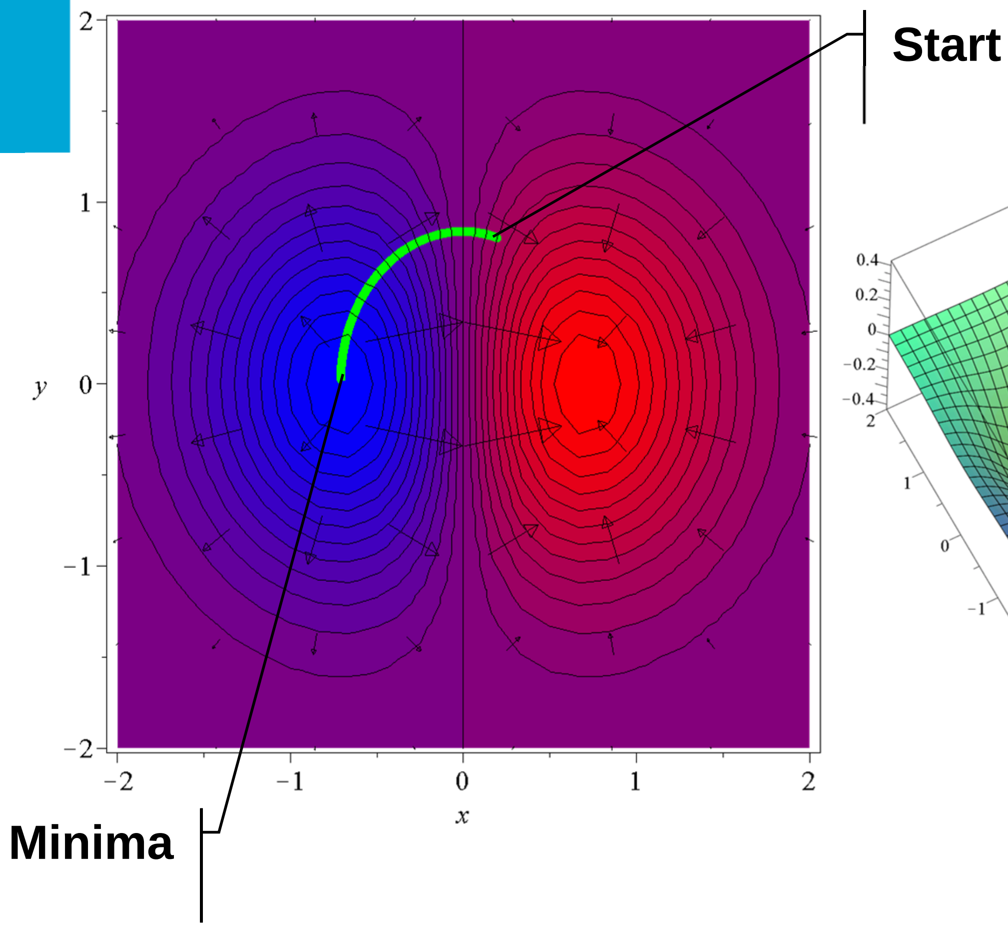

$$\frac{\partial}{\partial x} f(x,y)$$

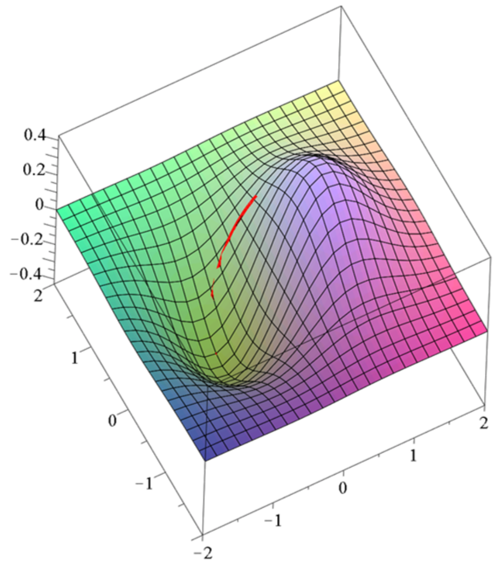
$$\frac{\partial}{\partial y} f(x,y)$$

$$-\nabla f(x,y)$$

$$= -\left(\frac{\partial}{\partial x} f(x,y), \frac{\partial}{\partial y} f(x,y)\right)$$

# 2D gradient descent method




Start with a point (guess)

