Advanced computational statistics, lecture 4

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LINKÖPING UNIVERSITY

Course schedule

- Topic 1: **Gradient based optimisation**
- Topic 2: **Stochastic gradient based optimisation**
- Topic 3: **Gradient free optimisation**
- Topic 4: **Optimisation with constraints**
- Topic 5: **EM algorithm and bootstrap**
- Topic 6: **Simulation of random variables**
- Topic 7: **Importance sampling**

Course homepage:
http://www.adoptdesign.de/frankmillereu/adcompstat2023.html

Includes schedule, reading material, lecture notes, assignments

Today’s schedule

Optimisation with constraints

- Equality constraints
  - Transformation to an unconstrained problem
  - Modification of iterative algorithm to handle constraints
  - Lagrange multipliers
- Inequality constraints
  - Karush–Kuhn–Tucker approach
  - penalty method
  - barrier method
- Combinatorial constrained optimisation

Optimisation with equality constraints

- Optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$ (equality constraints)

Optimisation with equality constraints

- Optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, $g\colon \mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$ (equality constraints)
- Approaches:
  - Transformation to an unconstrained problem (problem specific approach)
  - Modification of iterative algorithm to handle constraints (algorithm specific approach)
  - Lagrange multipliers (general approach)
- $\mathbb{S} = \{\boldsymbol{x} \in \mathbb{R}^p | h_i(\boldsymbol{x}) = 0,\ i = 1, \dots, m\}$ called <u>feasible points</u>

Equality constraints: transformation

- Example: Cubic regression model for fertilizer-yield-relation-ship with fertilizer $x \in [0,1.2]$. Experiment planned with
    - proportion w_1 of observations using $x_1 = 0$,
    - proportion w_2 using $x_2 = 0.4$,
    - proportion w_3 using $x_3 = 0.8$,
    - proportion w_4 using $x_4 = 1.2$.
- Note that $w_1 + w_2 + w_3 + w_4 = 1$.
- Information matrix $\boldsymbol{M}$ (proportional to inverse of covariance matrix for $\left(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3\right)^T$):
  $\boldsymbol{M} = \boldsymbol{X}^T \operatorname{diag}(w_1, \dots, w_4)\boldsymbol{X} = \sum_{i=1}^4 w_i \boldsymbol{f}(x_i)\, \boldsymbol{f}(x_i)^T$ with $\boldsymbol{f}(x) = (1, x, x^2, x^3)^T$
- The D-optimal design maximises
  $g(\boldsymbol{w}) = \det\left(\sum_{i=1}^4 w_i \boldsymbol{f}(x_i)\, \boldsymbol{f}(x_i)^T\right)$ subject to $h_1(\boldsymbol{w}) = 1 - \sum_{i=1}^4 w_i = 0$

Equality constraints: transformation

- The D-optimal design maximises
  $g(\boldsymbol{w}) = \det\left(\sum_{i=1}^{4} w_i \boldsymbol{f}(x_i)\,\boldsymbol{f}(x_i)^T\right)$ subject to $h_1(\boldsymbol{w}) = 1 - \sum_{i=1}^{4} w_i = 0$
- Transformation: $1 - \sum_{i=1}^{4} w_i = 0 \;\Rightarrow\; w_4 = 1 - w_1 - w_2 - w_3$
  $\tilde{g}(w_1, w_2, w_3) = \det\left(\sum_{i=1}^{3} w_i \boldsymbol{f}(x_i)\,\boldsymbol{f}(x_i)^T + (1 - w_1 - w_2 - w_3)\boldsymbol{f}(x_4)\boldsymbol{f}(x_4)^T\right)$
- The <u>constrained</u> optimisation problem
  max. $g(w_1, w_2, w_3, w_4)$ subj. to $h_1(w_1, w_2, w_3, w_4) = 1 - \sum_{i=1}^{4} w_i = 0$
  is equivalent to the <u>unconstrained</u> optimisation problem
  maximise $\tilde{g}(w_1, w_2, w_3)$.
- Solution with **`optim`**: $(w_1, w_2, w_3) = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $w_4 = 1 - \frac{3}{4} = \frac{1}{4}$

