A Short Course In Nonlinear Optimization

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Introduction

Nonlinear optimization problems:

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

x	Variables
$f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$	Objective function
$c(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^m$	Equality constraints
$d(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^p$	Inequality constraints

- We assume that all functions are C^2, but can be nonlinear
- Interested in large problem ($n = 100, \ldots, 10^7$)

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- Interested in large problem ($n = 100, \ldots, 10^7$)
- MINLP: Some of the x variables are required to be integer
- Goal of this course: Provide understanding, how
  - non-convex NLPs (software: IPOPT)
  - convex MINLP (software: BONMIN)

  can be solved numerically
- This is not a comprehensive course on (MI)NLP

Outline

1. Unconstrained Optimization

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

- Optimality conditions
- Newton's method
- Line search

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- Optimality conditions
- Sequential quadratic programming
- Merit functions and filter methods

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3. Inequality Constrained Optimization

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

- Optimality conditions
- Active set methods
- Interior point methods

Outline (cont.)

4. IPOPT: Open source software for non-convex NLP

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ s.t. \quad & c(x) = 0 \\ & x_L \leq x \leq x_U \end{aligned}$$

- Algorithm details
- Implementation
- Adaptive choice of barrier parameter

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5. Industrial applications for NLP

- Examples
- Circuit tuning

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6. (Convex) Mixed-Integer Nonlinear Programming (MINLP)

$$\begin{aligned} \min_{x \in \mathbb{R}^n, y \in \mathbb{R}^p} \quad & f(x, y) \\ s.t. \quad & c(x, y) = 0 \\ & x_L \leq x \leq x_U \\ & y \in \{0, 1\}^p \end{aligned}$$

- Branch and bound
- Outer approximation
- A new hybrid approach
- The BONMIN package

Unconstrained Optimization

Unconstrained Optimization

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For this short course we assume:

- Smoothness:
  - $f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$ is C^2
- Computational availability of functions and derivatives:
  - $f(x_k)$, $\nabla f(x_k)$ and $\nabla^2 f(x_k)$ can be evaluated for given x_k

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- Not covered here:
  - Nonsmooth optimization, e.g., $f(x)$ as "kinks"
  - Derivative-Free Optimization
    - $\nabla f(x_k)$ and $\nabla^2 f(x_k)$ cannot be computed
  - Quasi-Newton Methods
    - $\nabla^2 f(x_k)$ cannot be computed
    - approximate $W_k \approx \nabla^2 f(x_k)$

Optimality Conditions

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Characterizing "local solutions" x_*: $f(x) \geq f(x_*)$ for x in neighborhood of x_*.

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- 1st order necessary condition:

$$x_* \text{ is local solution of } f(x) \quad \Longrightarrow \quad \nabla f(x_*) = 0$$

At x_* there is no "descent direction" (up to first order).
Such x_* is called "stationary point".

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- 2nd order sufficient condition:

  $$\left.\begin{array}{l} \nabla f(x_*) = 0 \\ \nabla^2 f(x_*) \succ 0 \end{array}\right\} \quad \Longrightarrow \quad x_* \text{ is local solution of } f(x)$$

Comments

- If $f(x)$ is convex:
  - Every stationary point is a global solution
  - There are no maxima or saddle point points
  - 1st order optimality conditions are sufficient for x_* being a global solution

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- If $f(x)$ is non-convex:
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  - Might have many local solutions x_* with different $f(x_*)$

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Usually, numerical methods for finding a local solution

- seek point x_* with $\nabla f(x_*) = 0$
- try to avoid convergence to maxima

Newton's Method

- Numerical method for solving nonlinear system of equations

$$F(x_*) = 0$$

- Iterative method:
  - Given starting point x_0
  - Generate sequence $\{x_k\}$ of improved "guesses" of the solution

