Last Time:

- Root Finding
- Minimization
- Newton's Method
- Regularization
- Line Search

Today:

- Constrained Minimization
- Equality constraints
- Inequality Constraints

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* Equality Constraints

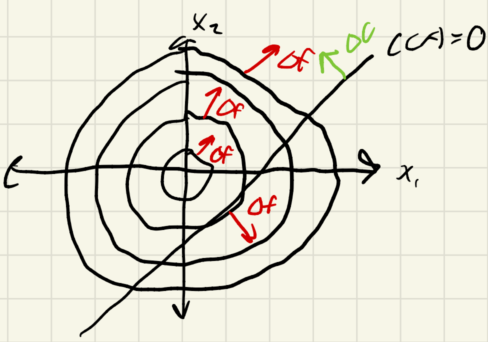
$$\min_x \quad f(x) \quad \leftarrow \quad f(x) : \mathbb{R}^n \to \mathbb{R}$$

$$\text{s.t.} \quad c(x) = 0 \quad \leftarrow \quad c(x) : \mathbb{R}^n \to \mathbb{R}^m$$

- First-Order necessary conditions

1) Need $\nabla f(x^*) = 0$ in <u>free</u> directions

2) Need $c(x^*) = 0$



$f(x) : \mathbb{R}^2 \to \mathbb{R}$

$c(x) : \mathbb{R}^2 \to \mathbb{R}$

* Any non-zero component of ∇f must be normal to the constraint surface/manifold

$$\Rightarrow \quad \nabla f + \underbrace{\lambda}_{\text{“Lagrange multiplier”/“dual variable”}} \nabla c = 0 \quad \text{for some } \lambda \in \mathbb{R}$$

- In general:

$$\frac{\partial f}{\partial x} + \lambda^T \frac{\partial c}{\partial x} = 0 \; , \quad \lambda \in \mathbb{R}^m$$

- Based on this gradient condition, we define

$$\underbrace{L(x,\lambda)}_{\text{“Lagrangian”}} = f(x) + \lambda^T c(x)$$

- Such that:

$$\left.\begin{aligned} \nabla_x L(x,\lambda) &= \nabla f + \left(\frac{\partial c}{\partial x}\right)^T \lambda = 0 \\ \nabla_\lambda L(x,\lambda) &= c(x) = 0 \end{aligned}\right\} \text{“KKT conditions”}$$

- We can solve this with Newton:

$$\nabla_x L(x+\Delta x, \lambda+\Delta\lambda) \approx \nabla_x L(x,\lambda) + \frac{\partial^2 L}{\partial x^2}\Delta x + \underbrace{\frac{\partial^2 L}{\partial x \partial \lambda}}_{\left(\frac{\partial c}{\partial x}\right)^T} \Delta\lambda = 0$$

$$\nabla_\lambda L(x+\Delta x, \lambda+\Delta\lambda) \approx \underbrace{c(x) + \frac{\partial c}{\partial x}\Delta x = 0}$$

$$\Rightarrow \frac{\partial c}{\partial x}\Delta x = -c(x)$$

$$\underbrace{\begin{bmatrix} \frac{\partial^2 L}{\partial x^2} & \left(\frac{\partial c}{\partial x}\right)^T \\ \frac{\partial c}{\partial x} & 0 \end{bmatrix}}_{\text{"KKT System"}} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} -\nabla_x L(x,\lambda) \\ -c(x) \end{bmatrix}$$

* Gauss-Newton Method:

$$\frac{\partial^2 L}{\partial x^2} = \nabla^2 f + \underbrace{\frac{\partial}{\partial x}\left[\left(\frac{\partial c}{\partial x}\right)^T \lambda\right]}_{\text{This term is expensive to compute}}$$

- We often drop the 2nd "constraint curvature" term.
- Called "Gauss-Newton"
- Slightly slower convergence than full Newton (more iterations), but cheaper per iteration

$\Rightarrow$ Often wins in wall-clock time

* Example

- Start at $[-1, -1]$, $\underbrace{[-3, 2]}_{\text{Newton gets stuck, Gauss-Newton doesn't}}$

* Take-Away Message

- May still need to regularize $\frac{\partial^2 c}{\partial x^2}$ in Newton, even if $\nabla^2 f > 0$

- Gauss-Newton is often used in practice.