Equality constraints: modification of algorithms

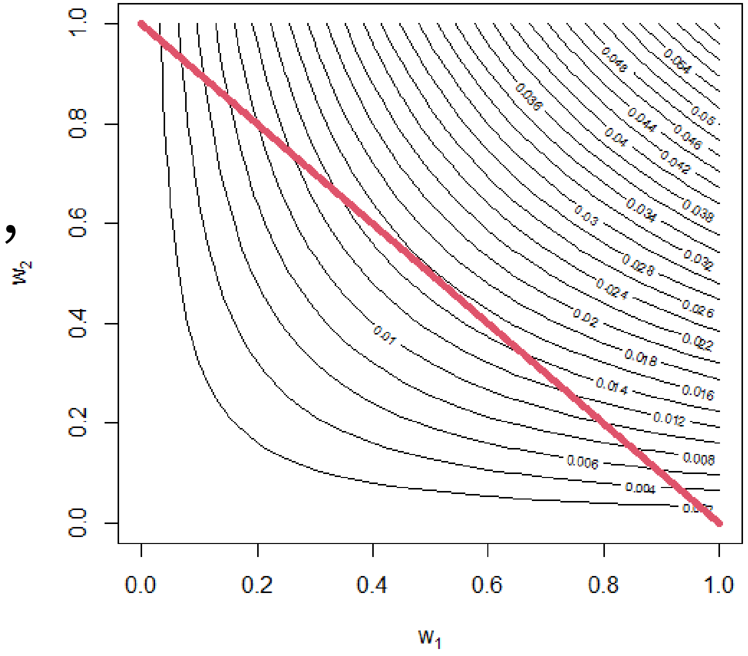
- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \rightarrow \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $\boldsymbol{Ax}^* - \boldsymbol{b} = \boldsymbol{0}$, $\boldsymbol{A} \in \mathbb{R}^{m \times p}, \boldsymbol{b} \in \mathbb{R}^m$ (linear equality constraints)
- Example: Particle Swarm Optimisation (see L3)
- Movement of particle i at iteration t+1:
  - $\boldsymbol{x}_i^{(t+1)} = \boldsymbol{x}_i^{(t)} + \boldsymbol{v}_i^{(t+1)}$
  - $\boldsymbol{v}_i^{(t+1)} = \mathrm{w}\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\,i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$

Scalar random variables (SPSO2011), not random vectors (SPSO2007)

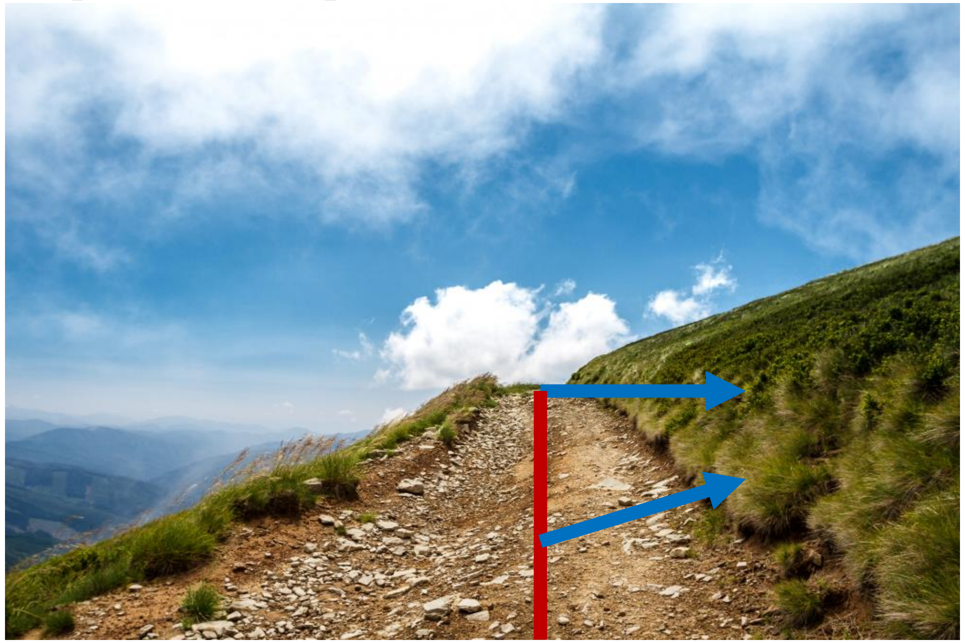
- $R_1^{(t+1)}$ and $R_2^{(t+1)}$ are uniformly distributed, `runif()`
- Ensure that $\boldsymbol{Ax}_i^{(0)} = \boldsymbol{b}$ and $\boldsymbol{Av}_i^{(0)} = \boldsymbol{0}$, then $\boldsymbol{Ax}_i^{(t)} = \boldsymbol{b}$ for all i and t

