

# Constrained Nonlinear Optimization Algorithms

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# Constrained Nonlinear Optimization Problems

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

$$\text{s.t. } c_E(x) = 0$$

$$c_I(x) \leq 0$$

(NLP)

$$f : \mathbb{R}^n \longrightarrow \mathbb{R}$$

$$c_E : \mathbb{R}^n \longrightarrow \mathbb{R}^{m_E}$$

$$c_I : \mathbb{R}^n \longrightarrow \mathbb{R}^{m_I}$$

- ▶ We assume that all functions are twice continuously differentiable.

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- ▶ No is convexity required.
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  - ▶ theoretical convergence guarantee only to stationary points;
  - ▶ ingredients that steer towards local minimizers.

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Applications

Equality-Constrained Quadratic Programming

Active-Set Quadratic Programming Solvers

SQP for Equality-Constrained NLPs

SQP for Inequality-Constrained NLPs

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Software

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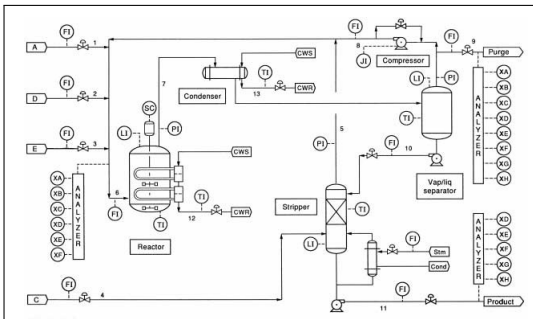
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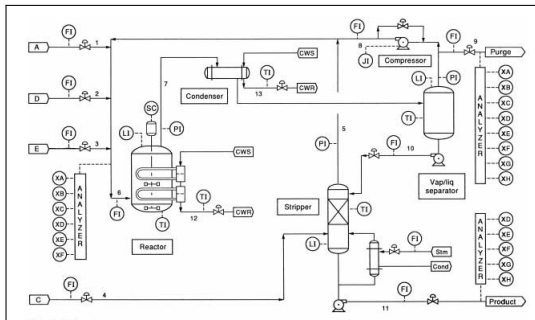
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# Design and Operation of Chemical Plant





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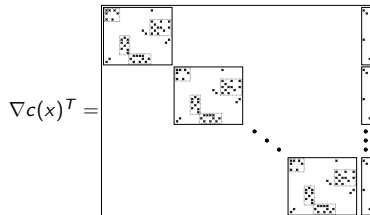
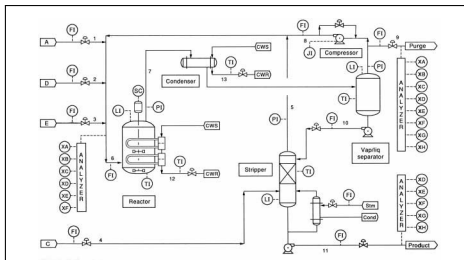


- ▶ Minimize “Costs – Profit”
- ▶ Variables: Physical quantities
- ▶ Constraints: physical relationships  
(conservation laws; thermodyn. rel.)
- ▶ Limits (physical and operational)
- ▶  $< 10^5$  variables; few degrees of freedom





# Design Under Uncertainty



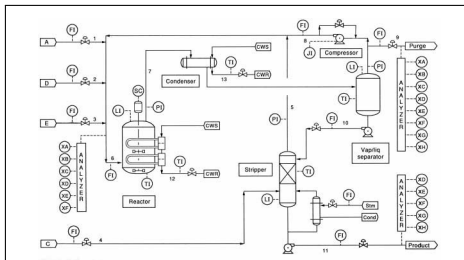
► Scenario parameters:  $F_{in}^l, x_{in}^l, T_{env}^l, p_{env}^l, \dots$  (given)  
(defining scenarios  $l = 1, \dots, L$ )

► Design variables:  $V_{react}, D_{dist}, h_{tank}, \dots$

► Control variables:  $Q_{heat}^l, r_{refl}^l, v_{valve}^l, \dots$

► State variables:  $x_{str}^l, F_{str}^l, L_{tank}^l, T^l, p^l, \dots$

# Optimal Control / Dynamic Optimization



$$\min_{z, y, u, p} f(z(t_f), y(t_f), u(t_f), p)$$

$$\text{s.t. } F(\dot{z}(t), z(t), y(t), u(t), p) = 0$$

$$G(z(t), y(t), u(t), p) = 0$$

$$z(0) = z_{init}$$

bound constraints

$u : [0, t_f] \rightarrow \mathbb{R}^{n_u}$  control variables

$z : [0, t_f] \rightarrow \mathbb{R}^{n_z}$  differentiable state variables

$y : [0, t_f] \rightarrow \mathbb{R}^{n_y}$  algebraic state variables

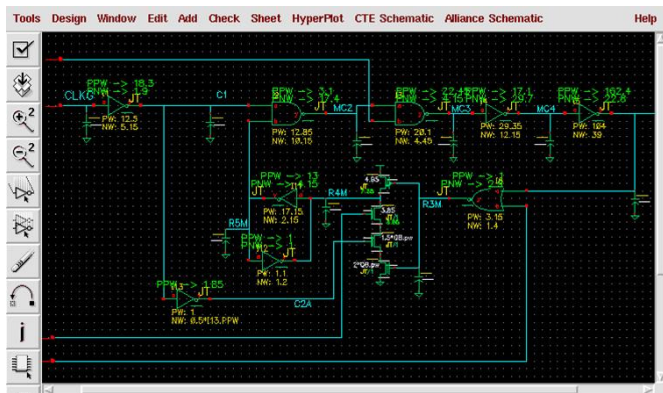
$p \in \mathbb{R}^{n_p}$  time-independent parameters

$z_{init}$  initial conditions

$t_f$  final time

- Large-scale NLPs arise from discretization.

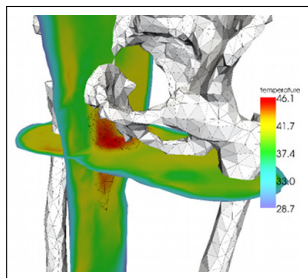
# Circuit Tuning



- ▶ Model consists of network of gates.
- ▶ Gate delays computed by simulation (expensive, noisy).
- ▶ Model has many variables (up to 1,000,000).
- ▶ Implemented in IBM's circuit tuning tool EinsTuner.

# Hyperthermia Treatment Planning

$$\begin{aligned} \min_{T(x), u} \quad & \frac{1}{2} \int_{\Omega} (T(x) - T_{\text{target}}(x))^2 dx \\ \text{s.t.} \quad & -\Delta T(x) - w(T(x) - T_{\text{blood}}) = u^* M(x) u \quad \text{in } \Omega \\ & \nabla T(x) \cdot n = T_{\text{exterior}} - T(x) \quad \text{on } \partial\Omega \\ & T(x) \leq T_{\text{max}} \quad \text{in } \Omega \setminus \Omega_{\text{Tumor}} \end{aligned}$$



- ▶ Heat tumors with microwaves (support chemo- and radio-therapy).
- ▶ Model is a PDE with
  - ▶ controls: Application  $u$  of microwave antennas.
  - ▶ states: Temperature  $T(x)$  defined over domain  $\Omega$ .
- ▶ Finite-dimensional problem obtained by discretization.
  - ▶ e.g., finite differences, finite elements
- ▶ Resulting NLP is usually very large.

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# Quadratic Programming

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} x^T Q x + g^T x$$

$$\text{s.t. } A_E x + b_E = 0$$

$$A_I x + b_I \leq 0$$

(QP)

$$Q \in \mathbb{R}^{n \times n} \text{ symmetric}$$

$$A_E \in \mathbb{R}^{m_E \times n} \quad b_E \in \mathbb{R}^{m_E}$$

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- ▶ Important building block for methods for general NLP.
- ▶ Algorithms:
  - ▶ Active-set methods
  - ▶ Interior-point methods
- ▶ Let's first consider equality-constrained case.
- ▶ Assume: all rows of  $A_E$  are linearly independent.

# Equality-Constrained QP

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & \frac{1}{2}x^T Qx + g^T x \\ \text{s.t.} & Ax + b = 0 \end{array}$$

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First-order optimality conditions:

$$\begin{array}{l} Qx + g + A^T \lambda = 0 \\ Ax + b = 0 \end{array}$$

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First-order optimality conditions:

$$\begin{aligned} Qx + g + A^T \lambda &= 0 \\ Ax + b &= 0 \end{aligned}$$

Find stationary point  $(x^*, \lambda^*)$  by solving the linear system

$$\begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix} \begin{pmatrix} x^* \\ \lambda^* \end{pmatrix} = - \begin{pmatrix} g \\ b \end{pmatrix}.$$



# KKT System of QP

$$\begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix} \begin{pmatrix} x^* \\ \lambda^* \end{pmatrix} = - \begin{pmatrix} g \\ b \end{pmatrix}$$

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- ▶ Recall the second-order optimality conditions:
  - ▶ Let the columns of  $Z \in \mathbb{R}^{n \times (n-m)}$  be a basis of the null-space of  $A$ , so  $AZ = 0$  (“null-space matrix”).
  - ▶ Then  $x^*$  is a strict local minimizer of (EQP) if  $Z^T QZ \succ 0$ .

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- ▶ On the other hand:
  - ▶ If  $Z^T QZ$  has negative eigenvalue, then (EQP) is unbounded below.
- ▶ There are different ways to solve the KKT system
  - ▶ Best choice depends on particular problem

## Direct Solution of the KKT System

$$\underbrace{\begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix}}_{=:K} \begin{pmatrix} x^* \\ \lambda^* \end{pmatrix} = - \begin{pmatrix} g \\ b \end{pmatrix}$$

- ▶ How can we verify that  $x^*$  is local minimizer without computing  $Z$ ?