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* Inequality Constraints

$$\min_x \quad f(x)$$

$$\text{s.t.} \quad c(x) \geq 0$$

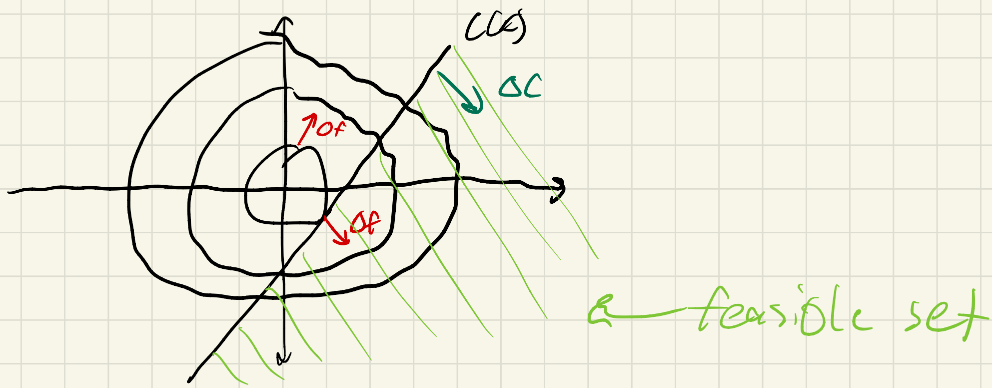
- we will just look at inequalities for now

- In general, we combine these methods with the previous ones for mixed equality/inequality constraints

* First-Order Necessary Conditions

1) $\nabla f = 0$ in <u>free</u> directions

2) $c(x) \geq 0$



KKT conditions
$$\begin{cases} \nabla f - \left(\frac{\partial c}{\partial x}\right)^T \lambda = 0 & \leftarrow \text{"stationarity"} \\ c(x) \geq 0 & \leftarrow \text{"primal feasibility"} \\ \lambda \geq 0 & \leftarrow \text{"dual feasibility"} \\ \lambda \odot c(x) = 0 & \leftarrow \text{"complementarity"} \end{cases}$$

$\odot$ "Hadamard" (element-wise) product

* Intuition
  - If constraint is "active" $\underbrace{(c(x) = 0) \Rightarrow \lambda > 0}_{\text{same as equality case}}$
  - If constraint is "inactive" $\underbrace{(c(x) > 0) \Rightarrow \lambda = 0}_{\text{same as unconstrained case}}$
  - Complementarity encodes "on/off switching"

* Algorithms:
  - Much harder than equality case
  - Can't just apply Newton to KKT conditions
  - Lot's of options w/ trade-offs

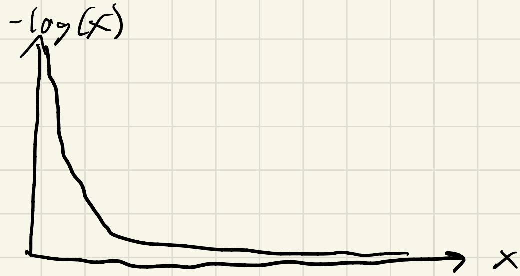
* Active-Set

  - Have some way of guessing active/inactive constraints
  - Just solve equality constrained problems
  - Very fast if you can guess well
  - Very bad otherwise

* Barrier/Interior Point

  - Replace inequalities with "barrier function" in objective that goes to infinity at constraint boundary

$$\left.\begin{array}{ll} \min & f(x) \\ \text{s.t.} & c(x) \geq 0 \end{array}\right\} \rightarrow \min_x f(x) - \sum_{i=1}^{m} \frac{1}{\rho} \log(c_i(x))$$

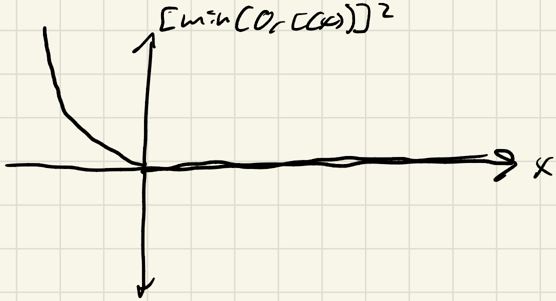


  - Gold standard for "small ~ medium size" convex problems
  - Requires lots of tricks/hacks for non-convex problems

* Penalty Methods

- Replace inequalities with objective term to penalize violations:

$$\left.\begin{array}{l} \min f(x) \\ \text{s.t. } c(x) \geq 0 \end{array}\right\} \to \min_x f(x) + \frac{\rho}{2}\left[\min(0, c(x))\right]^2$$



- Easy to implement
- Has issues with numerical ill-conditioning
- Difficult to achieve high accuracy