Optimisation algorithms in Statistics I, lecture 4

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Course schedule

- Topic 1: **Gradient based algorithms**
  Lectures: October 2; Time 10-12, 13-15 (online, Zoom)
- Topic 2: **Stochastic gradient based algorithms**
  Lecture: October 13; Time: 9-12 (online, Zoom)
- Topic 3: **Gradient free algorithms**
  Lecture: October 23; Time 9-12 (online, Zoom)
- Topic 4: **Optimisation with restrictions**
  Lecture: November 6, Time 9-12 (online, Zoom)

Course homepage: http://gauss.stat.su.se/phd/oasi/

Includes reading material, lecture notes, assignments

Today's schedule

- Optimisation with constraints
  - Equality constraints
  - Inequality constraints

- Remarks
  - Simulated annealing

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 $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \ldots, m$ (equality constraints)

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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)

- Approaches:
  - Transformation to an unconstrained problem (problem specific approach)
  - Modification of iterative algorithm to reflect 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 feasible points

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Optimisation with equality constraints – transformation

- Example: Cubic regression model for fertilizer-yield-relationship 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 M (proportional to inverse of covariance matrix for $\left(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3\right)^T$): $M = X^T \mathrm{diag}(w_1, \dots, w_4) X = \sum_{i=1}^4 w_i \boldsymbol{f}(x_i)\, \boldsymbol{f}(x_i)^T$ 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 $h_1(\boldsymbol{w}) = 1 - \sum_{i=1}^4 w_i = 0$

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Optimisation with 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 constrained 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 unconstrained optimisation problem
  maximise $\tilde{g}(w_1, w_2, w_3)$.

- Solution with **`optim`**: $(w_1, w_2, w_3) = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $w_4 = 1 - \frac{3}{4} = \frac{1}{4}$

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Optimisation with equality constraints – modification of algorithms

- 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 $\boldsymbol{A}\boldsymbol{x}^* - \boldsymbol{b} = \boldsymbol{0}$, $\boldsymbol{A} \in \mathbb{R}^{m \times p}, \boldsymbol{b} \in \mathbb{R}^m$ (linear equality constraints)
- Example: Particle Swarm Optimisation (see L3)
- Movement of particle *i* at iteration t+1:
  - $\boldsymbol{x}_i^{(t+1)} = \boldsymbol{x}_i^{(t)} + \boldsymbol{v}_i^{(t+1)}$
  - $\boldsymbol{v}_i^{(t+1)} = \mathrm{w}\boldsymbol{v}_i^{(t)} + c_1 R_1^{(t+1)} (\boldsymbol{p}_{\text{best},\, i}^{(t)} - \boldsymbol{x}_i^{(t)}) + c_2 R_2^{(t+1)} (\boldsymbol{g}_{\text{best}}^{(t)} - \boldsymbol{x}_i^{(t)})$
- $R_1^{(t+1)}$ and $R_2^{(t+1)}$ are uniformly distributed, **`runif()`**
- Ensure that $\boldsymbol{A}\boldsymbol{x}_i^{(0)} = \boldsymbol{b}$ and $\boldsymbol{A}\boldsymbol{v}_i^{(0)} = \boldsymbol{0}$,
  then $\boldsymbol{A}\boldsymbol{x}_i^{(t)} = \boldsymbol{b}$ for all *i* and *t*