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### Definition

Let  $n_+$ ,  $n_-$ ,  $n_0$  be the number of positive, negative, and zero eigenvalues of a matrix  $M$ . Then  $\text{In}(M) = (n_+, n_-, n_0)$  is the inertia of  $M$ .

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### Theorem

*Suppose that  $A$  has full rank. Then:  $\text{In}(K) = \text{In}(Z^T Q Z) + (m, m, 0)$ .*

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## Corollary

*If  $\text{In}(K) = (n, m, 0)$ , then  $x^*$  is the unique global minimizer.*



# Computing the Inertia

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- ▶ Symmetric indefinite factorization  $PKP^T = LBL^T$ 
  - ▶  $P$ : permutation matrix
  - ▶  $L$ : unit lower triangular matrix
  - ▶  $B$ : block diagonal matrix with  $1 \times 1$  and  $2 \times 2$  diagonal blocks

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- ▶ Obtain inertia simply from counting eigenvalues of the blocks in  $B$ .
- ▶ Used also to solve the linear system.
- ▶ Will be important later when we need to “convexify” QPs  
( $Q \leftarrow Q + \gamma I$ ).

# Schur-Complement Method

$$\begin{aligned} Qx + g + A^T \lambda &= 0 \\ Ax + b &= 0 \end{aligned}$$

- ▶ Assume,  $Q$  is positive definite. Then  $AQ^{-1}A^T$  is nonsingular.

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$$[AQ^{-1}A^T]\lambda^* = b - AQ^{-1}g$$



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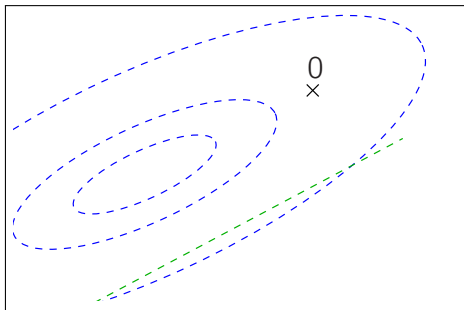
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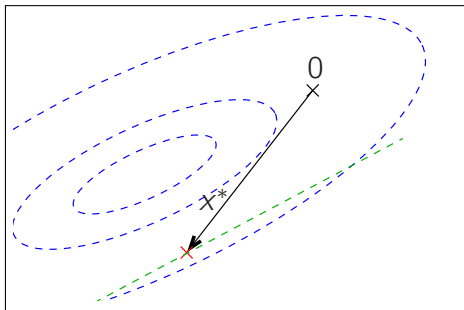
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  - ▶ Need to compute  $[AQ^{-1}A^T]$  and solve linear system with it
  - ▶ Works best if  $m$  is small

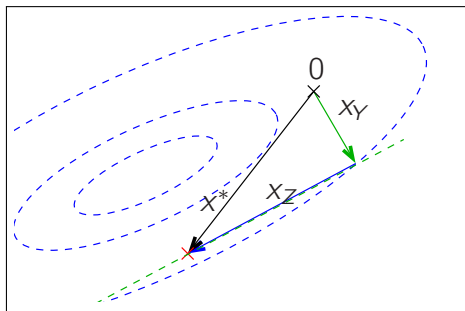
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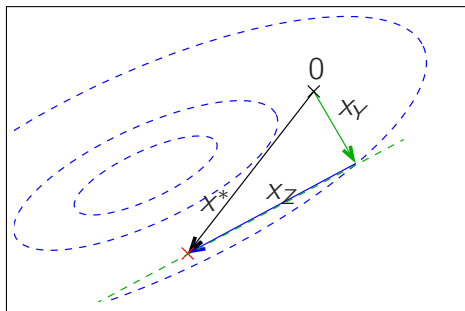


# Step Decomposition



- ▶ Decompose  $x^* = x_Y + x_Z$  into two steps:
  - ▶ “range-space step”  $x_Y$ : step into constraints
  - ▶ “null-space step”  $x_Z$ : optimize within null space

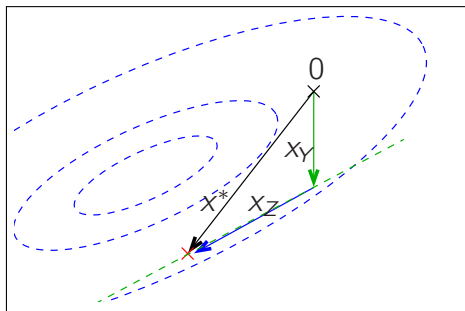
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- ▶  $x_Y = Yp_Y$  and  $x_Z = Zp_Z$ 
  - ▶ where  $[Y \ Z]$  is basis of  $\mathbb{R}^n$  and  $Z$  is null space matrix for  $A$ .



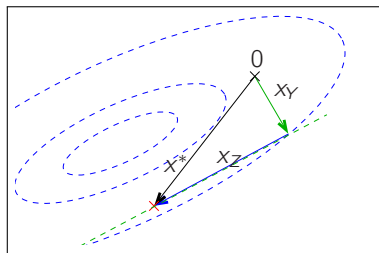
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  - ▶ “null-space step”  $x_Z$ : optimize within null space
- ▶  $x_Y = Yp_Y$  and  $x_Z = Zp_Z$ 
  - ▶ where  $[Y \ Z]$  is basis of  $\mathbb{R}^n$  and  $Z$  is null space matrix for  $A$ .
- ▶ Decomposition depends on choice of  $Y$  and  $Z$

# Step Decomposition

$$\begin{aligned} Qx + g + A^T \lambda &= 0 \\ Ax + b &= 0 \end{aligned}$$

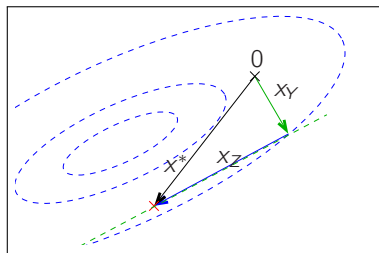


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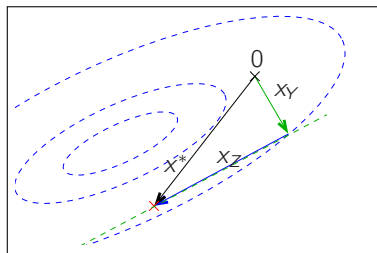


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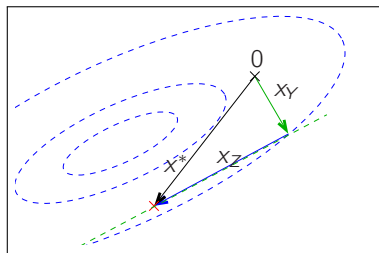
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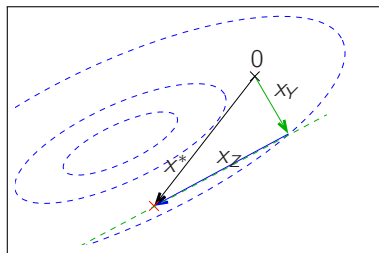
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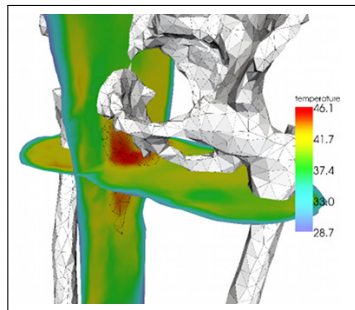
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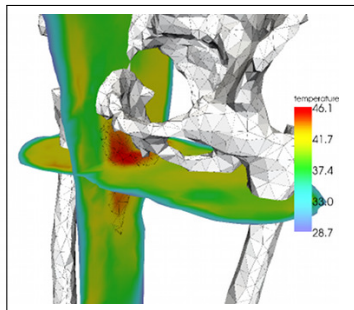
## Example: PDE-Constrained Optimization

$$\begin{aligned} \min_{T,u} \quad & \frac{1}{2} \int (T(z) - \hat{T}(z))^2 dz + \frac{\alpha}{2} \|u\|^2 \\ \text{s.t.} \quad & -\Delta T(z) = \sum_{i=1}^{n_u} k_i(z) u_i \text{ on } \Omega \\ & T(z) = b(z) \text{ on } \partial\Omega \end{aligned}$$



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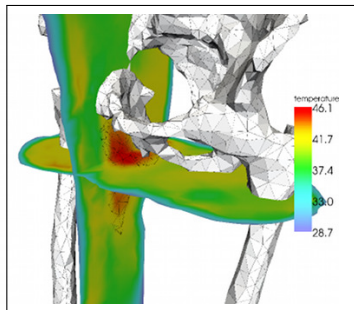


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## Discretized PDE-Constrained Problem

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- ▶ We could just eliminate  $t$  and solve lower-dimensional problem in  $u$

## Generalization: Elimination of Variables

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & \frac{1}{2} (x_B^T \ x_N^T) Q \begin{pmatrix} x_B \\ x_N \end{pmatrix} + g_B^T x_B + g_N^T x_N \\ \text{s.t.} \quad & Bx_B + Nx_N + b = 0 \end{aligned}$$

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- ▶ Tailored implementation for “simulation” often already exist.
- ▶ Exploit problem structure!



# Solution of EQP Summary

- ▶ Direct method:
  - ▶ Factorize KKT matrix
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- ▶ Null-space method
  - ▶ Step decomposition into range-space step and null-space step
  - ▶ Permits exploitation of constraint matrix structure
  - ▶ Number of degrees of freedom ( $n - m$ ) should not be large

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SQP for Inequality-Constrained NLPs

Interior Point Methods

Software

# Inequality-Constrained QPs

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} x^T Q x + g^T x$$

$$\text{s.t. } a_i^T x + b_i = 0 \text{ for } i \in \mathcal{E}$$

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- ▶ We know how to solve equality-constrained QPs.
  - ▶ Can we use that here?