Equality constraints: Lagrange multipliers

- Example: D-optimal design for quadratic regression without intercept. Experiment planned on $x \in [0,1]$ with
  - prop. w_1 of observations using $x_1 = 0.5$,
  - prop. w_2 using $x_2 = 1$,
  - $w_1 + w_2 = 1$.
- $g(\boldsymbol{w}) = \det(w_1 \begin{pmatrix} \frac{1}{4} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{16} \end{pmatrix} + w_2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix})$
- $h(\boldsymbol{w}) = 1 - w_1 - w_2$



Equality constraints: Lagrange multipliers



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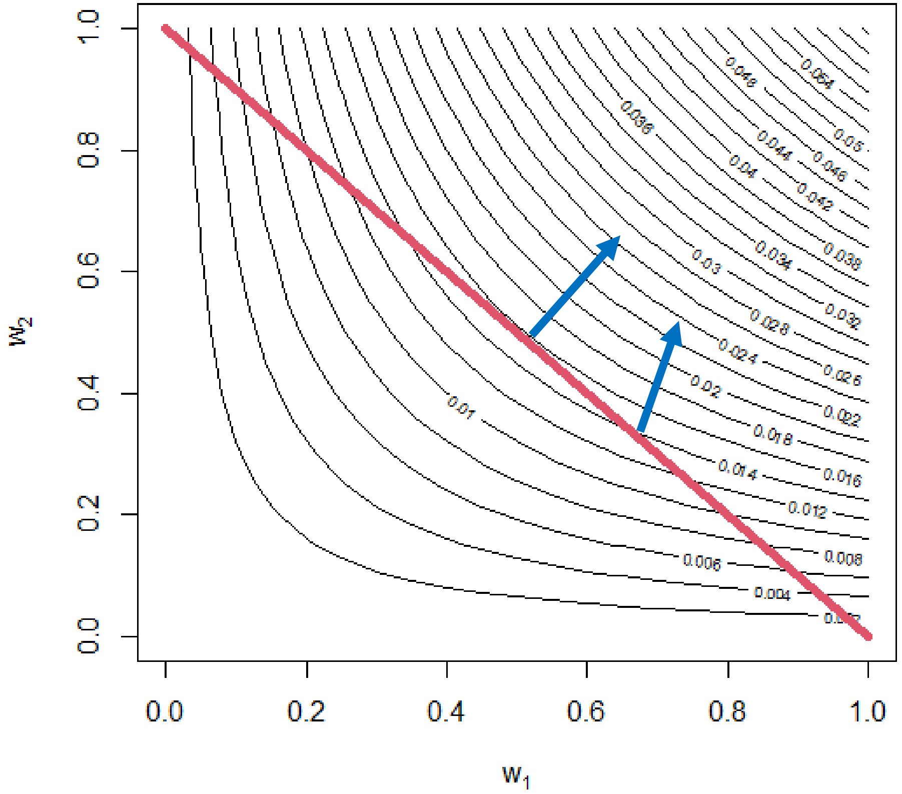
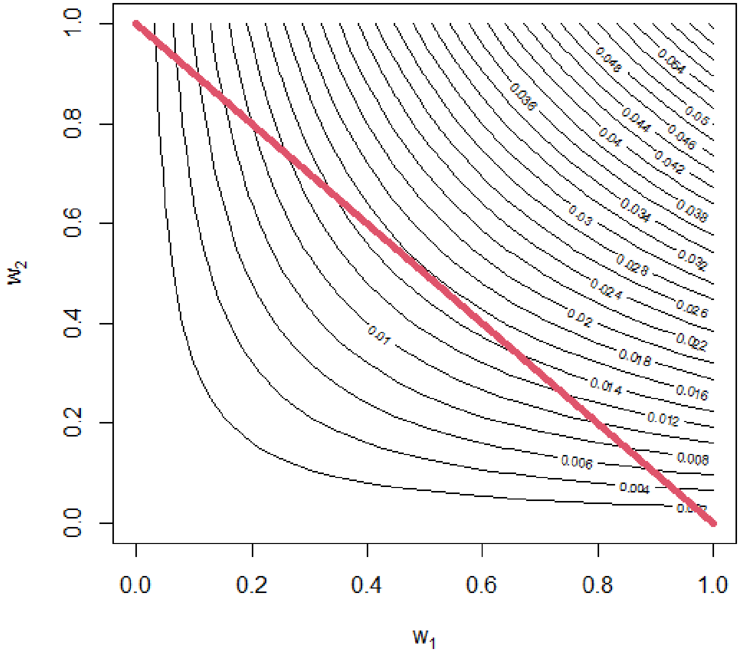


- Feasible points **w** (h(**w**)=0)
- Direction of steepest ascent, g'(**w**)

These two are orthogonal at constrained max.; direction orthogonal to feasible points is h'(**w**)