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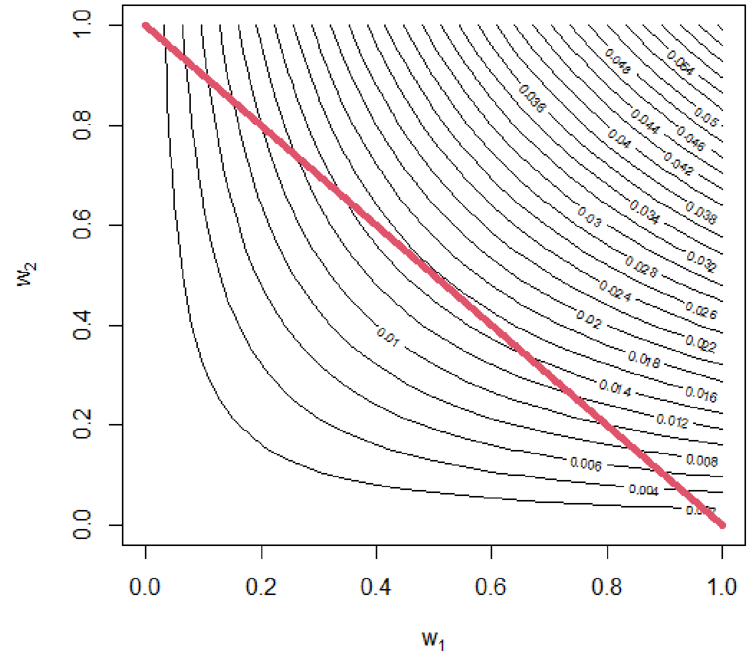
Optimisation with equality constraints – Lagrange multipliers

- 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 $x_2 = 1$,
  - $w_1 + w_2 = 1$.

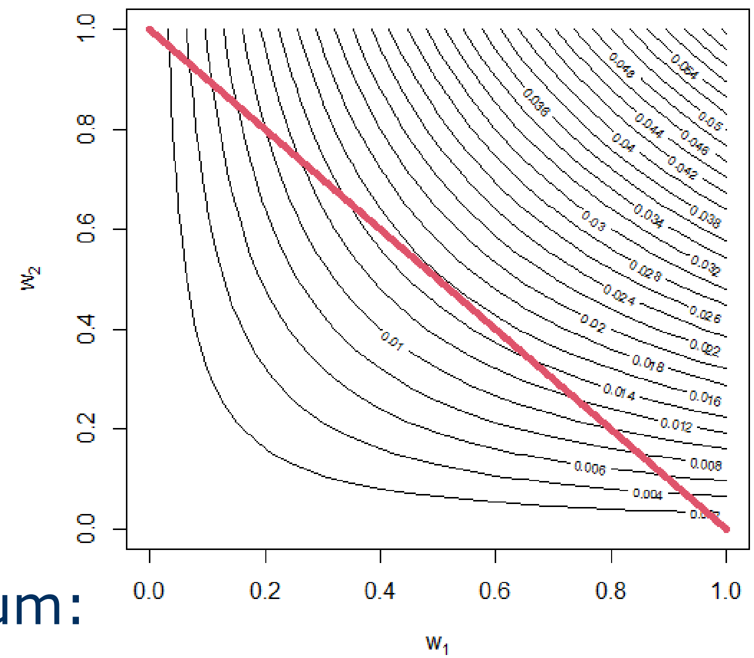


- $g(\boldsymbol{w}) = \det\left(w_1 \begin{pmatrix} \frac{1}{4} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{16} \end{pmatrix} + w_2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right)$

- $h(\boldsymbol{w}) = 1 - w_1 - w_2$

Optimisation with 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
- $h'(\boldsymbol{w})=(-1,-1)^T$



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

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Optimisation with 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 $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = g(\boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x})$, $\boldsymbol{h}(\boldsymbol{x}) = (h_1(\boldsymbol{x}), \dots, h_m(\boldsymbol{x}))^T, \boldsymbol{\lambda} \in \mathbb{R}^{\boldsymbol{m}}$ and $g, h_1, \dots, h_m$ are continuously differentiable. If g has a local maximum at some point $\boldsymbol{x}^*$ with $\boldsymbol{h}(\boldsymbol{x}^*) = \boldsymbol{0}$ (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 $\mathcal{L}'(\boldsymbol{x}^*, \boldsymbol{\lambda}) = \boldsymbol{0}$ (i.e. stationary point in the unconstrained problem).