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- Step: Given x_k, set up local linear "model" of $F(x)$

$$m_k(x) = F(x_k) + \nabla F(x_k)^T (x - x_k)$$

From Taylor expansion: $\|m_k(x) - F(x)\| = O(\|x - x_k\|^2)$

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$$0 = m_k(x) = F(x_k) + \nabla F(x_k)^T (x - x_k)$$

$$\Longrightarrow \qquad d_k = -[\nabla F(x_k)]^{-T} F(x_k)$$

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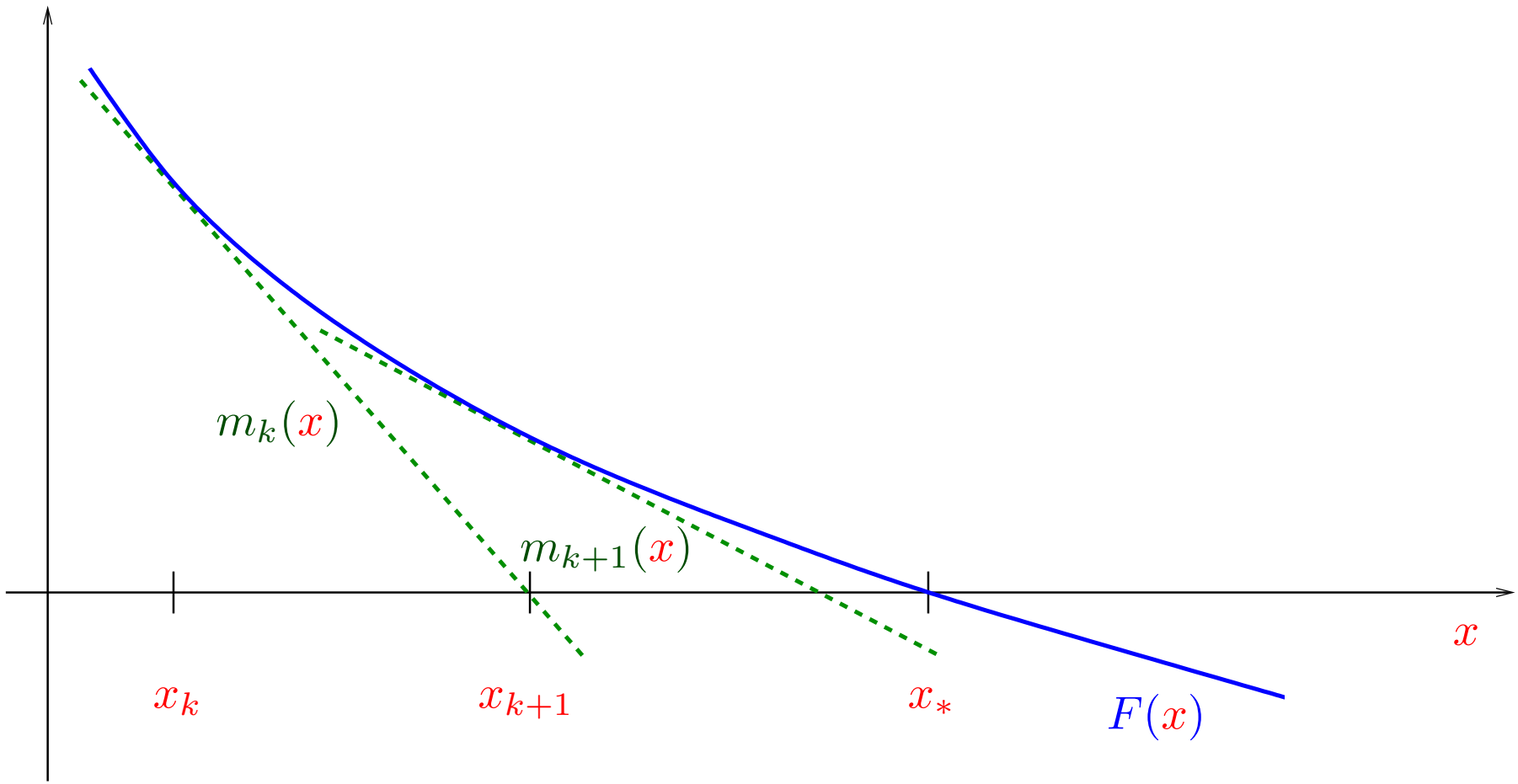
- Set $x_{k+1} = x_k + d_k$

Newton's Method For Equations



Newton's Method For Optimization

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Newton's Method For Optimization