## Working Set

Choose working set  $\mathcal{W} \subseteq \mathcal{I}$  and solve

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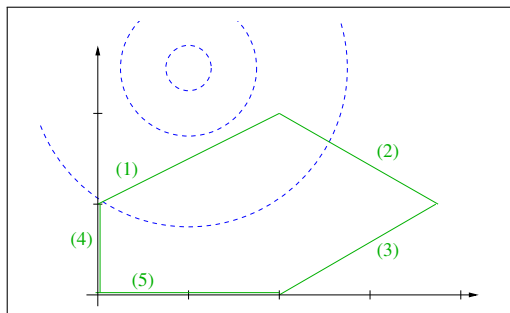
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- ▶ If satisfied,  $(x, \lambda)$  is the (unique) optimal solution
- ▶ Otherwise, let's try a different working set

## Example QP



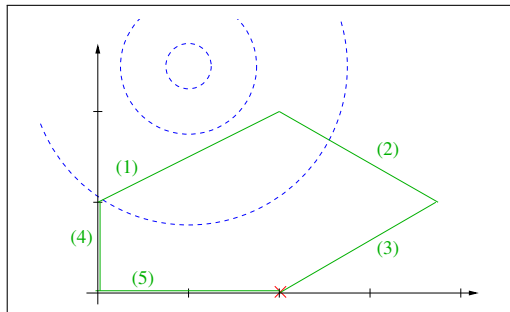
$$\min (x_1 - 1)^2 + (x_2 - 2.5)^2$$

$$\text{s.t. } -x_1 + 2x_2 - 2 \leq 0 \quad (1) \qquad -x_1 \leq 0 \quad (4)$$

$$x_1 + 2x_2 - 6 \leq 0 \quad (2) \qquad -x_2 \leq 0 \quad (5)$$

$$x_1 - 2x_2 - 2 \leq 0 \quad (3)$$

# Primal Active-Set QP Solver Iteration 1



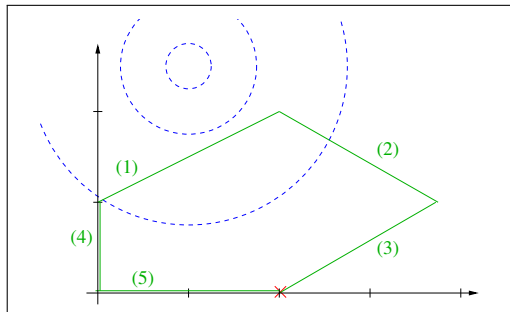
Initialization:

Choose feasible starting iterate  $x$

$$x = (0, 2)$$



# Primal Active-Set QP Solver Iteration 1



$$\mathcal{W} = \{3, 5\}$$

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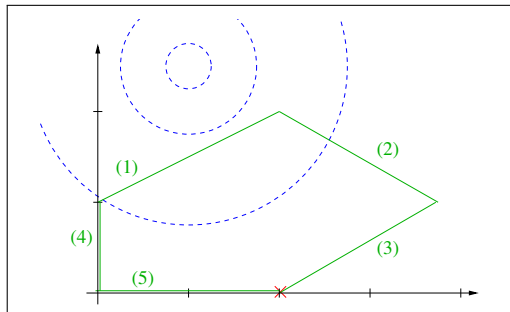
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(Algorithm will maintain these properties)

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$$\mathcal{W} = \{3, 5\}$$

$$x = (0, 2)$$

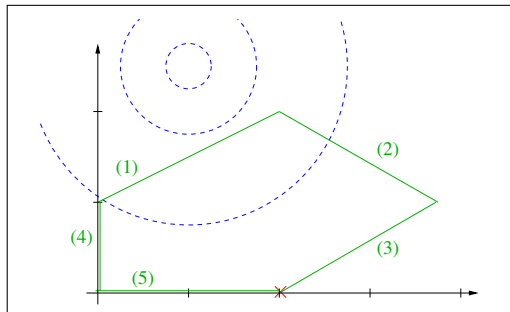
$$x^{\text{EQP}} = (0, 2)$$

Solve (EQP)

$$\lambda_3 = -2$$

$$\lambda_5 = -1$$

# Primal Active-Set QP Solver Iteration 1



Status: Current iterate is optimal for (EQP).

$$\mathcal{W} = \{3, 5\}$$

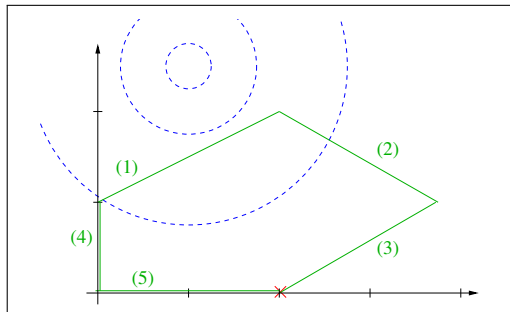
$$x = (0, 2)$$

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# Primal Active-Set QP Solver Iteration 1



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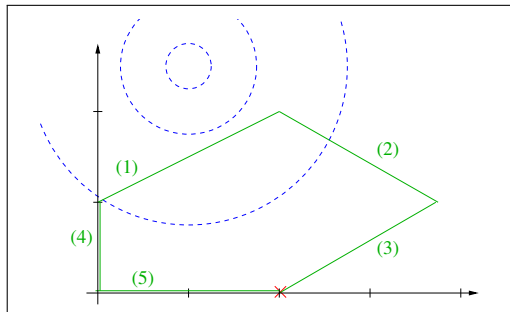
$$\lambda_5 = -1$$

Status: Current iterate is optimal for (EQP).

Release Constraint:

- Pick constraint  $i$  with  $\lambda_i < 0$ .

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$$\mathcal{W} = \{3, 5\}$$

$$x = (0, 2)$$

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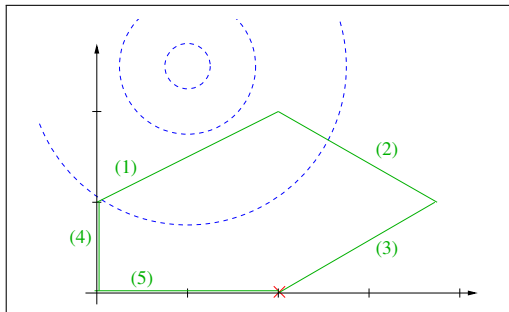
Status: Current iterate is optimal for (EQP).

Release Constraint:

- ▶ Pick constraint  $i$  with  $\lambda_i < 0$ .
- ▶ Remove  $i$  from working set:

$$\mathcal{W} \leftarrow \mathcal{W} \setminus \{3\} = \{5\}$$

# Primal Active-Set QP Solver Iteration 1



$$\mathcal{W} = \{3, 5\}$$

$$x = (0, 2)$$

$$x^{\text{EQP}} = (0, 2)$$

$$\lambda_3 = -2$$

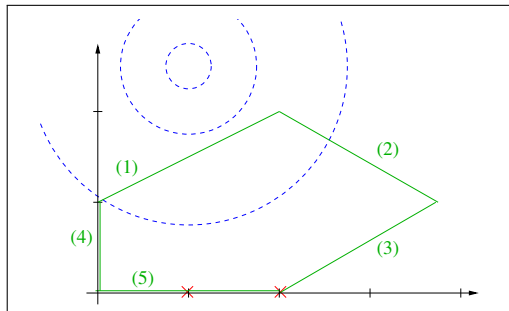
$$\lambda_5 = -1$$

Status: Current iterate is optimal for (EQP).

Release Constraint:

- ▶ Pick constraint  $i$  with  $\lambda_i < 0$ .
- ▶ Remove  $i$  from working set:  
$$\mathcal{W} \leftarrow \mathcal{W} \setminus \{3\} = \{5\}$$
- ▶ Keep iterate  $x = (0, 2)$ .

## Primal Active-Set QP Solver Iteration 2



$$\mathcal{W} = \{5\}$$

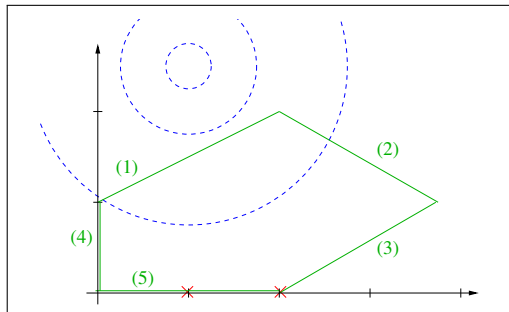
$$x = (2, 0)$$

$$x^{\text{EQP}} = (1, 0)$$

$$\lambda_5 = -5$$

Solve (EQP)

## Primal Active-Set QP Solver Iteration 2



$$\mathcal{W} = \{5\}$$

$$x = (2, 0)$$

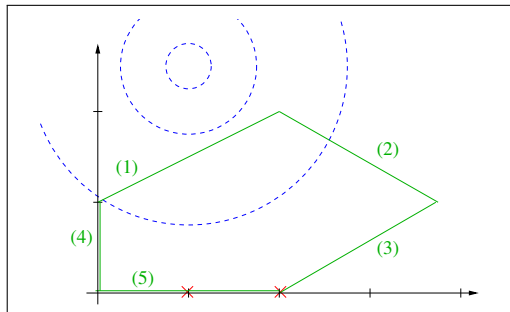
$$x^{\text{EQP}} = (1, 0)$$

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Status: Current iterate is not optimal for (EQP).



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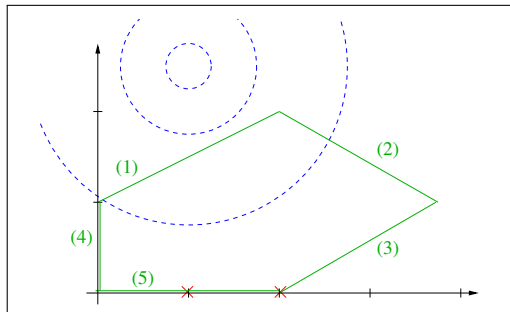
$$\lambda_5 = -5$$

Status: Current iterate is not optimal for (EQP).