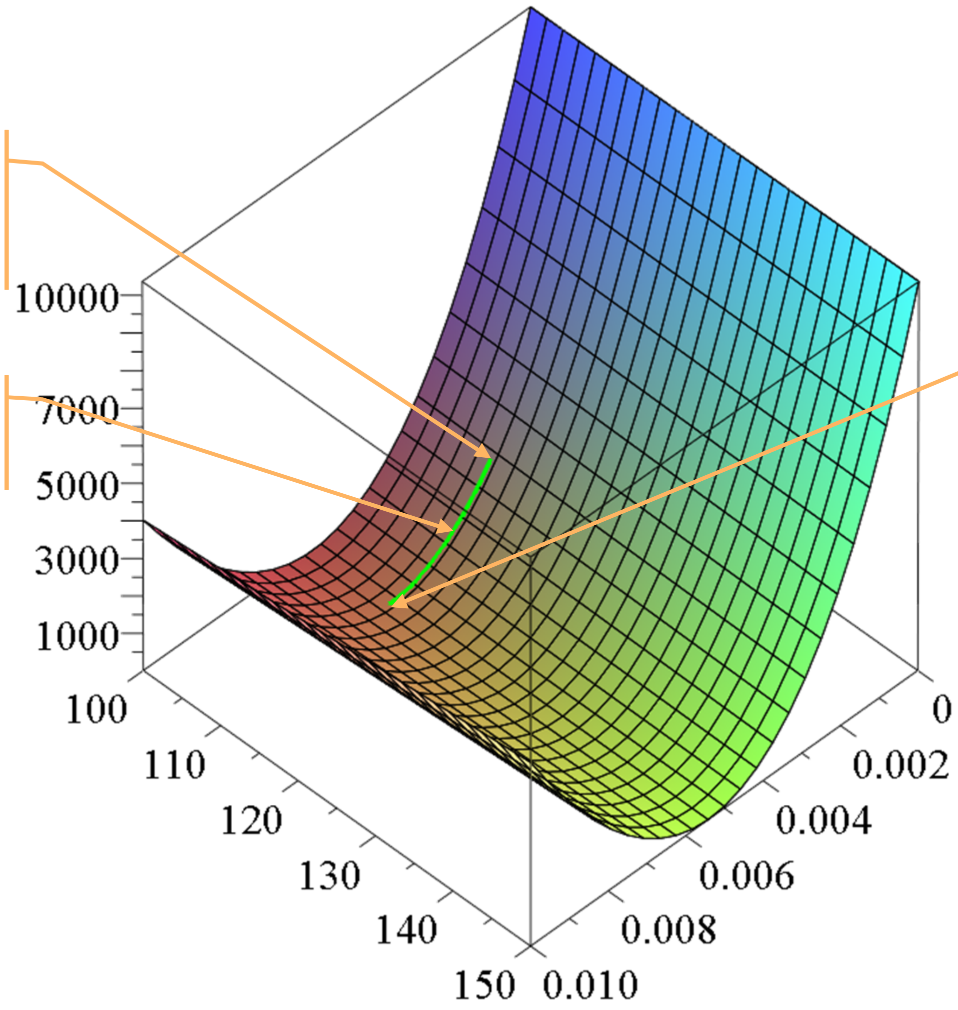
Repeat
- Determine a decent direction
- Choose a step
- Update

Until stopping criterion is satisfied

# Solving our design problem: The coffee cups

Guess
$M_{steam}$ = 0.003
$T_{steaminitial}$=110

Gradient decent path





The minimum value of the objective function is 6

# Wishes vs Designs

Put real optimal parameters in side

## Design brief

In the new generation of Douwe Egberts® coffee machine, the preheat coffee cup feature is introduced. In the preheating process, water steam from the nozzle preheats the cup to a certain temperature before the coffee is served.

Experiments indicate that:
1. if the cup is preheated to **92°C** , the best coffee can be served;
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Besides, Douwe Egberts® also manufactures its own coffee cups with different sizes and materials, for example, the Hollandsche series and the Standard series.

You are asked to find the initial temperature and the amount of steam that should be produced in order to **preheat either of the two types of cups as close as possible to 92°C (minimize the deviation)**.

**Output of the optimised design**

**Hollandsche cup final temperature**

$$T_{Hfinal}(m_{steam}, T_{\text{steaminitial}}) = 89.5°C$$


$$T_{Sfinal}(m_{steam}, T_{\text{steaminitial}}) = 94.3°C$$

**Standard cup final temperature**

# Generalised form

To optimise a function: $\min f(p_1, p_2, \ldots p_n)$

$$(p_1^0, p_2^0, \ldots p_n^0)$$

Start with a point (guess)

$$-\nabla f\big|_{(p_1^m, p_2^m, \ldots p_n^m)}$$

$$step_m$$

$$(p_1^{m+1}, p_2^{m+1}, \ldots p_n^{m+1}) = (p_1^m, p_2^m, \ldots p_n^m) + step_m(-\nabla f\big|_{p_1^m, p_2^m, \ldots p_n^m})$$