- Numerical method for solving nonlinear optimization problem

$$\min_{x \in \mathbb{R}^n} f(x) \qquad \nabla f(x_*) = 0$$

- Iterative method:
  - Given starting point x_0
  - Generate sequence $\{x_k\}$ of improved "guesses" of the solution
- Step: Given x_k, set up local quadratic "model" of $f(x)$

$$m_k(x) = f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k)$$

From Taylor expansion: $\|\nabla m_k(x) - \nabla f(x)\| = O(\|x - x_k\|^2)$

- Find minimizer $\tilde{x}_{k+1} = x_k + d_k$ of model $m_k(x)$ (assume convex)

$$0 = \nabla m_k(x) = \nabla f(x_k) + \nabla^2 f(x_k)(x - x_k)$$

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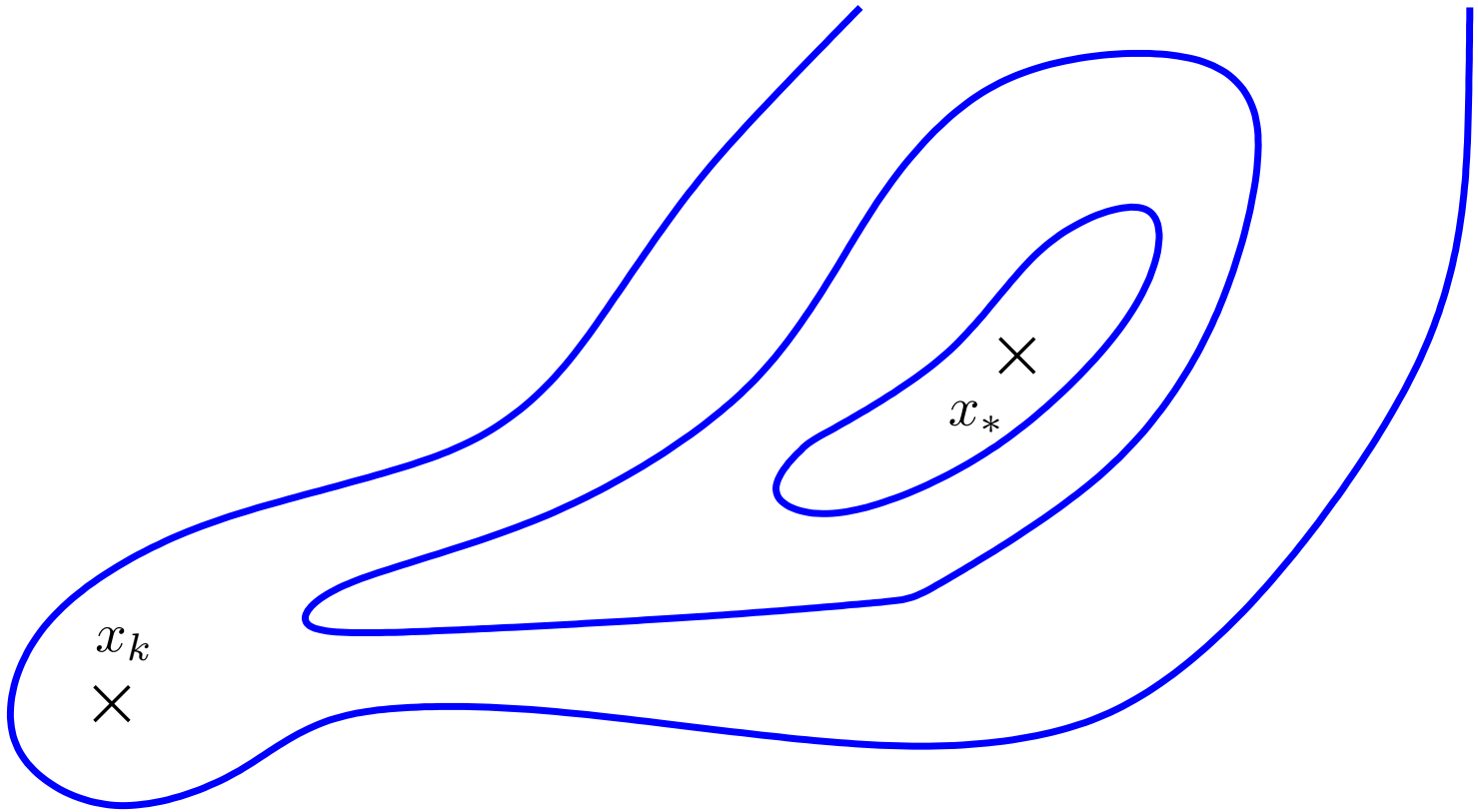