Equality constraints: Lagrange multipliers

- $g(\boldsymbol{w}) = \det\left(w_1 \begin{pmatrix} \frac{1}{4} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{16} \end{pmatrix} + w_2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right)$



- $h(\boldsymbol{w}) = 1 - w_1 - w_2$
- $g'(\boldsymbol{w})$ direction of steepest ascent
- $h'(\boldsymbol{w})=(-1,-1)^T$ (orthogonal to feasible points)

- Condition for constrained maximum: $g'(\boldsymbol{w}) = \lambda\, h'(\boldsymbol{w})$
- $g'(\boldsymbol{w}) - \lambda\, h'(\boldsymbol{w})=0$
- Define $\mathcal{L}(\boldsymbol{w}, \lambda) = g(\boldsymbol{w}) - \lambda\, h(\boldsymbol{w})$ and determine stationary point

Equality constraints: Lagrange multipliers

- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$ (equality constraints)
- Lagrange:
  Let $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = g(\boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x})$, $\boldsymbol{h}(\boldsymbol{x}) = (h_1(\boldsymbol{x}), \dots, h_m(\boldsymbol{x}))^T, \boldsymbol{\lambda} \in \mathbb{R}^m$ and $g, h_1, \dots, h_m$ are continuously differentiable. If g has a local maximum at some point $\boldsymbol{x}^*$ with $\boldsymbol{h}(\boldsymbol{x}^*) = \mathbf{0}$ (i.e. in the constrained maximisation problem) and at which the gradients of $h_1, \dots, h_m$ are linearly independent, then there exists a $\boldsymbol{\lambda}$ such that gradient $\mathcal{L}'(\boldsymbol{x}^*, \boldsymbol{\lambda}) = \mathbf{0}$ (i.e. stationary point in the unconstrained problem).

Equality constraints: Lagrange multipliers

- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, $g\colon\ \mathbb{R}^p \rightarrow \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$ (equality constraints)
- Unconstrained problem:
  Search stationary point $(\boldsymbol{x}^*, \boldsymbol{\lambda})$ of $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = g(\boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x})$.
- Note:
  - $\frac{\partial}{\partial \lambda_i}\mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}) = 0$ ensures $h_i(\boldsymbol{x}^*) = 0$
  - $\frac{\partial}{\partial x_i}\mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}) = 0$ ensures that gradient $g'(\boldsymbol{x}^*)$ is orthogonal to the set $\mathbb{S}$ of feasible points at $\boldsymbol{x} = \boldsymbol{x}^*$

Equality constraints: Comparison

- Recall example about D-optimal design for quadratic regression without intercept; optimal values for w_1 and w_2 are of interest (p=2, m=1).

In general:

- Transformation method: optimize over w_1 — dim = p – m,
- Modification of algorithm: optimize over (w_1, w_2) — dim = p,
- Lagrange multiplier method: search space is (w_1, w_2, λ) — dim = p + m

- If transformation method possible and not too complicated, it has potential to deliver results fastest
- Transformation and modification methods require creativity; Lagrange can be applied generally

Optimisation with inequality constraints

- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, $g\colon\ \mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$
  - and $q_i(\boldsymbol{x}^*) \leq 0,\ i = 1, \dots, n$ (inequality constraints)
- Set of feasible points $\mathbb{S} = \{\boldsymbol{x} \in \mathbb{R}^p | h_i(\boldsymbol{x}) = 0,\ i = 1, \dots, m; q_i(\boldsymbol{x}) \leq 0,\ i = 1, \dots, n\}$

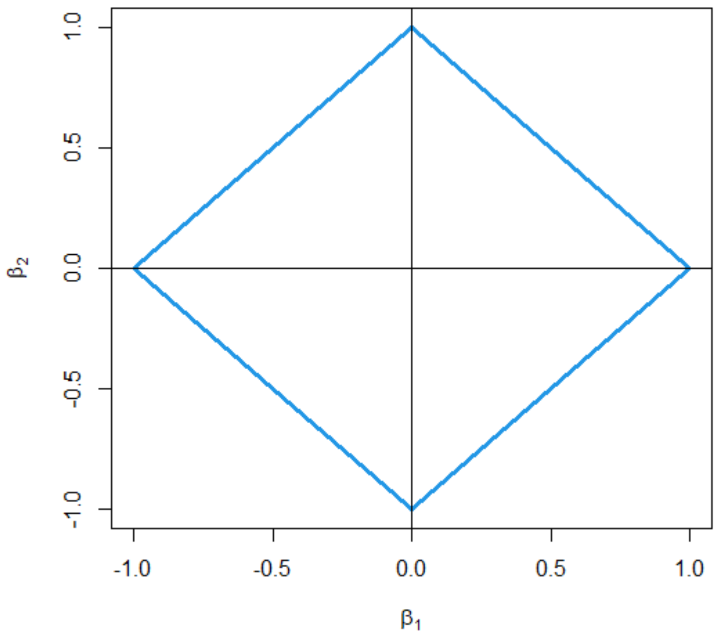
- An inequality constrained $q_\mathrm{i}(\boldsymbol{x})$ is called active, if $q_\mathrm{i}(\boldsymbol{x}^*) = 0$
- If it is not active ($q_\mathrm{i}(\boldsymbol{x}^*) < 0$), $\boldsymbol{x}^*$ is a local optimum of the unconstrained optimisation problem