Repeat

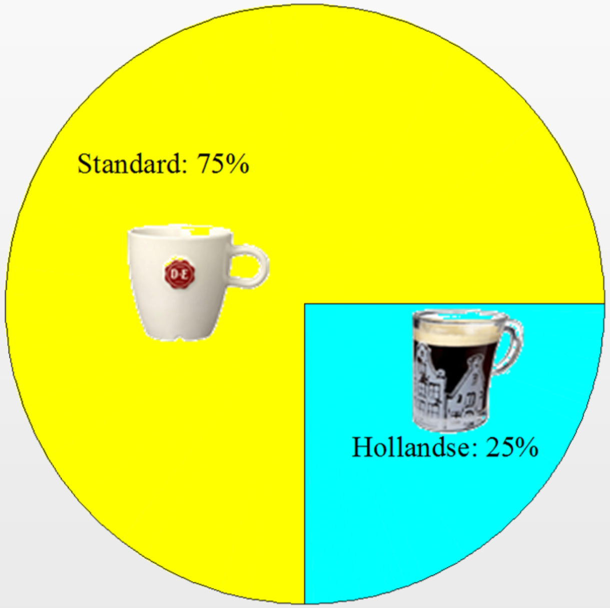
- Determine a decent direction
- Choose a step
- Update

$$\left\| \nabla f\big|_{p_1^{m+1}, p_2^{m+1}, \ldots p_n^{m+1}} \right\| < \varepsilon$$

Until stopping criterion is satisfied

# Question!
# Weights in the objective function

**The market share**




We can emphasise a wish by increasing Its relative weight

# Question! Weights in the objective function

Put real optimal parameters in side

$$\min f(m_{steam}, T_{\text{steaminitial}})$$

where

And compare to previous

$$\min f(m_{steam}, T_{\text{steaminitial}}) = W_1 (T_{\text{Hfinal}}(m_{steam}, T_{\text{steaminitial}}) - 92)^2 + W_2 (T_{\text{Sfinal}}(m_{steam}, T_{\text{steaminitial}}) - 92)^2$$

**Weight Value = 0.25**

**Weight Value = 0.75**

**Output of the optimised design**

**Hollandsche cup final temperature**

$$T_{Hfinal}(m_{steam}, T_{\text{steaminitial}}) = 88.4°C$$

**Standard cup final temperature**

$$T_{Sfinal}(m_{steam}, T_{\text{steaminitial}}) = 93.1°C$$

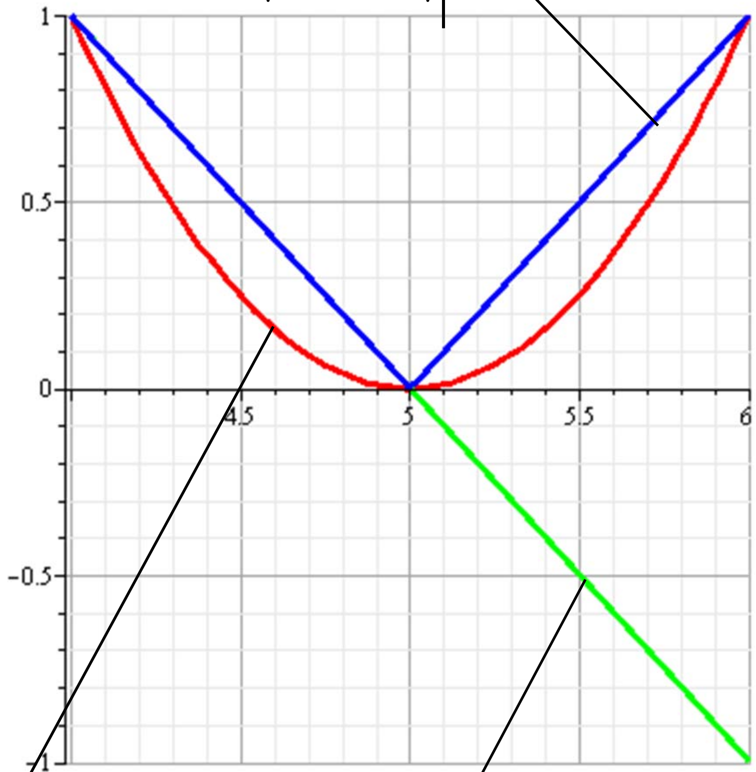
# Question! Square in the metrics

$$M_1 = (T_{Hfinal}(m_{steam}, T_{\text{steaminitial}}) - 92)^2$$

**Why square instead of absolute value?**

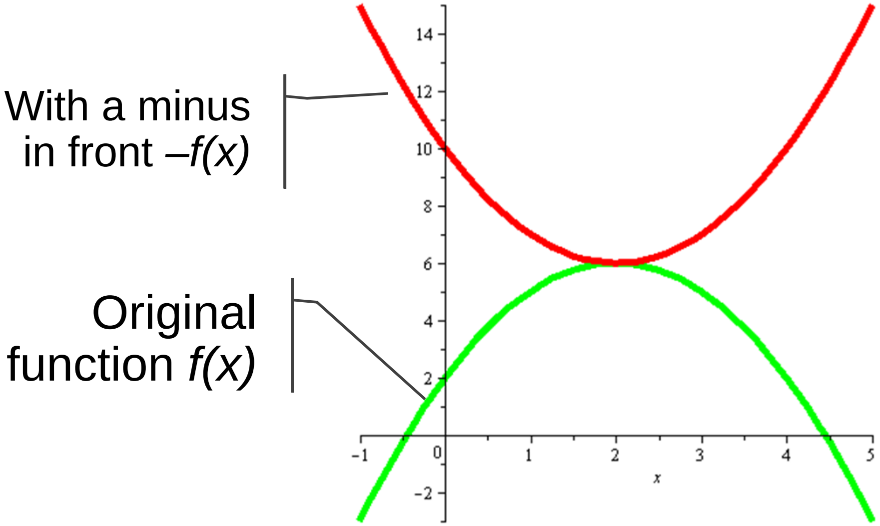
$$M_2 = (T_{Sfinal}(m_{steam}, T_{\text{steaminitial}}) - 92)^2$$