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Optimisation with equality constraints – Lagrange multipliers

- 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 $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$ (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 $\boldsymbol{x} = \boldsymbol{x}^*$

Optimisation with inequality constraints

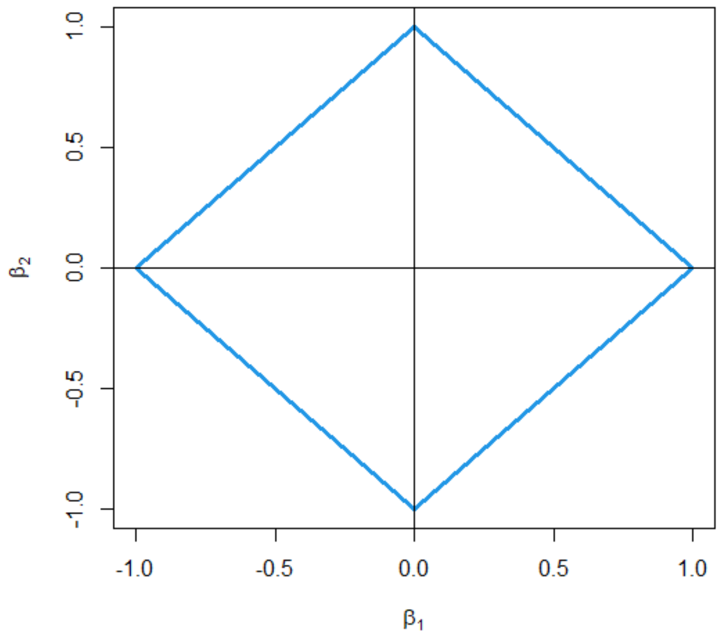
- Constrained optimisation problem:
  - $\boldsymbol{x}$ p-dimensional vector, $g: \mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $h_i(\boldsymbol{x}^*) = 0,\ i = 1, \dots, m$
  - and $q_i(\boldsymbol{x}^*) \leq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

  $\mathbb{S} = \{\boldsymbol{x} \in \mathbb{R}^p | h_i(\boldsymbol{x}) = 0,\ i = 1, \dots, m; q_i(\boldsymbol{x}) \leq 0,\ i = 1, \dots, n\}$

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

Optimisation with inequality constraints – lasso example

- Lasso's objective function to minimise:
  $g(\widehat{\boldsymbol{\beta}}) = \left\|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{y}\right\|^2 + \lambda \sum_{i=1}^{p} \left|\widehat{\beta}_i\right|$
- Alternatively, one can solve the constrained problem:
  minimise: $g(\widehat{\boldsymbol{\beta}}) = \left\|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{y}\right\|^2$
  subject to $\sum_{i=1}^{p} \left|\widehat{\beta}_i\right| \leq t$
- For p=2 and t=1, the set of feasible points $\mathbb{S} = \left\{\widehat{\boldsymbol{\beta}} \in \mathbb{R}^p \,\middle|\, \sum_{i=1}^{p} \left|\widehat{\beta}_i\right| \leq t\right\}$ is inside of the blue area



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Optimisation with inequality constraints – Karush–Kuhn–Tucker approach

- 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 $(\boldsymbol{x}^*, \boldsymbol{\lambda}, \boldsymbol{\mu} \geq \boldsymbol{0})$ 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 $\mu_i = 0$"