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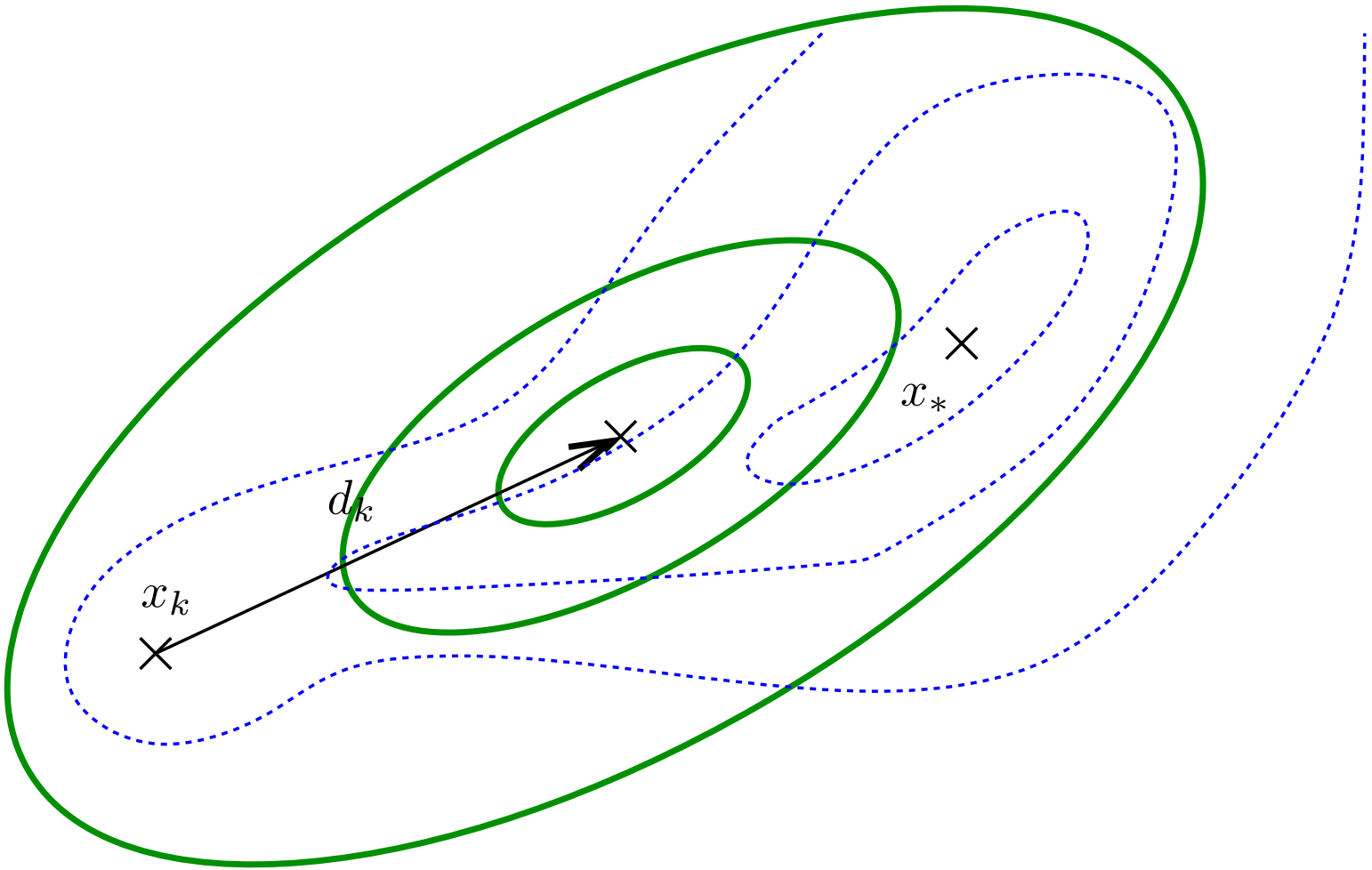