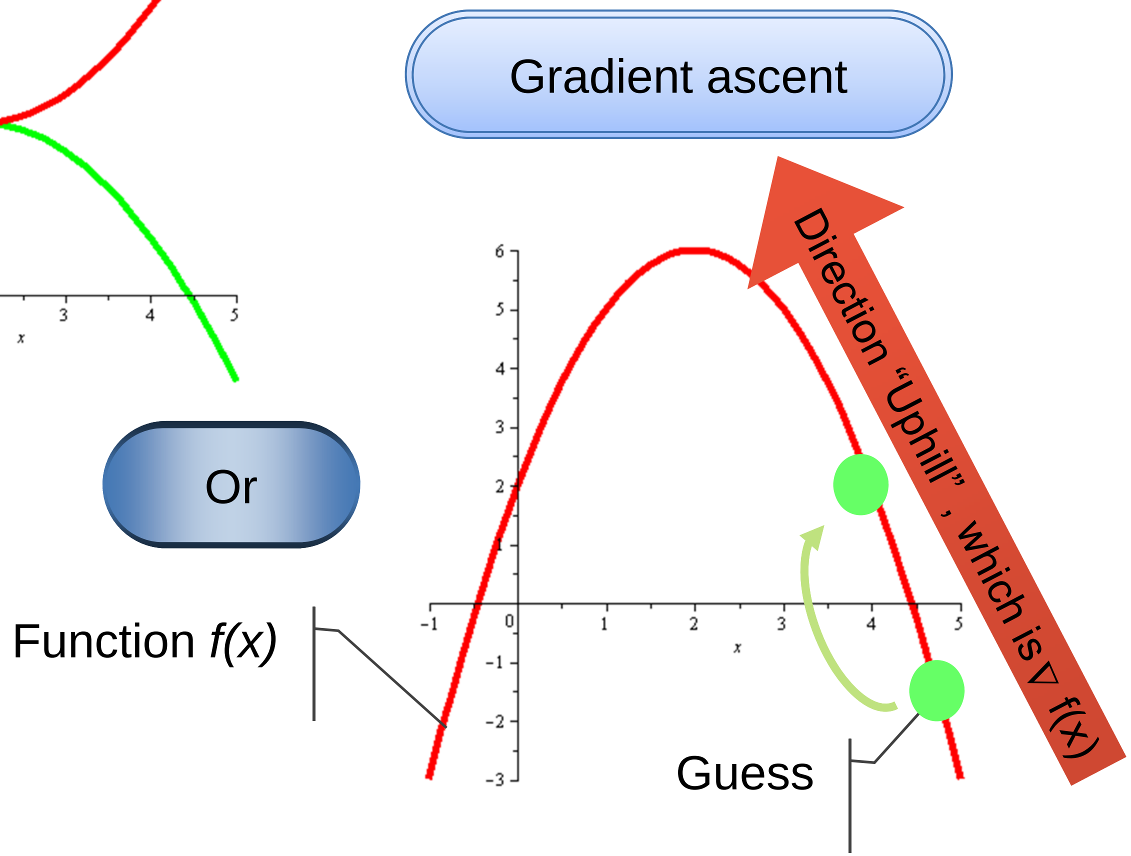
$$y(x) = \left|-x+5\right|$$




$$y(x) = (-x+5)^2 \qquad y(x) = -x+5$$

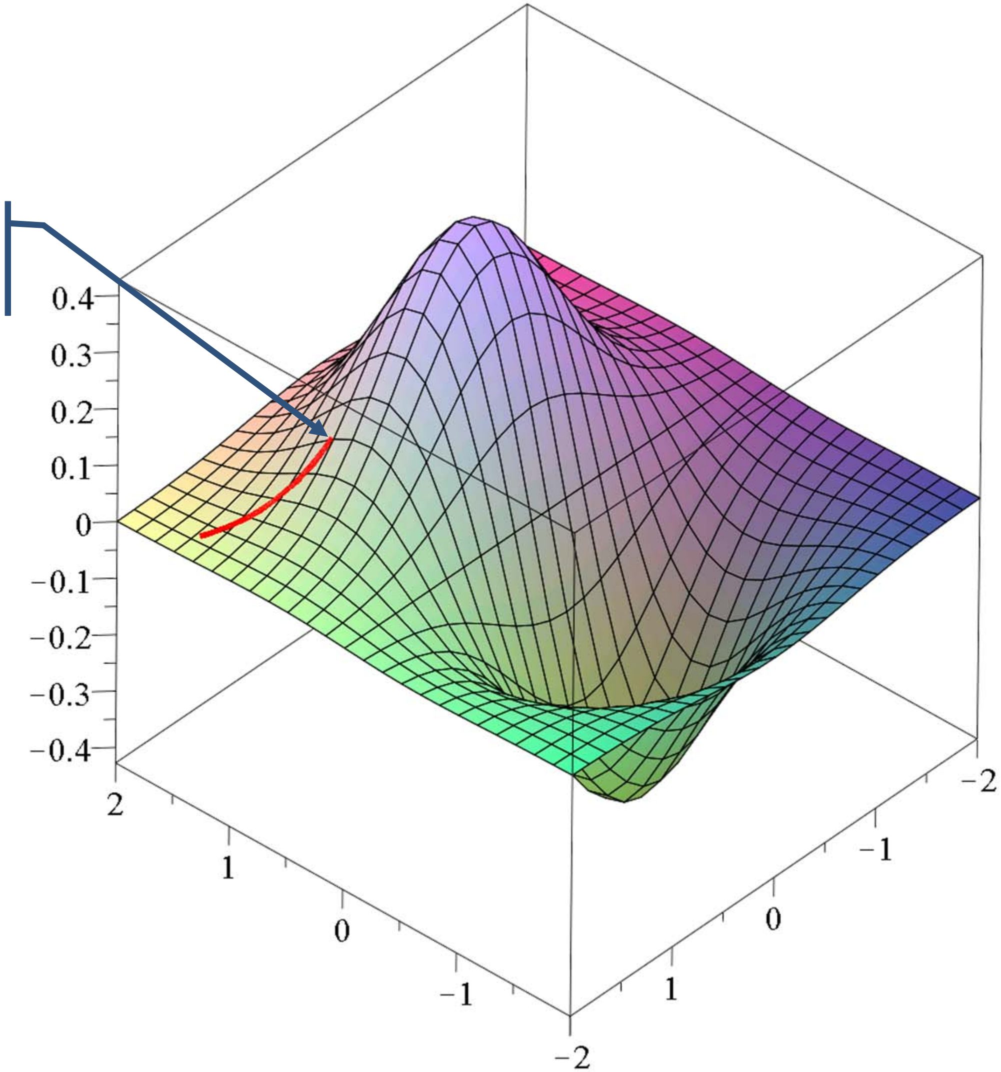
# Problem: find the maxima



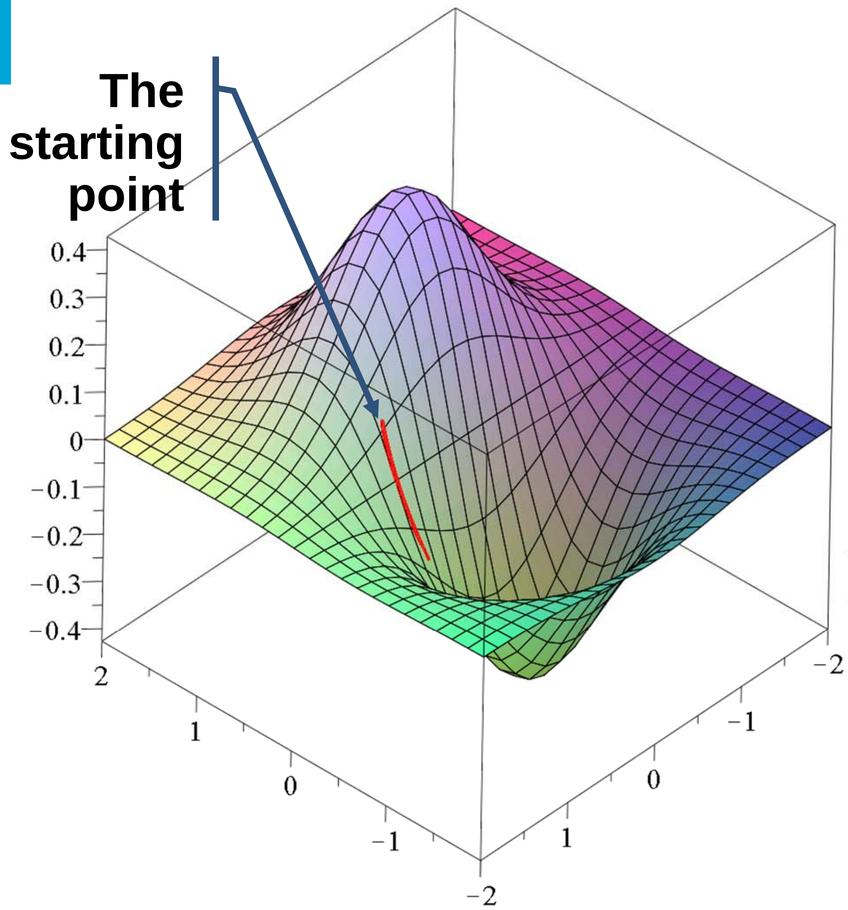
# Problems: Guess the starting point

**The starting point is not good**

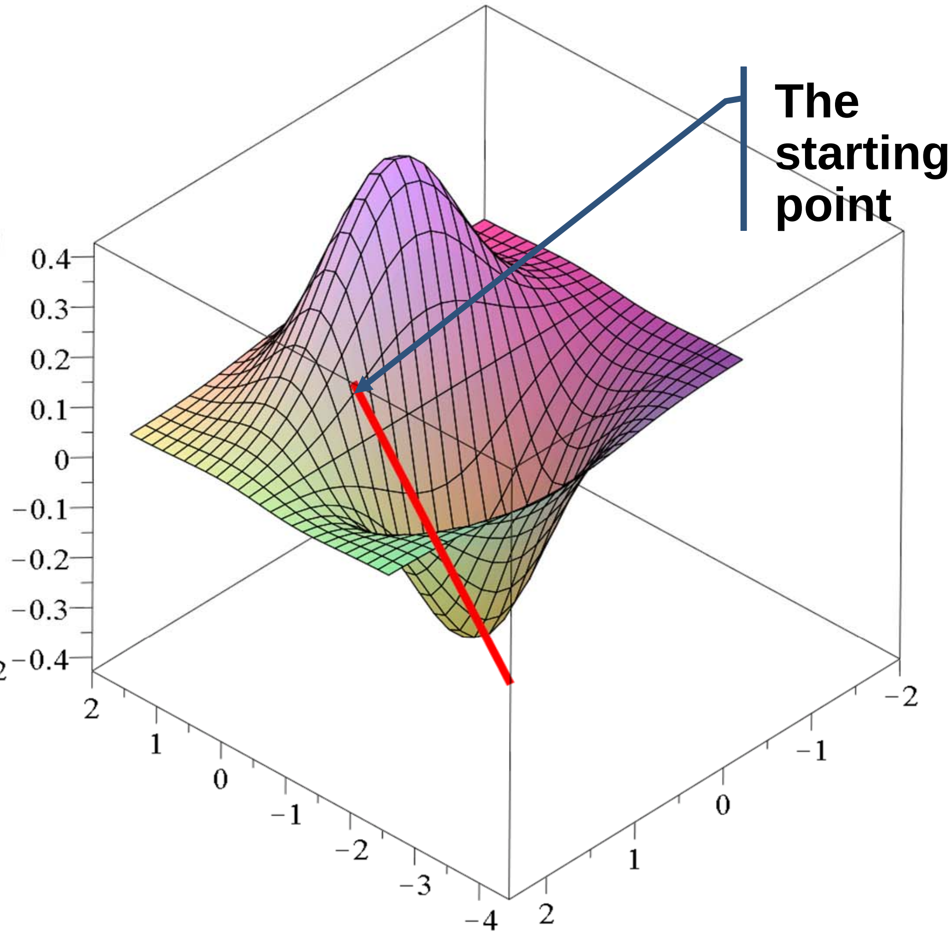