Optimisation with inequality constraints – penalty and barrier methods

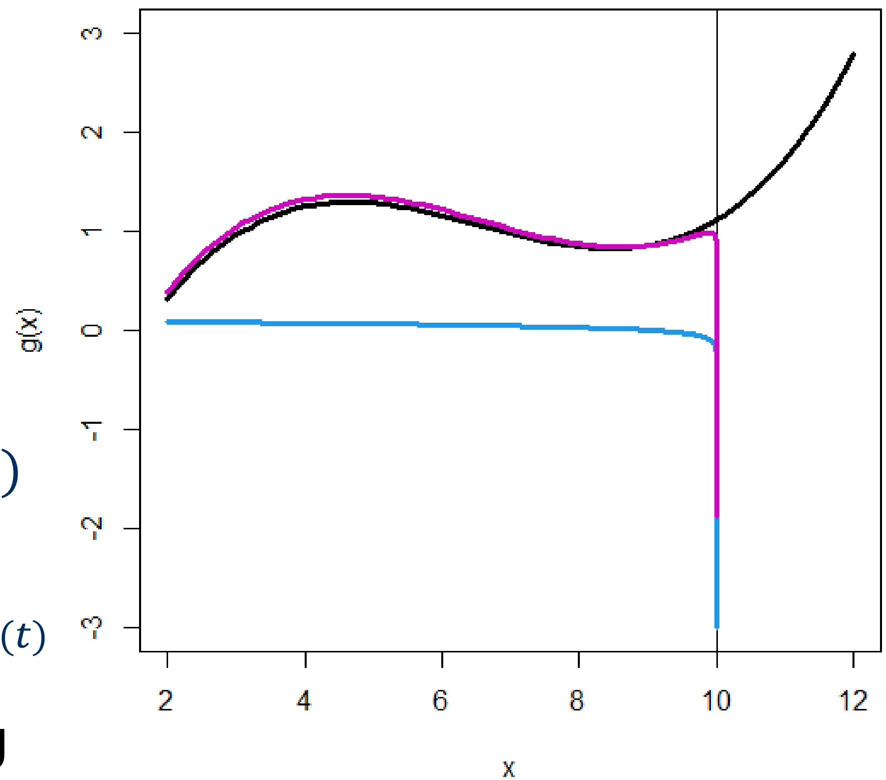
- Constrained optimisation problem:
  - $\boldsymbol{x}$ *p*-dimensional vector, $g: \mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
  - Subject to $q_i(\boldsymbol{x}^*) \geq 0,\ i = 1, \ldots, n$ (inequality constraints)

- Idea: Modify *g* to $\tilde{g}$ such that the algorithm finds only local maxima which fulfil $q_i(\boldsymbol{x}^*) \geq 0,\ i = 1, \ldots, n$, even if optimisation done unconstrained

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

Optimisation with inequality constraints – Barrier method (interior-point 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 <u>at the boundary</u> and <u>in the interior</u>



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

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

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Optimisation with linear inequality constraints – R-function `constrOptim`

- 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 $\boldsymbol{U}\boldsymbol{x}^* - \boldsymbol{c} \geq \boldsymbol{0}$, $\boldsymbol{U} \in \mathbb{R}^{n\times p}, \boldsymbol{c} \in \mathbb{R}^n$ (linear inequality constraints; rows of 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: $\mu^{(t)}$ decreases
- E.g: $\tilde{g}(\boldsymbol{x}) = g(\boldsymbol{x}) + \mu^{(t)} \sum_{i=1}^{n} \log(\boldsymbol{u}_i^T \boldsymbol{x} - c_i)$ (for maximisation; $g(\boldsymbol{x}) - \mu^{(t)}$ … for minimisation)

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Optimisation with linear inequality constraints – barrier method

- Example: Quadratic regression for fertilizer-yield-relationship with fertilizer $x \in [0,1.2]$. Experiment planned with
  - proportion w_i of observations using $x_i \in [0,1.2]$ (<u>can be chosen by experimenter</u>), 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 $\boldsymbol{U}\boldsymbol{y} - \boldsymbol{c} \geq \boldsymbol{0}$

Optimisation with 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 $x_i \geq 0$, $1.2 - x_i \geq 0$, $w_1 \geq 0$, $w_2 \geq 0$, $1 - w_1 - w_2 \geq 0$
- $\boldsymbol{U}\boldsymbol{y} - \boldsymbol{c} \geq \boldsymbol{0}$ with