Inequality constraints – lasso example

- Lasso's objective function to minimise:
  $g(\widehat{\boldsymbol{\beta}}) = \|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{y}\|^2 + \lambda \sum_{i=1}^{p} |\widehat{\beta}_i|$

- Alternatively, one can solve the constrained problem:
  minimise: $g(\widehat{\boldsymbol{\beta}}) = \|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{y}\|^2$
  subject to $\sum_{i=1}^{p} |\widehat{\beta}_i| \leq t$

- For p=2 and t=1, the set of feasible points $\mathbb{S} = \{\widehat{\boldsymbol{\beta}} \in \mathbb{R}^p | \sum_{i=1}^{p} |\widehat{\beta}_i| \leq t\}$ is inside of the blue area



Optimisation with inequality constraints

- Approaches to handle inequality constraints:
  - Generalisation of Lagrange multipliers (Karush–Kuhn–Tucker approach)
  - penalty method
  - barrier method (also called: interior-point method)

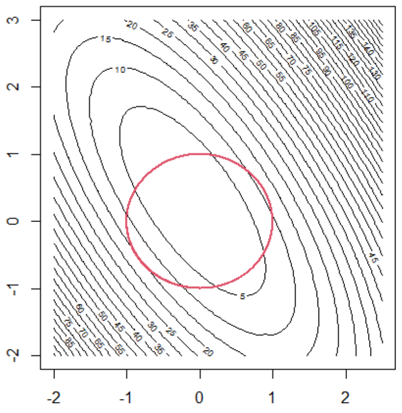
Inequality constraints: Karush-Kuhn-Tucker appr.

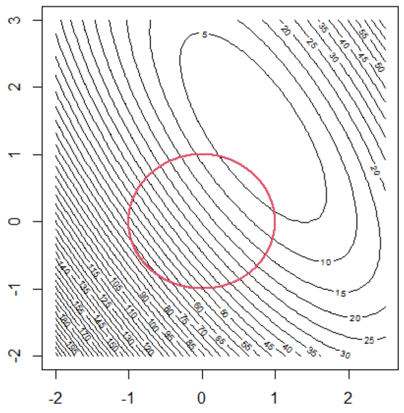
- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$
  - and $q_i(\boldsymbol{x}^*) \leq 0,\ i = 1, \dots, n$ (inequality constraints)

- Karush–Kuhn–Tucker (KKT) approach uses generalised Lagrangian $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = g(\boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x}) - \boldsymbol{\mu}^T \boldsymbol{q}(\boldsymbol{x})$ with $\boldsymbol{h}(\boldsymbol{x}) = (h_1(\boldsymbol{x}), \dots, h_m(\boldsymbol{x}))^T, \boldsymbol{\lambda} \in \mathbb{R}^{\boldsymbol{m}}, \boldsymbol{q}(\boldsymbol{x}) = (q_1(\boldsymbol{x}), \dots, q_n(\boldsymbol{x}))^T, \boldsymbol{\mu} \in \mathbb{R}^{\boldsymbol{n}}$
- Instead of above constrained optimisation, search stationary point $(\boldsymbol{x}^*, \boldsymbol{\lambda}, \boldsymbol{\mu} \geq \mathbf{0})$ of $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = g(\boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x}) - \boldsymbol{\mu}^T \boldsymbol{q}(\boldsymbol{x})$.
  For $\boldsymbol{x}^*$ being a solution of the constrained problem, following condition required: "for all i=1,…,n: $q_i(\boldsymbol{x}^*) = 0$ or $\mu_i = 0$"