# Problems: Choice of the sizes of steps

**Small steps: inefficient**

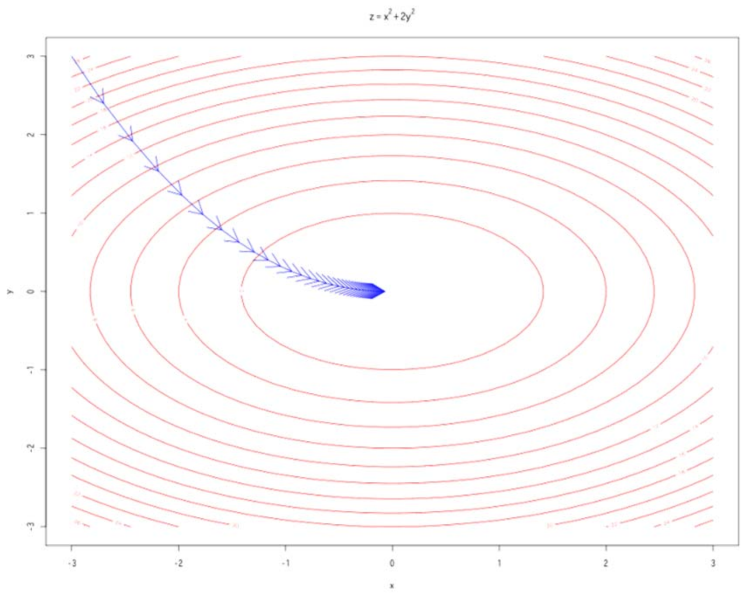



**Large steps: potential risks**



# Advanced: Dynamic steps

$$-\frac{\nabla f|_{(p_1^m, p_2^m, \ldots p_n^m)}}{\left\|\nabla f|_{(p_1^m, p_2^m, \ldots p_n^m)}\right\|}$$



Acquire the direction

Assign the initial step

If the step is too large, reduce the step to a certain percentage

# Problems: The stopping criterion

Intuitive criterion

$$\|\nabla f\| < \varepsilon$$

$$\|\nabla f\| = \sqrt{\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2} = \sqrt{\left(\frac{\partial f}{\partial x_1}\right)^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \cdots \left(\frac{\partial f}{\partial x_N}\right)^2} < \varepsilon$$