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

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Optimisation with 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 is algebraically known based on optimal design theory
  ```

Optimisation with 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

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Other topics

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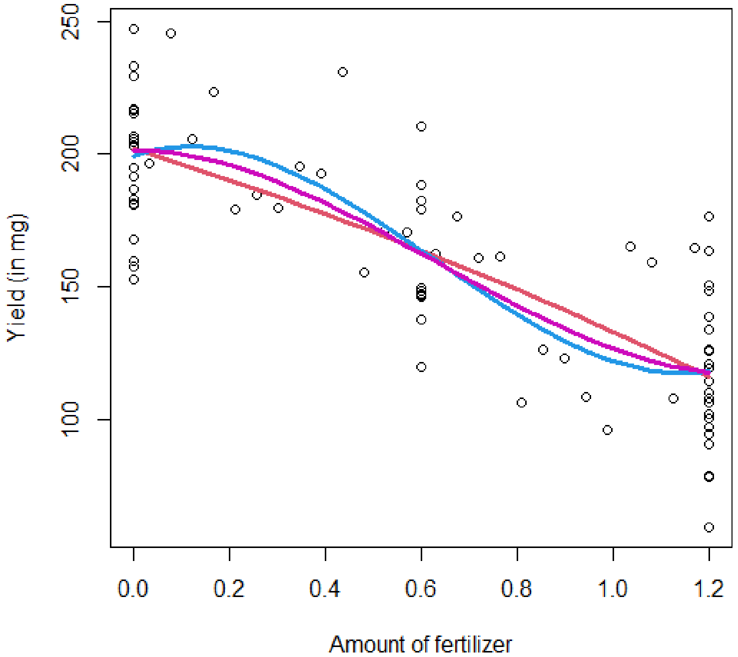
About the cress experiment – Problem 3.3

- Design chosen has some optimality property assuming a quadratic regression with some robustness if other model valid
- Regressions: quadratic; cubic; cubic without linear term



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Gradient free optimisation – Simulated annealing

- Start value $x^{(0)}$; Stage j=0,1,2,… has m_j iterations; set j=0
- Given iteration $x^{(t)}$, generate $x^{(t+1)}$ as follows:

1. Sample a candidate x^* from a proposal distribution $p(\cdot|x^{(t)})$
2. Compute $h\left(x^{(t)}, x^*\right) = \exp(\frac{g(x^*)-g\left(x^{(t)}\right)}{\tau_j})$

   $g\left(x^{(t)}\right) - g(x^*)$ for minimisation

3. Define next iteration $x^{(t+1)}$ according to

$$x^{(t+1)} = \begin{cases} x^*, \text{with probability} \min\{h\left(x^{(t)}, x^*\right), 1\} \\ x^{(t)}, \text{otherwise} \end{cases}$$

4. Set `t <- t+1` and repeat 1.-3. m_j times
5. Update $\tau_j = \alpha(\tau_{j-1})$ and $m_j = \beta(m_{j-1})$; set `j <- j+1`; go to 1

τ_j is temperature; function α should slowly decrease it

Function β should be increasing

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Markov Chain Monte Carlo (MCMC) – Metropolis-Hastings algorithm

- Metropolis-Hastings (MH) algorithm:
- A starting value $x^{(0)}$ is generated from some starting distribution
- Given observation $x^{(t)}$, generate $x^{(t+1)}$ as follows:

1. Sample a candidate x^* from a proposal distribution $g(\cdot|x^{(t)})$
2. Compute the MH ratio $R\left(x^{(t)}, x^*\right) = \dfrac{f(x^*)\, g\left(x^{(t)} \middle| x^*\right)}{f\left(x^{(t)}\right) g\left(x^* \middle| x^{(t)}\right)}$
3. Sample $x^{(t+1)}$ according to

$$x^{(t+1)} = \begin{cases} x^*, \text{with probability} \min\{R\left(x^{(t)}, x^*\right), 1\} \\ x^{(t)}, \text{otherwise} \end{cases}$$

4. If more observations needed, set `t <- t+1`; go to 1

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Remarks