Inequality constraints: KKT, example

- **Constrained LS-<u>min</u>imisation**:
  - $\boldsymbol{x}$ p-dim., g: $\mathbb{R}^p \to \mathbb{R}$, $g(\boldsymbol{x}) = \left\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\right\|_2^2$ $\|\boldsymbol{x}\|_2 \leq 1$
  - $g(\boldsymbol{x}) = \min g(\boldsymbol{x})$ subject to $q_1(\boldsymbol{x}) = \|\boldsymbol{x}\|_2^2 - 1 \leq 0$ (inequality constraint)
- Generalised Lagrangian (KKT): $\mathcal{L}(\boldsymbol{x}, \mu) = \left\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\right\|_2^2 + \mu(\|\boldsymbol{x}\|_2^2 - 1)$ with $\mu \geq 0$
- $\frac{\partial}{\partial x}\mathcal{L}(\boldsymbol{x}, \mu) = \boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}^T\boldsymbol{b} + 2\mu\boldsymbol{x}$; setting this to 0 gives $\boldsymbol{x} = (\boldsymbol{A}^T\boldsymbol{A} + 2\mu\boldsymbol{I})^{-1}\,\boldsymbol{A}^T\boldsymbol{b}$
- $\frac{\partial}{\partial \mu}\mathcal{L}(\boldsymbol{x}, \mu) = 1 - \|\boldsymbol{x}\|_2^2$





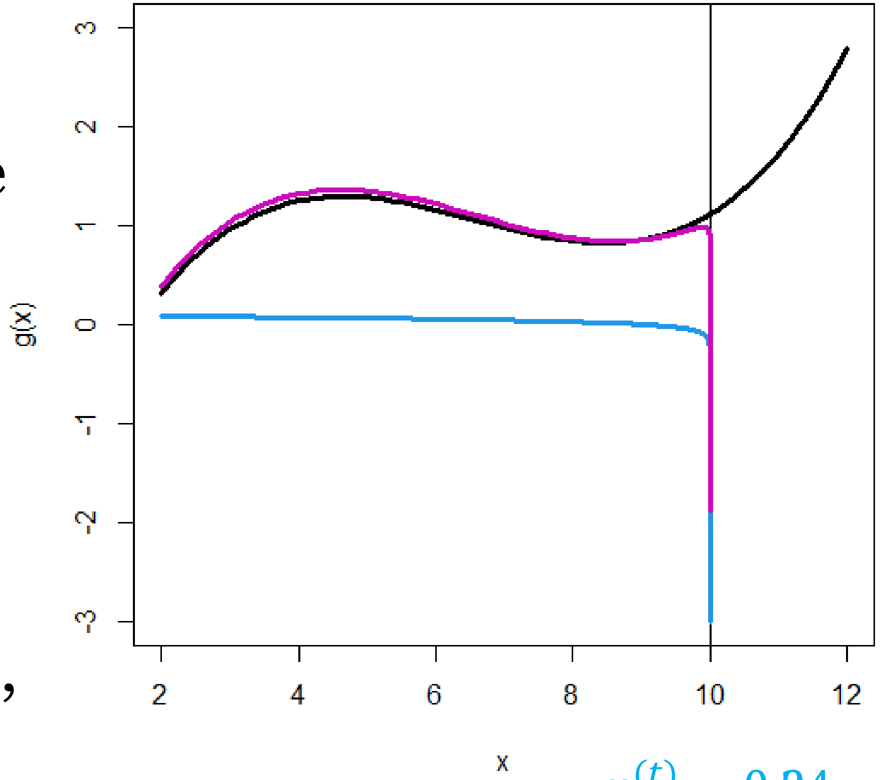
Inequality constraints: penalty and barrier methods

- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, $g\colon \mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $q_i(\boldsymbol{x}^*) \geq 0,\ i = 1, \dots, n$ (inequality constraints)
- Idea: Modify g to $\tilde{g}$ such that the algorithm finds only local maxima which fulfil $q_i(\boldsymbol{x}^*) \geq 0,\ i = 1, \dots, n$, even if optimisation done unconstrained

- Penalty methods: Set $\tilde{g} = g$ on $\mathbb{S} = \{\boldsymbol{x} | q_i(\boldsymbol{x}) \geq 0,\ i = 1, \dots, n\}$ and add a (negative) penalty if $q_i(\boldsymbol{x}) < 0$ for some $\boldsymbol{i}$
- Barrier methods: Set $\tilde{g} = -\infty$ if $q_i(\boldsymbol{x}) < 0$ for some $\boldsymbol{i}$ and g is modified on $\mathbb{S} = \{\boldsymbol{x} | q_i(\boldsymbol{x}) \geq 0,\ i = 1, \dots, n\}$