Other criteria

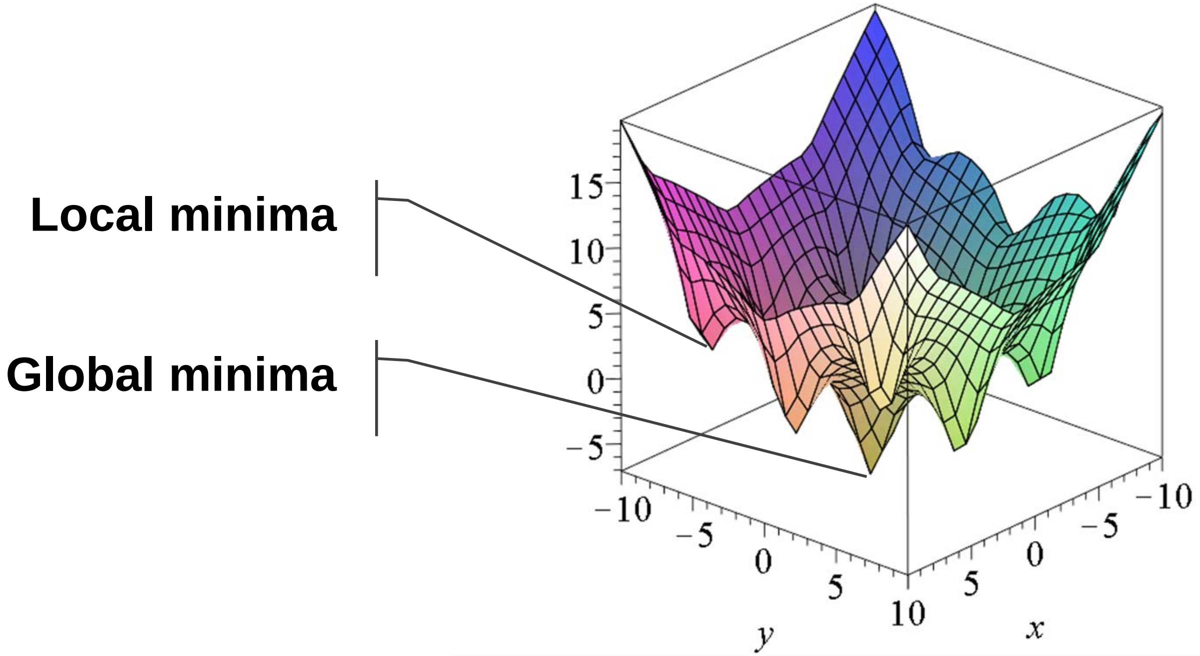
Example 1 $$\left|(p_1^{m+1}, p_2^{m+1}, \ldots p_n^{m+1}) - (p_1^{m}, p_2^{m}, \ldots p_n^{m})\right| < \varepsilon$$

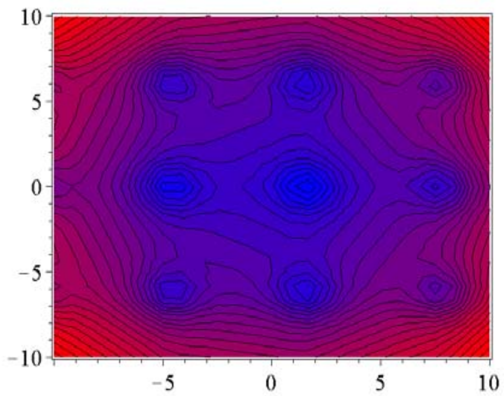
Example 2 $$\left|f(p_1^{m+1}, p_2^{m+1}, \ldots p_n^{m+1}) - f(p_1^{m}, p_2^{m}, \ldots p_n^{m})\right| < \varepsilon$$

…

# Fundamental problems: Local minima

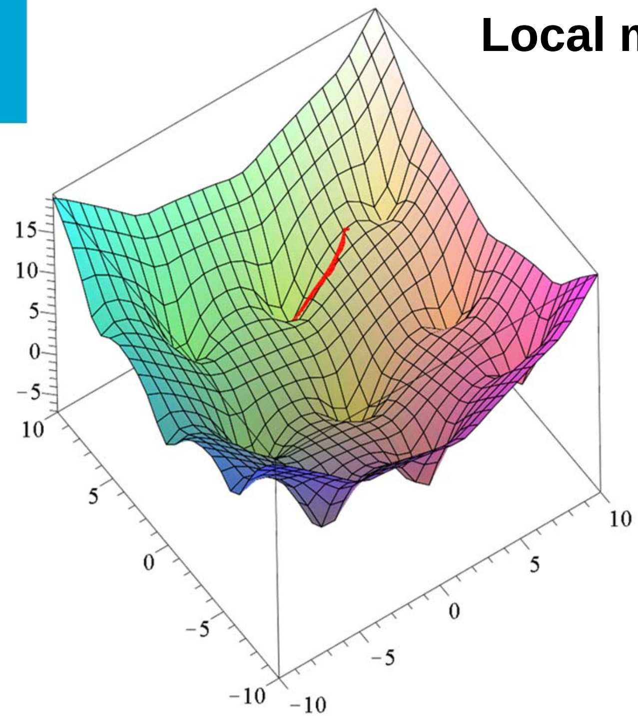
x, y → $f(x,y) = -e^{\sin(x)+\cos(y)} + 0.1(x^2 + y^2)$ → $f(x,y)$