Take step ( $x^{\text{EQP}}$  is feasible):

► Update iterate  $x \leftarrow x^{\text{EQP}}$

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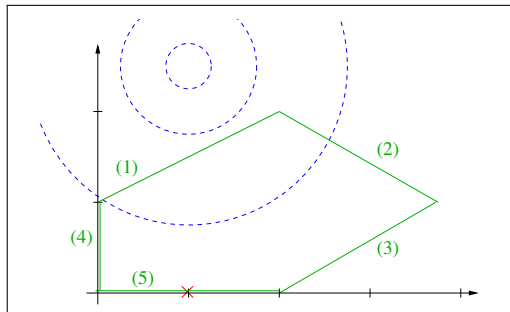
$$\lambda_5 = -5$$

Status: Current iterate is not optimal for (EQP).

Take step ( $x^{\text{EQP}}$  is feasible):

- Update iterate  $x \leftarrow x^{\text{EQP}}$
- Keep  $\mathcal{W}$

# Primal Active-Set QP Solver Iteration 3



$$\mathcal{W} = \{5\}$$

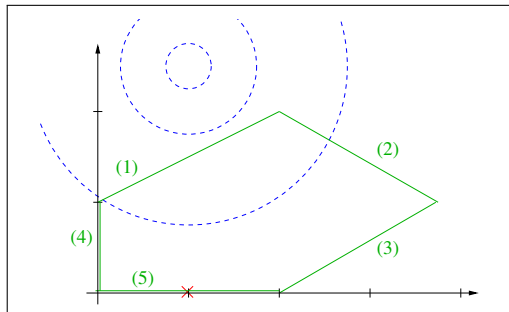
$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 0)$$

$$\lambda_5 = -5$$

Solve (EQP)

## Primal Active-Set QP Solver Iteration 3



Status: Current iterate is optimal for (EQP)

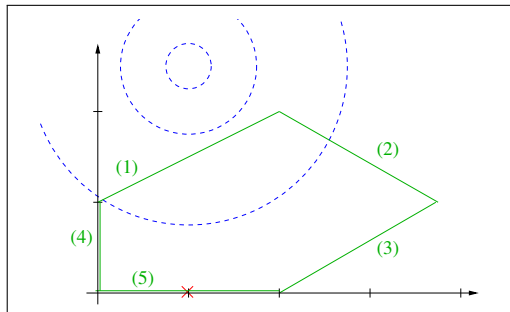
$$\mathcal{W} = \{5\}$$

$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 0)$$

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$$x = (1, 0)$$

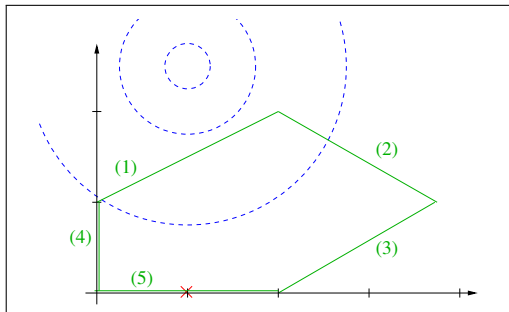
$$x^{\text{EQP}} = (1, 0)$$

$$\lambda_5 = -5$$

Release Constraint:

- Pick constraint  $i$  with  $\lambda_i < 0$ .

## Primal Active-Set QP Solver Iteration 3



Status: Current iterate is optimal for (EQP)

$$\mathcal{W} = \{5\}$$

$$x = (1, 0)$$

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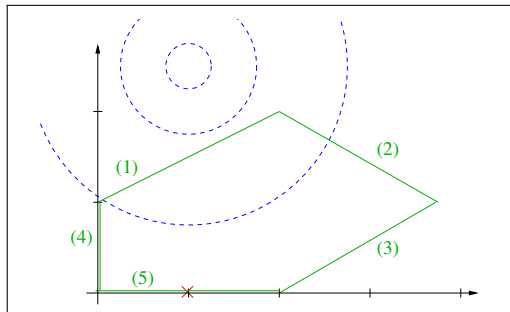
$$\lambda_5 = -5$$

Release Constraint:

- ▶ Pick constraint  $i$  with  $\lambda_i < 0$ .
- ▶ Remove  $i$  from working set:

$$\mathcal{W} \leftarrow \mathcal{W} \setminus \{5\} = \emptyset$$

# Primal Active-Set QP Solver Iteration 3



Status: Current iterate is optimal for (EQP)

$$\mathcal{W} = \{5\}$$

$$x = (1, 0)$$

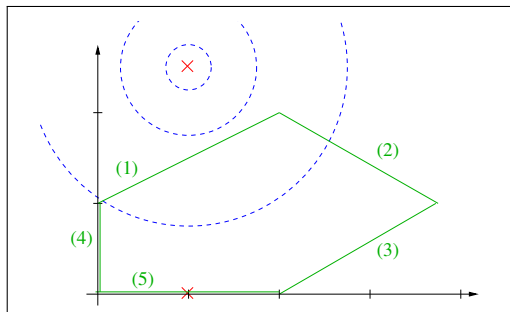
$$x^{\text{EQP}} = (1, 0)$$

$$\lambda_5 = -5$$

Release Constraint:

- ▶ Pick constraint  $i$  with  $\lambda_i < 0$ .
- ▶ Remove  $i$  from working set:  
$$\mathcal{W} \leftarrow \mathcal{W} \setminus \{5\} = \emptyset$$
- ▶ Keep iterate  $x = (1, 0)$ .

# Primal Active-Set QP Solver Iteration 4



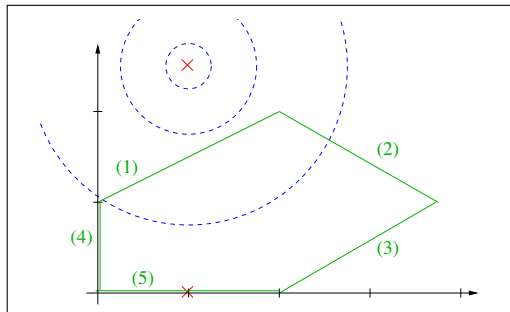
$$\mathcal{W} = \emptyset$$

$$x = (1, 0) \quad \text{Solve (EQP)}$$

$$x^{\text{EQP}} = (1, 2.5)$$



## Primal Active-Set QP Solver Iteration 4



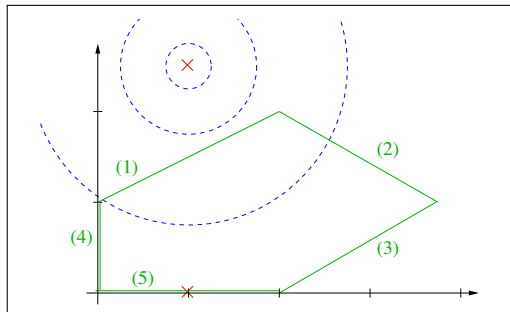
Status: Current iterate not optimal for (EQP)

$$\mathcal{W} = \emptyset$$

$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 2.5)$$

## Primal Active-Set QP Solver Iteration 4



Status: Current iterate not optimal for (EQP)

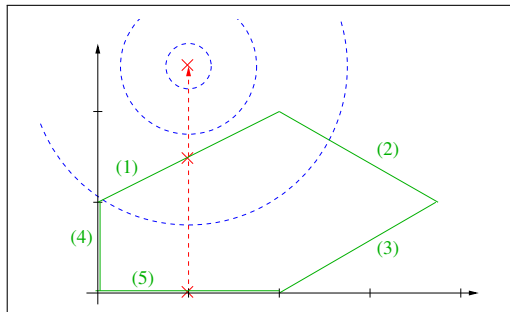
Take step ( $x^{\text{EQP}}$  not feasible):

$$\mathcal{W} = \emptyset$$

$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 2.5)$$

# Primal Active-Set QP Solver Iteration 4



Status: Current iterate not optimal for (EQP)

Take step ( $x^{\text{EQP}}$  not feasible):

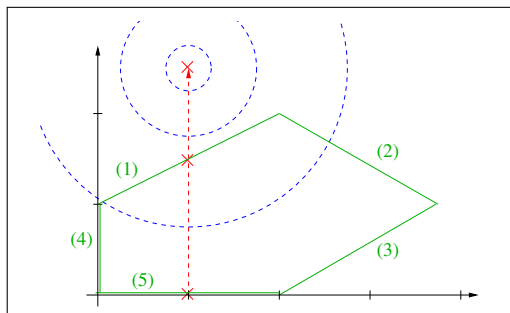
► Largest  $\alpha \in [0, 1]$ :  $x + \alpha(x^{\text{EQP}} - x)$  feasible

$$\mathcal{W} = \emptyset$$

$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 2.5)$$

# Primal Active-Set QP Solver Iteration 4



Status: Current iterate not optimal for (EQP)

Take step ( $x^{\text{EQP}}$  not feasible):

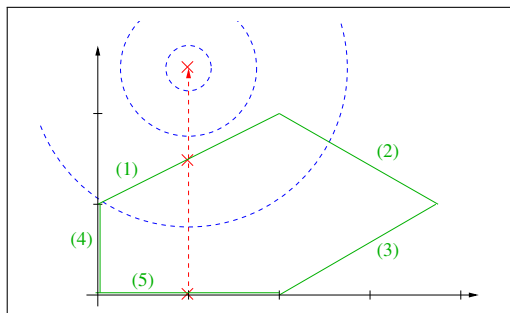
$$\mathcal{W} = \emptyset$$

$$x = (1, 0)$$

$$x^{\text{EQP}} = (1, 2.5)$$

- ▶ Largest  $\alpha \in [0, 1]$ :  $x + \alpha(x^{\text{EQP}} - x)$  feasible
- ▶ Update iterate  $x \leftarrow x + \alpha(x^{\text{EQP}} - x)$