Inequality constraints: Barrier method

- Example: maximise g(x) on range x ≤ 10
- Add barrier function $\mu^{(t)} b(x)$
- $\tilde{g}(x) = g(x) + \mu^{(t)} b(x)$ should be small close to 10, x<10, and $-\infty$ for x>10
- Log barrier: $b(x) = \log(10 - x)$
- Solve maximisation for $\tilde{g}(x)$
- Adapt barrier with smaller $\mu^{(t)}$
- If $\mu^{(t)} \to 0$, local maxima of g can be detected, both at the boundary and in the interior



$\mu^{(t)} = 0.04$

Two 2d-animations: http://apmonitor.com/me575/index.php/Main/InteriorPointMethod

Linear inequality constraints: R-function `constrOptim`

- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $\boldsymbol{U}\boldsymbol{x}^* - \boldsymbol{c} \geq \boldsymbol{0}$, $\boldsymbol{U} \in \mathbb{R}^{n \times p}, \boldsymbol{c} \in \mathbb{R}^n$ (linear inequality constraints; rows of $\boldsymbol{U}$ are $\boldsymbol{u}_i^T$)

- The R-function **`constrOptim`** uses log barrier functions
- **`constrOptim`** calls repeatedly **`optim`** for function $\tilde{g}$ with barrier; barrier adapted between iterations: $\mu^{(\boldsymbol{t})}$ decreases
- E.g: $\tilde{g}(\boldsymbol{x}) = g(\boldsymbol{x}) + \mu^{(\boldsymbol{t})} \sum_{i=1}^{n} \log(\boldsymbol{u}_i^T \boldsymbol{x} - c_i)$ (for maximisation; $g(\boldsymbol{x}) - \mu^{(\boldsymbol{t})}$ ... for minimisation)

Linear inequality constraints: barrier method

- Example: Quadratic regression for fertilizer-yield-relation-ship with fertilizer $x \in [0,1.2]$. Experiment planned with
  - proportion w_i of observations using $x_i \in [0,1.2]$ (can be chosen by experimenter), i=1,2,3; $w_3 = 1 - w_1 - w_2$.
- Parameters to be optimised: $\boldsymbol{y} = (x_1, x_2, x_3, w_1, w_2)^T$
- D-optimal design maximises $g(\boldsymbol{y}) = \det\left(\sum_{i=1}^{3} w_i \boldsymbol{f}(x_i)\, \boldsymbol{f}(x_i)^T\right)$ subject to $x_i \geq 0$, $1.2 - x_i \geq 0$, i=1,2,3, $w_1 \geq 0$, $w_2 \geq 0$, $1 - w_1 - w_2 \geq 0$
- Construct $\boldsymbol{U}$ and $\boldsymbol{c}$ such that constraints can be written as $\boldsymbol{U}\boldsymbol{y} - \boldsymbol{c} \geq \boldsymbol{0}$

Linear inequality constraints: barrier method

- $\boldsymbol{y} = (x_1, x_2, x_3, w_1, w_2)^T$, $w_3 = 1 - w_1 - w_2$
- D-optimal design maximises $g(\boldsymbol{y}) = \det\left(\sum_{i=1}^{3} w_i \boldsymbol{f}(x_i)\, \boldsymbol{f}(x_i)^T\right)$ subject to $x_i \geq 0$, $1.2 - x_i \geq 0$, i=1,2,3, $w_1 \geq 0$, $w_2 \geq 0$, $1 - w_1 - w_2 \geq 0$
- $\boldsymbol{U}\boldsymbol{y} - \boldsymbol{c} \geq \boldsymbol{0}$ with

$$\boldsymbol{U} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & -1 \end{pmatrix}, \boldsymbol{c} = \begin{pmatrix} 0 \\ -1.2 \\ 0 \\ -1.2 \\ 0 \\ -1.2 \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