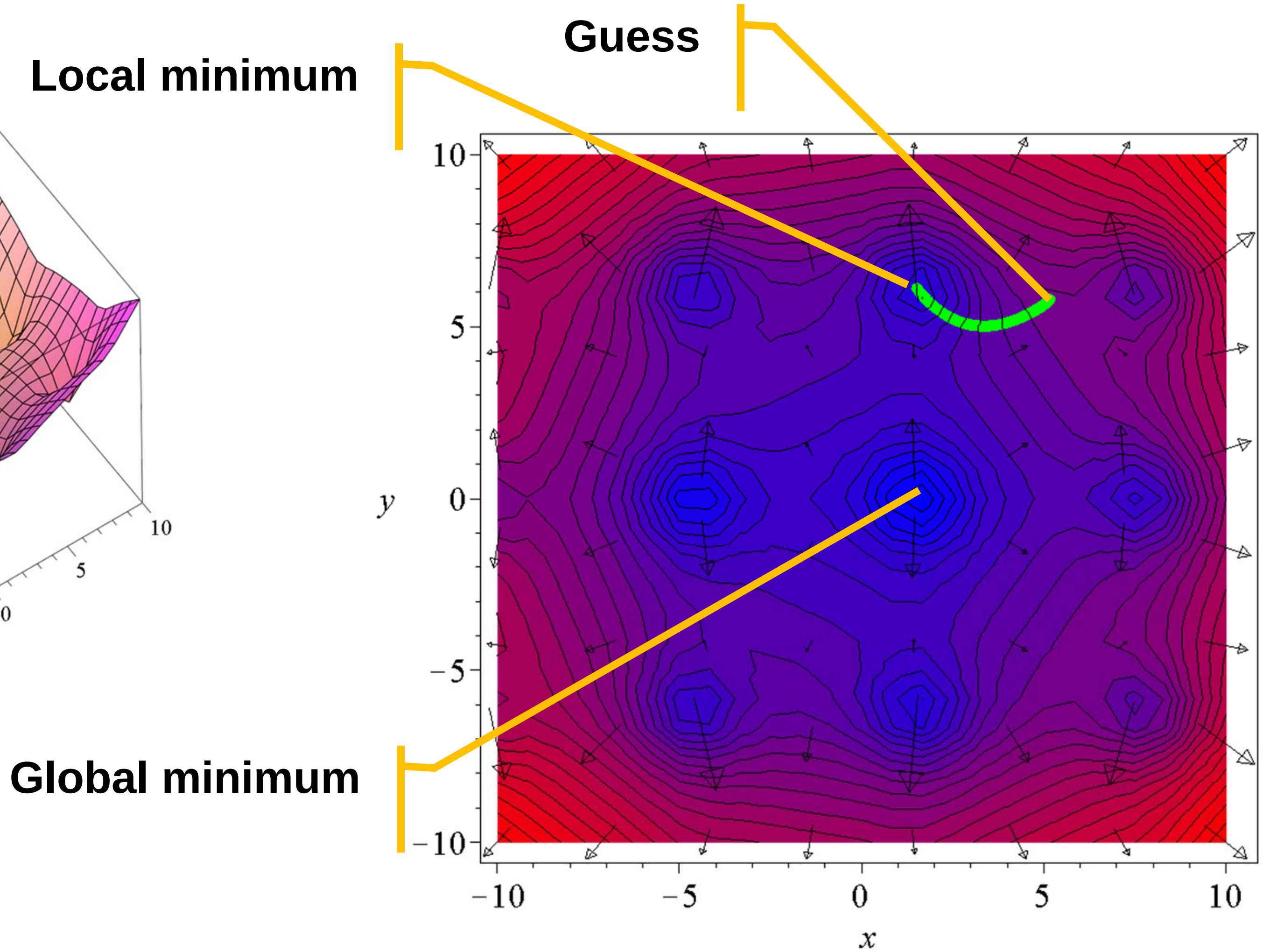



Top view

# Fundamental problems: Local minima





# The world is much larger

**Tools for Optimisation**

- Quasi-Newton / conjugate gradient methods
- Box (complex) / Hook-Jeeves
- Genetic algorithms (Evolution Strategy)
- and many more

# What did we learn today?

Formulate the objective function (metric) of your design

Gradient descent method is a possible way to find the minimum of your objective function

An optimum is (almost) always a compromise (competing metrics!)

Optimisation methods have limitations

# Success!

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