# Primal Active-Set QP Solver Iteration 4



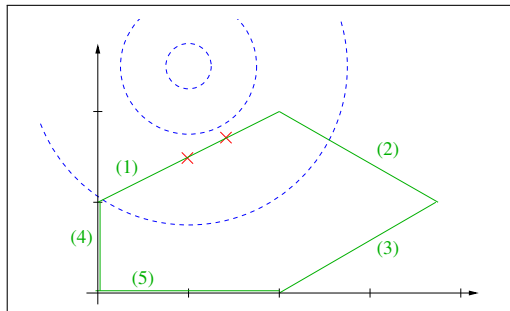
Status: Current iterate not optimal for (EQP)

Take step ( $x^{\text{EQP}}$  not feasible):

$$\begin{aligned}\mathcal{W} &= \emptyset \\ x &= (1, 0) \\ x^{\text{EQP}} &= (1, 2.5)\end{aligned}$$

- ▶ Largest  $\alpha \in [0, 1]$ :  $x + \alpha(x^{\text{EQP}} - x)$  feasible
- ▶ Update iterate  $x \leftarrow x + \alpha(x^{\text{EQP}} - x)$
- ▶ Update  $\mathcal{W} \leftarrow \mathcal{W} \cup \{i\} = \{1\}$ 
  - ▶ where constraint  $i = 1$  is “blocking”

# Primal Active-Set QP Solver Iteration 5



$$\mathcal{W} = \{1\}$$

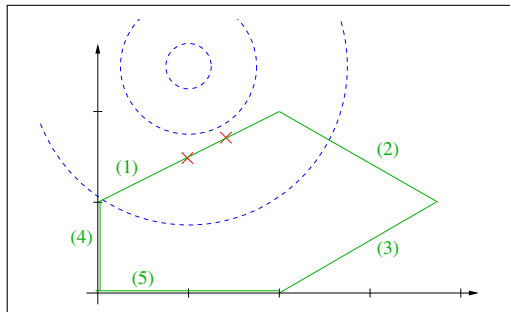
$$x = (1, 1.5)$$

$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Solve (EQP)

## Primal Active-Set QP Solver Iteration 5



$$\mathcal{W} = \{1\}$$

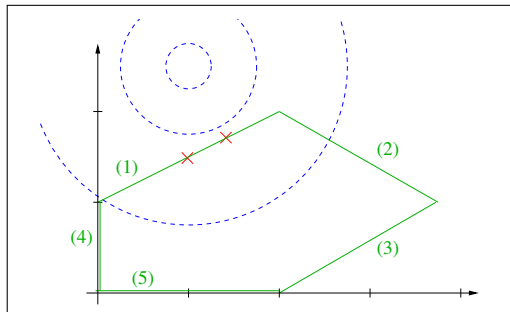
$$x = (1, 1.5)$$

$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Status: Current iterate is not optimal for (EQP).

# Primal Active-Set QP Solver Iteration 5



$$\mathcal{W} = \{1\}$$

$$x = (1, 1.5)$$

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$$\lambda_1 = 0.8$$

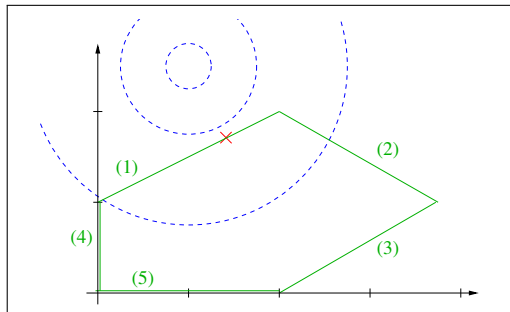
Status: Current iterate is not optimal for (EQP).

Take step ( $x^{\text{EQP}}$  feasible):

- Update iterate  $x \leftarrow x^{\text{EQP}}$ .
- Keep  $\mathcal{W}$ .



## Primal Active-Set QP Solver Iteration 6



$$\mathcal{W} = \{1\}$$

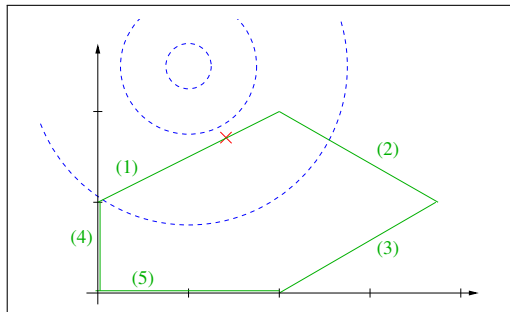
$$x = (1.4, 1.7)$$

$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Solve (EQP)

## Primal Active-Set QP Solver Iteration 6



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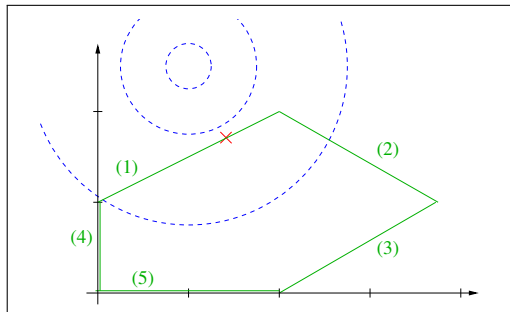
$$x = (1.4, 1.7)$$

$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Status: Current iterate is optimal for (EQP)

## Primal Active-Set QP Solver Iteration 6



$$\mathcal{W} = \{1\}$$

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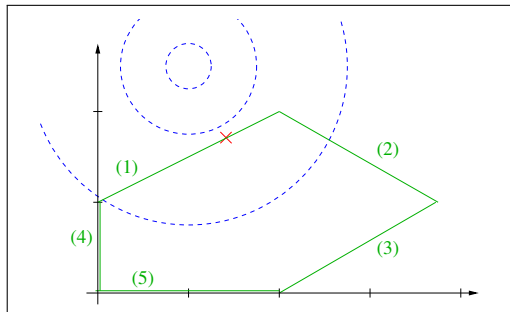
$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Status: Current iterate is optimal for (EQP)

►  $\lambda_i \geq 0$  for all  $i \in \mathcal{W}$ .

## Primal Active-Set QP Solver Iteration 6



$$\mathcal{W} = \{1\}$$

$$x = (1.4, 1.7)$$

$$x^{\text{EQP}} = (1.4, 1.7)$$

$$\lambda_1 = 0.8$$

Status: Current iterate is optimal for (EQP)

►  $\lambda_i \geq 0$  for all  $i \in \mathcal{W}$ .

Declare Optimality!

# Primal Active-Set QP Method

1. Select feasible  $x$  and  $\mathcal{W} \subseteq \mathcal{I} \cap \mathcal{A}(x)$ .

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  - ▶ If  $\lambda^{\text{EQP}} \geq 0$ : Done!



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  - ▶ Update  $x \leftarrow x + \alpha p$ .
5. Go to step 2.

# Active-Set QP Algorithms

- ▶ Primal active-set method:
  - ▶ Keeps all iterates feasible.
  - ▶ Changes  $\mathcal{W}$  by at most one constraint per iteration.
  - ▶  $\{a_i\}_{i \in \mathcal{E} \cup \mathcal{W}}$  remain linearly independent.

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  - ▶ Special handling of degeneracy necessary ( $\alpha = 0$  steps)

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  - ▶ Alternative: Interior-point QP solvers (polynomial complexity).
- ▶ There are variants that allow  $Q$  to be indefinite.

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SQP for Inequality-Constrained NLPs

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Software

# Equality-Constrained Nonlinear Problems

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c(x) = 0 \end{array}$$

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  - ▶ Mechanisms that encourage convergence to local minima

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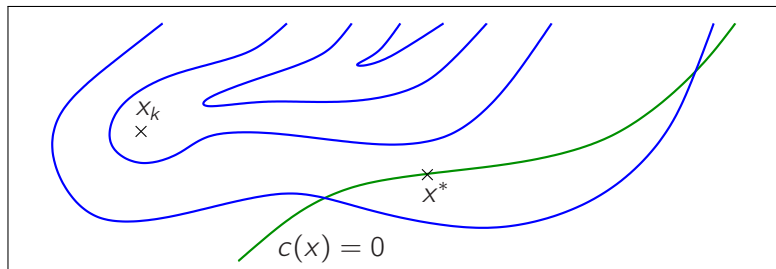
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- ▶ Newton step can be interpreted as solution of a local QP model!

# Local QP Model

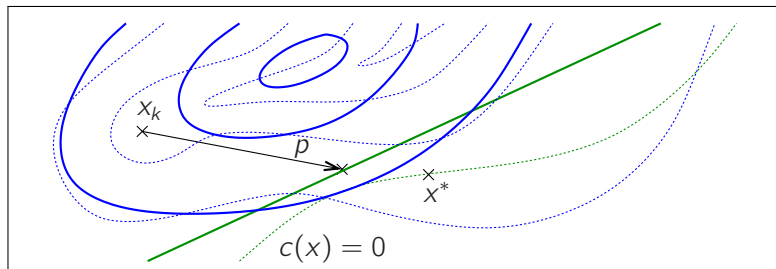


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- ▶ We can use decrease in  $\phi_\rho$  as a measure of progress towards a local minimizer of (NLP).

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6. Set  $k \leftarrow k + 1$  and to go Step 2.

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*In other words, each limit point of  $\{x_k\}$  is a stationary point for (NLP).*

## Choice of Hessian $H_k$

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- ▶  $H_k = \text{BFGS}$  approximation of  $\nabla_{xx}^2 \mathcal{L}(x_k, \lambda_k)$ .