Linear inequality constraints: R-function `constrOptim`

- R-code:
- ```
  U       <- matrix(0, nrow=9, ncol=5)
  U[1,1] <- U[3,2] <- U[5,3] <- U[7,4] <- U[8,5] <- 1
  U[2,1] <- U[4,2] <- U[6,3] <- U[9,4] <- U[9,5] <- -1
  d       <- c(rep(c(0, -1.2), 3), 0, 0, -1)

  startv <- c(0.2, 0.3, 0.4, 0.2, 0.2)

  # Nelder-Mead as inner optimisation method:
  res     <- constrOptim(startv, f=g, grad=NULL, ui=U, ci=d,
                         control=list(fnscale=-1))
  round(res$par, 3)
  ```
- Result: `0.000 0.597 1.200 0.331 0.333`
- Note: In this case, the solution can also be calculated algebraically (optimal design theory)
  ```

Linear inequality constraints: barrier method

- Limitations of barrier method (Lange, 2010, page 301):
  - Iterations within iterations necessary
  - No obvious choice how fast $\mu^{(t)}$ should go to 0
  - A too small value $\mu^{(t)}$ can lead to numerical instability

Combinatorial constrained optimisation

Recall L3 and Exercise 3.4: Maximising information of experimental designs

- Regression model **y**=**X β** + **ε**, $\mathrm{Cov}(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1} \cdot const$
- Example: cubic regression,

$$y_i = \beta_0 + \beta_1 w_i + \beta_2 w_i^2 + \beta_3 w_i^3 + \varepsilon_i, \quad \boldsymbol{X} = \begin{pmatrix} 1 & w_1 & w_1^2 & w_1^3 \\ 1 & w_2 & w_2^2 & w_2^3 \\ \dots & \dots & \dots & \dots \\ 1 & w_n & w_n^2 & w_n^3 \end{pmatrix}$$

  w_i can be chosen in [-1, 1], but practical circumstances require here a distance between design points of 0.05
- Therefore, we allow design points {-1, -0.95, -0.9, …, 1} a~~nd at most one observation can be done at each point~~

  $\mathbb{S} = \{(n_1, \dots, n_{41}), n_i \in \mathbb{N}_0\}$
- A design can be represented by a vector in ~~$\mathbb{S} = \{0, 1\}^{41}$~~ where 0 means that no observation is done at a design point and 1 means that one observation is made there
- Each observation has a cost; and we want to minimise the penalized D-optimality

$$\#\mathrm{observations} * 0.2 - \log\left(\det\left(\boldsymbol{X}^T\boldsymbol{X}\right)\right)$$

Constrained optimisation to determine design

- Regression model $\mathbf{y}=\mathbf{X}\,\boldsymbol{\beta}+\boldsymbol{\varepsilon}$, $\mathrm{Cov}(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\cdot const$
- Example: cubic regression,

$$y_i = \beta_0 + \beta_1 w_i + \beta_2 w_i^2 + \beta_3 w_i^3 + \varepsilon_i, \quad \boldsymbol{X} = \begin{pmatrix} 1 & w_1 & w_1^2 & w_1^3 \\ 1 & w_2 & w_2^2 & w_2^3 \\ \dots & \dots & \dots & \dots \\ 1 & w_n & w_n^2 & w_n^3 \end{pmatrix}$$

  w_i can be chosen in [-1, 1], but practical circumstances require here a distance between design points of 0.05; hence, we allow design points {-1, -0.95, -0.9, ..., 1}
- A design can be represented by a vector in $\mathbb{S} = \{(n_1, \dots, n_{41}), n_i \in \mathbb{N}_0\}$ with n_1 being number of observations made at w_i
- We have a restricted budget allowing for n observations, i.e. $\sum_{i=1}^{41} n_i = n$.
- We want to minimise the D-criterion $-\log\left(\det(\boldsymbol{X}^T\boldsymbol{X})\right)$

Constrained optimisation to determine design

- We can easily adjust the simulated annealing algorithm for combinatorial optimisation to handle the equality constraint $\sum_{i=1}^{41} n_i = n$:
  - Start with a design fulfilling the constraint
  - Define neighbourhood of a design such that all neighbours fulfil restriction (proposal distribution has probability 1 on designs with $\sum_{i=1}^{41} n_i = n$)
  - An intuitive possibility is to **exchange** observations:

    (2, 0, 0, 4, 5, 0, 0, 0, 3, 1, 0, ..., 0, 4) ->
    (2, 1, 0, 4, 4, 0, 0, 0, 3, 1, 0, ..., 0, 4)
  - Search randomly a location (here of the 41 w_i's) which has $n_i > 0$ where an observation is removed and another location where one is added

Constrained optimisation to determine design

- Start design fulfilling constraint

```
des     <- rep(0, 41)
indices <- 1:41
for (i in 1:n){
  ind      <- sample(indices, size=1)
  des[ind] <- des[ind]+1
}
```

- Determine randomly a neighbour (exchanging points of observation)

```
irem         <- sample(indices[des>0], size=1)
iadd         <- sample(indices, size=1)
desnew       <- des
desnew[irem] <- desnew[irem]-1
desnew[iadd] <- desnew[iadd]+1
```

Constrained optimisation to determine design

- Design space
```
w   <- seq(-1, 1, by=0.05)
```
- The vector of observational points inclusive duplicates can be generated by
```
xv <- rep(w, des)
```