Fast Congergence of Newton's Method

Assume:

- x_* is second order sufficient solution for $\min_{x \in \mathbb{R}^n} f(x)$
- x_0 is sufficiently close to x_*
- $x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$

Then:

- $\lim_k x_k = x_*$
- $\{x_k\}$ converges quadratically to x_*, i.e.,

$$\exists\, C > 0 : \quad \|x_{k+1} - x_*\| \leq C \|x_k - x_*\|^2$$

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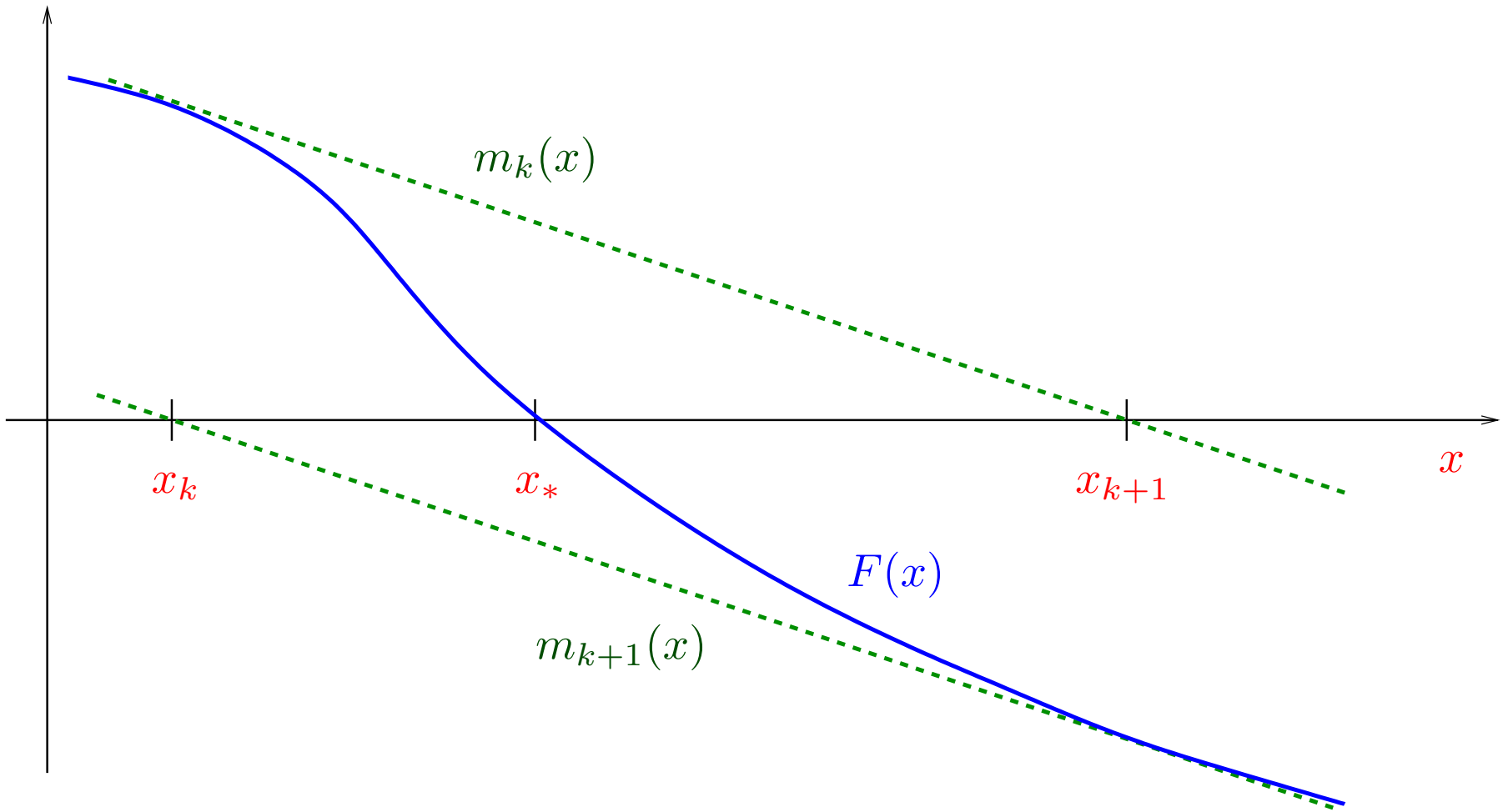
But what happens if x_0 is not close to x_*?