## Choice of Hessian $H_k$

$$\begin{array}{ll} \min_{p \in \mathbb{R}^n} & \frac{1}{2} p^T H_k p + \nabla f_k^T p \\ \text{s.t.} & \nabla c_k^T p + c_k = 0 \end{array} \quad (\text{QP}_k)$$

- ▶ For fast local convergence, want to choose  $H_k = \nabla_{xx}^2 \mathcal{L}_k$ .
- ▶  $\nabla_{xx}^2 \mathcal{L}_k$  is positive definite, if  $f$  and  $c$  are convex.
- ▶ In general,  $\nabla_{xx}^2 \mathcal{L}_k$  might be indefinite.
  - ▶  $(\text{QP}_k)$  might be unbounded.
  - ▶  $p_k$  might not be a descent direction for  $\phi_p$ .
  - ▶ Would like  $Z_k^T H_k Z_k \succ 0$  ( $Z_k$  null-space matrix for  $\nabla c_k^T$ ).
- ▶  $H_k = \text{BFGS}$  approximation of  $\nabla_{xx}^2 \mathcal{L}(x_k, \lambda_k)$ .
  - ▶ Potentially slow local convergence, since  $\nabla_{xx}^2 \mathcal{L}(x^*, \lambda^*)$  may be indefinite.

# Regularization

$$\begin{aligned} \min_{p \in \mathbb{R}^n} \quad & \frac{1}{2} p^T H_k p + \nabla f_k^T p \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = 0 \end{aligned}$$

Recall optimality conditions

$$\underbrace{\begin{bmatrix} H_k & \nabla c_k \\ \nabla c_k^T & 0 \end{bmatrix}}_{=: K_k} \begin{pmatrix} p_k \\ \tilde{\lambda}_{k+1} \end{pmatrix} = - \begin{pmatrix} \nabla f_k \\ c_k \end{pmatrix}$$



# Regularization

$$\begin{aligned} \min_{p \in \mathbb{R}^n} \quad & \frac{1}{2} p^T (H_k + \gamma I) p + \nabla f_k^T p \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = 0 \end{aligned}$$

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- Choose  $\gamma \geq 0$

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- ▶ Then  $Z_k^T H_k Z_k$  is positive definite.

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  - ▶ E.g.: Trial and error, computing inertia via factorization
- ▶ Then  $Z_k^T H_k Z_k$  is positive definite.
- ▶ No regularization necessary close to second-order sufficient solution.

## Step Decomposition Revisited

$$\begin{aligned} \min_{p \in \mathbb{R}^n} \quad & \frac{1}{2} p^T H_k p + \nabla f_k^T p \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = 0 \end{aligned}$$

(QP<sub>k</sub>)

Decomposition  $p_k = Y_k p_{Y,k} + Z_k p_{Z,k}$

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$$p_{Y,k} = -[\nabla c_k^T Y_k]^{-1} \nabla f_k$$

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# Trust-Region SQP Method

$$\min_{p \in \mathbb{R}^n} \frac{1}{2} p^T H_k p + \nabla f_k^T p$$

$$\text{s.t. } \nabla c_k^T p + c_k = 0, \quad \|p\| \leq \Delta_k$$

(QP<sub>k</sub>)

- ▶ Trust-region radius  $\Delta_k$ , updated throughout iterations

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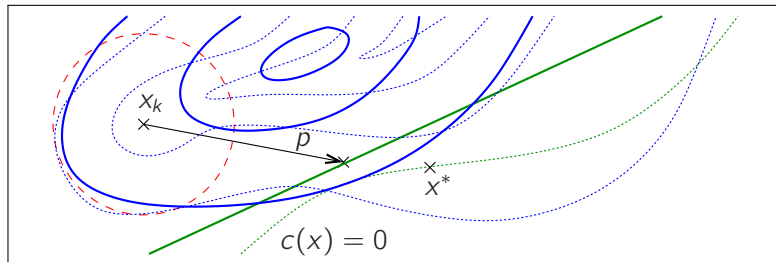
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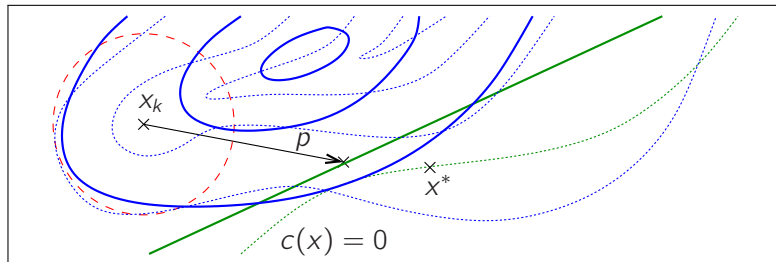
- ▶ Otherwise, decrease  $\Delta_k$

# Inconsistent QPs



- ▶ If  $x_k$  is not feasible and  $\Delta_k$  small,  $(QP_k)$  might not be feasible

# Inconsistent QPs

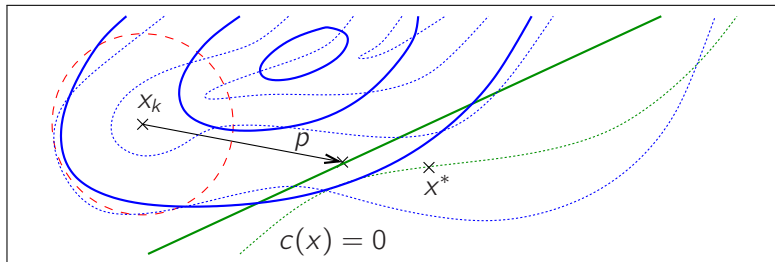


- ▶ If  $x_k$  is not feasible and  $\Delta_k$  small,  $(QP_k)$  might not be feasible
- ▶ One remedy: Penalize constraint violation

$$\begin{aligned} \min_{p \in \mathbb{R}^n} \quad & \frac{1}{2} p^T H_k p + \nabla f_k^T p \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = 0 \\ & \|p\| \leq \Delta_k \end{aligned}$$



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$$\begin{aligned} \min_{p \in \mathbb{R}^n; t, s \in \mathbb{R}^m} \quad & \frac{1}{2} p^T H_k p + \nabla f_k^T p + \rho \sum_{j=1}^m (s_j + t_j) \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = s - t \\ & \|p\| \leq \Delta_k, \quad s, t \geq 0 \end{aligned}$$

# Fletcher's $S\ell_1$ QP

$$\begin{aligned} \min_{p \in \mathbb{R}^n; t, s \in \mathbb{R}^m} \quad & \frac{1}{2} p^T H_k p + \nabla f_k^T p + \rho \sum_{j=1}^m (s_j + t_j) \\ \text{s.t.} \quad & \nabla c_k^T p + c_k = s - t \\ & \|p\| \leq \Delta_k, \quad s, t \geq 0 \end{aligned}$$

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is equivalent to

$$\min_{p \in \mathbb{R}^n} m_k(p) = f_k + \nabla f_k^T p + \frac{1}{2} p^T H_k p + \rho \|c_k + \nabla c_k^T p\|_1$$

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- Natural algorithm for minimizing  $\phi_\rho(x)$ .

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- ▶ Natural algorithm for minimizing  $\phi_\rho(x)$ .
- ▶ Difficulty: Selecting sufficiently large value of  $\rho$ .

# Fletcher's $S\ell_1$ QP

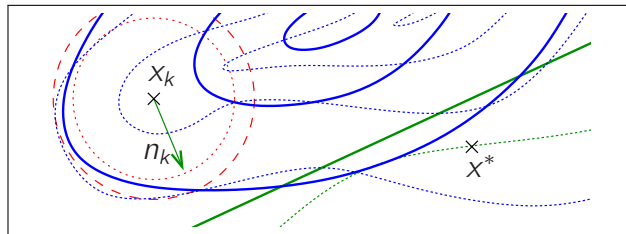
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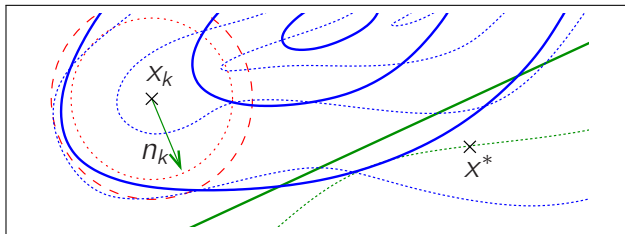
- ▶ Natural algorithm for minimizing  $\phi_\rho(x)$ .
- ▶ Difficulty: Selecting sufficiently large value of  $\rho$ .
  - ▶ This motivated the invention of *filter methods*.

# Byrd-Omojokun Trust-Region Algorithm



- Decompose step  $p_k = n_k + t_k$

# Byrd-Omojokun Trust-Region Algorithm

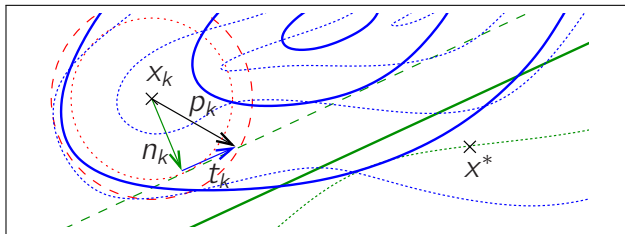


- Decompose step  $p_k = n_k + t_k$

Normal component  $n_k$   
towards feasibility



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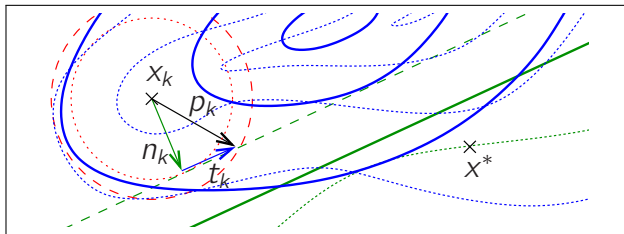


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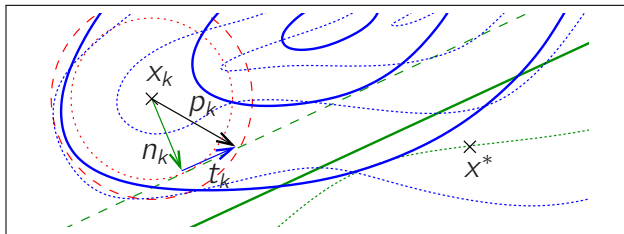
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- ▶ Strong convergence result:
  - ▶ If (NLP) is infeasible, limit points of  $\{x_k\}$  are stationary points for infeasibility minimization problem  $\min_x \|c(x)\|_2^2$ .

# Maratos Effect

- ▶ Even arbitrarily close to solution, full step  $\alpha = 1$  might be rejected because the non-smooth merit function  $\phi_\rho$  increases.
- ▶ Degrades fast local convergence.
- ▶ Remedies: Second-order correction steps or “watchdog” method.

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# SQP For Inequality-Constrained Nonlinear Problems

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c_E(x) = 0 \end{array}$$

Compute  $p_k$  from local QP model

$$\begin{array}{ll} \min_{p \in \mathbb{R}^n} & \frac{1}{2} p^T H_k p + \nabla f(x_k)^T p \\ \text{s.t.} & \nabla c_E(x_k)^T p + c_E(x_k) = 0 \end{array} \quad (\text{QP}_k)$$

# SQP For Inequality-Constrained Nonlinear Problems

$$\begin{aligned} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c_E(x) = 0 \\ & c_I(x) \leq 0 \end{aligned}$$

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# Local Behavior

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

$$\text{s.t. } c_i(x) = 0 \quad i \in \mathcal{E}$$

$$c_i(x) \leq 0 \quad i \in \mathcal{I}$$

# Local Behavior

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

$$\text{s.t. } c_i(x) = 0 \quad i \in \mathcal{E}$$

$$c_i(x) \leq 0 \quad i \in \mathcal{A}_*^{\text{NLP}}$$

$$c_i(x) \leq 0 \quad i \in \overline{\mathcal{A}}_*^{\text{NLP}}$$

$$\mathcal{A}_*^{\text{NLP}} = \{i \in \mathcal{I} : c_i(x^*) = 0\}$$

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## Lemma

Suppose  $x^*$  is a local minimizer satisfying the sufficient second-order optimality conditions, at which LICQ and strict optimality hold. Then  $\mathcal{A}_*^{\text{NLP}} = \mathcal{A}_*^{\text{QP}_k}$  for all  $x_k$  sufficiently close to  $x_*$ .

## Back to Newton's Method

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

$$\text{s.t. } c_i(x) = 0 \quad i \in \mathcal{E}$$

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- ▶ When  $x_k$  is close to  $x^*$ ,  $(\text{QP}_k)$  produces the same steps as SQP for equality-constrained NLP.

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- ▶ When  $x_k$  is close to  $x^*$ ,  $(\text{QP}_k)$  produces the same steps as SQP for equality-constrained NLP.
- ▶ We are back to Newton's method...
- ▶ Fast local convergence!

# Global Convergence

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c_E(x) = 0 \\ & c_I(x) \leq 0 \end{array}$$

Methods for equality constraints can be generalized.

- ▶ For example, penalty function

$$\phi_\rho(x) = f(x) + \rho \|c_E(x)\|_1 + \rho \|\max\{c_I(x), 0\}\|_1.$$

# Global Convergence

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$$\phi_\rho(x) = f(x) + \rho \|c_E(x)\|_1 + \rho \|\max\{c_I(x), 0\}\|_1.$$

$$\begin{aligned} \min_{p \in \mathbb{R}^n; t, s \in \mathbb{R}^{m_E}; r \in \mathbb{R}^{m_I}} & \frac{1}{2} p^T H_k p + \nabla f_k^T p + \rho \sum_{j=1}^{m_E} (s_j + t_j) + \rho \sum_{j=1}^{m_I} r_j \\ \text{s.t.} & \nabla c_{E,k}^T p + c_{E,k} = s - t \\ & \nabla c_{E,k}^T p + c_{E,k} \leq r \\ & \|p\| \leq \Delta_k, \quad s, t, r \geq 0 \end{aligned}$$



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→

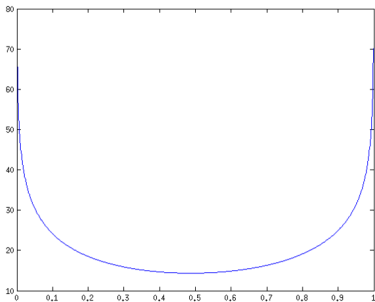
$$\begin{aligned} \min_{x \in \mathbb{R}^n} f(x) - \mu \sum_{i=1}^n \log(x_i) \\ \text{s.t. } c(x) = 0 \end{aligned}$$

# Barrier Problem

$$\begin{array}{ll} \min_{x \in \mathbb{R}} & f(x) \\ \text{s.t.} & x \geq 0 \\ & x \leq 10 \end{array}$$



$$\min_{x \in \mathbb{R}} f(x) - \mu \log(x) - \mu \log(10 - x)$$



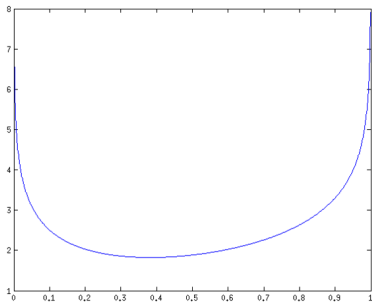
$$\mu = 10$$

# Barrier Problem

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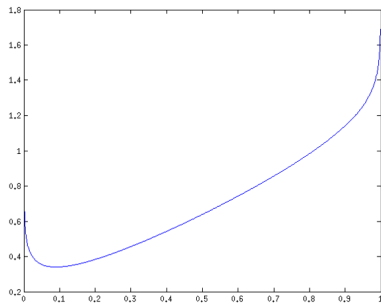
$$\mu = 1$$

# Barrier Problem

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$$\min_{x \in \mathbb{R}} f(x) - \mu \log(x) - \mu \log(10 - x)$$



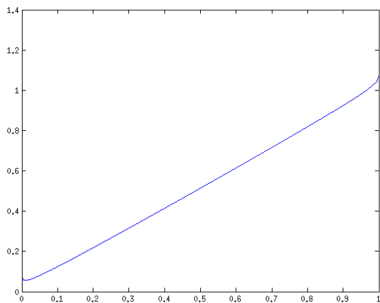
$$\mu = 0.1$$

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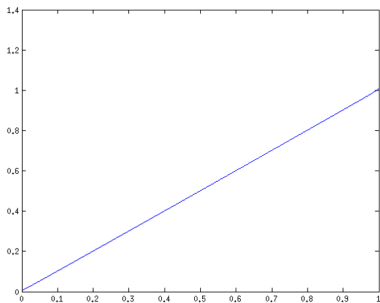
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# Barrier Method

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c(x) = 0 \\ & x \succeq 0 \end{array}$$

→

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Basic Algorithm:

1. Choose  $x_0 \in \mathbb{R}^n$ ,  $\mu_0 > 0$ ,  $\epsilon_0 > 0$ . Set  $k \leftarrow 0$ .

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3. Decrease  $\mu_{k+1} < \mu_k$  and  $\epsilon_{k+1} < \epsilon_k$ ; set  $k \leftarrow k + 1$ ; go to 2.  
(Ensure  $\mu_k \rightarrow 0$  and  $\epsilon_k \rightarrow 0$ .)

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→ Use SQP techniques
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# SQP Techniques for Solving the Barrier Problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \varphi_\mu(x) &= f(x) - \mu \sum_{i=1}^n \log(x_i) \\ \text{s.t. } c(x) &= 0 \end{aligned}$$

Can re-use SQP techniques:

- ▶ Step computation
  - ▶ KKT system with regularization
  - ▶ Decomposition

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  - ▶ Exact penalty function
  - ▶ Filter method

# Barrier Term Considerations

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- ▶ Fraction-to-the-boundary rule  $(\tau \in (0, 1), \text{ e.g., } \tau = 0.99)$

$$\alpha_k^{\max} = \arg \max \{ \alpha \in (0, 1] : x_k + \alpha p_k \geq (1 - \tau)x_k \}$$

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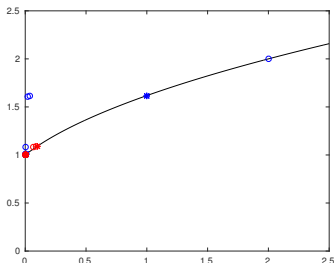
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- ▶ Ill-conditioning in linear system

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# Example

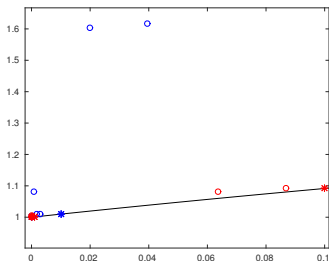
$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & x_1 + (x_2 - 1)^2 \\ \text{s.t.} \quad & x \geq 0 \end{aligned}$$



k	mu_k	f_k	( x_k(1), x_k(2) )	( p_k(1), p_k(2) )	err_barr	alpha
0	1.00e+00	2.50e+00	( 2.00e+00, 2.00e+00 )	( 0.00e+00, 0.00e+00 )	7.07e-01	0.00e+00
1	1.00e+00	2.02e-01	( 2.00e-02, 1.60e+00 )	( -2.00e+00, -4.00e-01 )	2.04e+00	9.90e-01
2	1.00e+00	2.31e-01	( 3.96e-02, 1.62e+00 )	( 1.96e-02, 1.40e-02 )	2.41e-02	1.00e+00
3	1.00e-01	6.69e-02	( 6.35e-02, 1.08e+00 )	( 2.39e-02, -5.36e-01 )	5.36e-01	1.00e+00
4	1.00e-01	9.09e-02	( 8.67e-02, 1.09e+00 )	( 2.32e-02, 9.33e-03 )	2.50e-02	1.00e+00
5	1.00e-02	4.15e-03	( 8.67e-04, 1.08e+00 )	( -6.65e-01, -8.18e-02 )	6.70e-01	1.29e-01
6	1.00e-02	1.71e-03	( 1.66e-03, 1.01e+00 )	( 7.92e-04, -7.12e-02 )	7.12e-02	1.00e+00
...						
12	3.16e-05	2.70e-05	( 2.70e-05, 1.00e+00 )	( 7.45e-06, 2.95e-11 )	7.45e-06	1.00e+00
13	1.78e-07	4.98e-10	( 4.81e-12, 1.00e+00 )	( -4.09e-03, -3.14e-05 )	4.09e-03	6.62e-03
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND = 1.300371e-16.						
14	1.78e-07	9.63e-12	( 9.62e-12, 1.00e+00 )	( 4.81e-12, -3.12e-05 )	3.12e-05	1.00e+00
15	1.78e-07	1.93e-11	( 1.92e-11, 1.00e+00 )	( 9.62e-12, 9.44e-17 )	9.62e-12	1.00e+00
16	7.50e-11	3.35e-11	( 3.35e-11, 1.00e+00 )	( 1.43e-11, -1.78e-07 )	1.78e-07	1.00e+00

# Example

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & x_1 + (x_2 - 1)^2 \\ \text{s.t.} \quad & x \geq 0 \end{aligned}$$



k	mu_k	f_k	( x_k(1), x_k(2) )	( p_k(1), p_k(2) )	err_barr	alpha
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1	1.00e+00	2.02e-01	( 2.00e-02, 1.60e+00 )	( -2.00e+00, -4.00e-01 )	2.04e+00	9.90e-01
2	1.00e+00	2.31e-01	( 3.96e-02, 1.62e+00 )	( 1.96e-02, 1.40e-02 )	2.41e-02	1.00e+00
3	1.00e-01	6.69e-02	( 6.35e-02, 1.08e+00 )	( 2.39e-02, -5.36e-01 )	5.36e-01	1.00e+00
4	1.00e-01	9.09e-02	( 8.67e-02, 1.09e+00 )	( 2.32e-02, 9.33e-03 )	2.50e-02	1.00e+00
5	1.00e-02	4.15e-03	( 8.67e-04, 1.08e+00 )	( -6.65e-01, -8.18e-02 )	6.70e-01	1.29e-01
6	1.00e-02	1.71e-03	( 1.66e-03, 1.01e+00 )	( 7.92e-04, -7.12e-02 )	7.12e-02	1.00e+00
...						
12	3.16e-05	2.70e-05	( 2.70e-05, 1.00e+00 )	( 7.45e-06, 2.95e-11 )	7.45e-06	1.00e+00
13	1.78e-07	4.98e-10	( 4.81e-12, 1.00e+00 )	( -4.09e-03, -3.14e-05 )	4.09e-03	6.62e-03
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND = 1.300371e-16.						
14	1.78e-07	9.63e-12	( 9.62e-12, 1.00e+00 )	( 4.81e-12, -3.12e-05 )	3.12e-05	1.00e+00
15	1.78e-07	1.93e-11	( 1.92e-11, 1.00e+00 )	( 9.62e-12, 9.44e-17 )	9.62e-12	1.00e+00
16	7.50e-11	3.35e-11	( 3.35e-11, 1.00e+00 )	( 1.43e-11, -1.78e-07 )	1.78e-07	1.00e+00

# Primal-Dual System

$$\begin{array}{ll} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & c(x) = 0 \\ & x \geq 0 \end{array}$$

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## Newton Steps

$$\begin{bmatrix} \nabla_{xx}^2 \mathcal{L}_k & \nabla c_k & -I \\ \nabla c_k^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{pmatrix} p_k \\ p_k^\lambda \\ p_k^z \end{pmatrix} = - \begin{pmatrix} \nabla f_k + \nabla c_k \lambda_k - z_k \\ c_k \\ X_k Z_k e - \mu e \end{pmatrix}$$

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## Block elimination

$$\begin{bmatrix} \nabla_{xx}^2 \mathcal{L}_k + X_k^{-1} Z_k & \nabla c_k \\ \nabla c_k^T & 0 \end{bmatrix} \begin{pmatrix} p_k \\ \tilde{\lambda}_{k+1} \end{pmatrix} = - \begin{pmatrix} \nabla f_k - \mu X_k^{-1} e \\ c_k \end{pmatrix}$$

# Primal-Dual Steps

$$\begin{bmatrix} \nabla_{xx}^2 \mathcal{L}_k + \Sigma_k & \nabla c_k \\ \nabla c_k^T & 0 \end{bmatrix} \begin{pmatrix} p_k \\ \tilde{\lambda}_{k+1} \end{pmatrix} = - \begin{pmatrix} \nabla f_k - \mu X_k^{-1} e \\ c_k \end{pmatrix}$$

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- ▶ Barrier Hessian term:
  - ▶  $\Sigma_k = X_k^{-2}$ : primal
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- ▶ Now: Fast local convergence.

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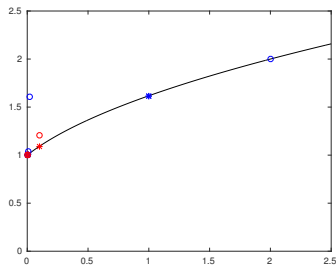
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- ▶ Now: Fast local convergence.
- ▶ Ill-conditioning in KKT system is benign for direct linear solvers.



# Example Revisited with Primal-Dual Method

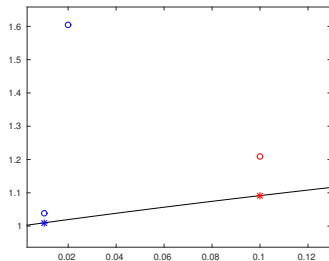
$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & x_1 + (x_2 - 1)^2 \\ \text{s.t.} \quad & x \geq 0 \end{aligned}$$



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Interior Point Methods

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(very rough guide. . .)

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  - ▶ Byrd-Omojokun decomposition
  - ▶ other algorithmic options: direct method; SLP-EQP method

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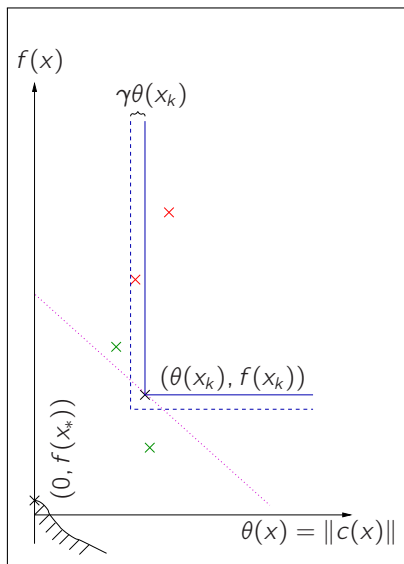
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- ▶ MINOS [Murtagh, Sanders]
  - ▶ linearly-constrained augmented Lagrangian method
  - ▶ line search

Thank You!

# A Filter Line Search Method



Idea: Bi-objective optimization

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & c(x) = 0 \end{array}$$

$$\min \theta(x)$$

$$\min f(x)$$

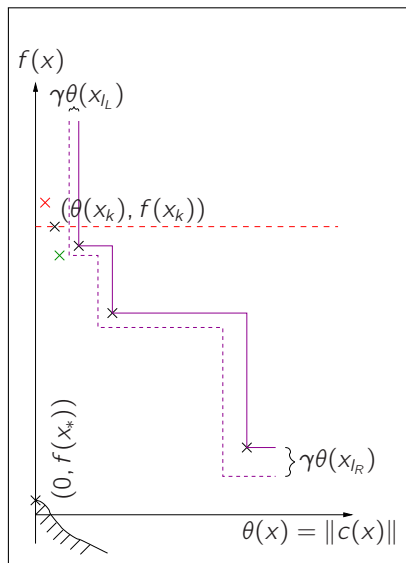








# A Filter Line Search Method (“ $f$ -type”)



If *switching condition*

$$-\alpha \nabla f(x_k)^T d_k^x > \delta [\theta(x_k)]^{s_\theta}$$

holds ( $s_\theta > 1$ ):

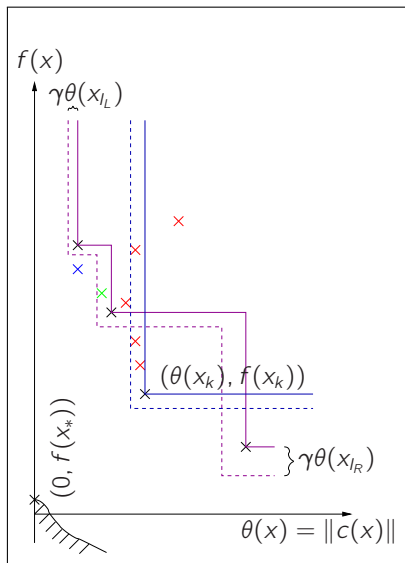
Require Armijo-condition on  $f(x)$ :

$$f(x_{tr}) \leq f(x_k) + \eta \alpha \nabla f(x_k)^T d_k^x$$

$\implies$  Don't augment  $\mathcal{F}_k$  in that case

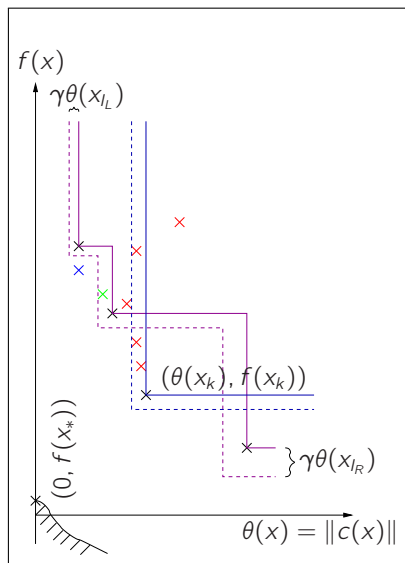


# A Filter Line Search Method (Restoration)



If no admissible step size  $\alpha_k$  can be found

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Revert to  
feasibility restoration phase:

Decrease  $\theta(x)$  until

- ▶ found acceptable new iterate  $x_{k+1}$ , or
- ▶ converged to local minimizer of constraint violation