What can go wrong



Line Search

- Want to guarantee "global convergence" (convergence from any x_0)
- Consider Newton direction $d_k^N = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$
- How does $f(x)$ behave in direction d_k^N?

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  - Define $\Phi_k(\alpha) := f(x_k + \alpha d_k^N)$
  - Then

$$\begin{aligned} \Phi_k'(\alpha) &= \nabla f(x_k)^T d_k^N \\ &= -\nabla f(x_k)^T [\nabla^2 f(x_k)]^{-1} \nabla f(x_k) \\ &< 0 \end{aligned}$$

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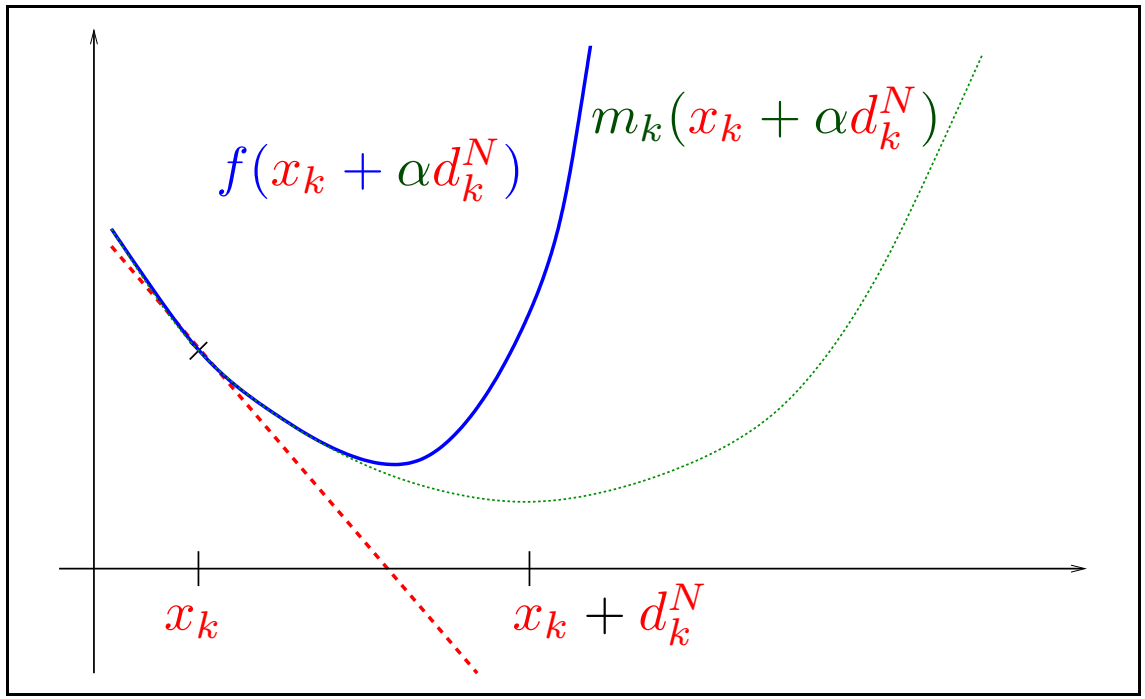
  - Therefore, d_k^N is a "descent direction" for $f(x)$
  - Idea: Choose "step size" $\alpha_k \in (0, 1]$, so that

$$\boxed{x_{k+1} = x_k + \alpha_k d_k^N}$$

    gives "sufficient decrease" in $f(x)$

Armijo Condition



- We have linearization $f(x_k + \alpha d_k^N) \approx f(x_k) + \alpha \nabla f(x_k)^T d_k^N$

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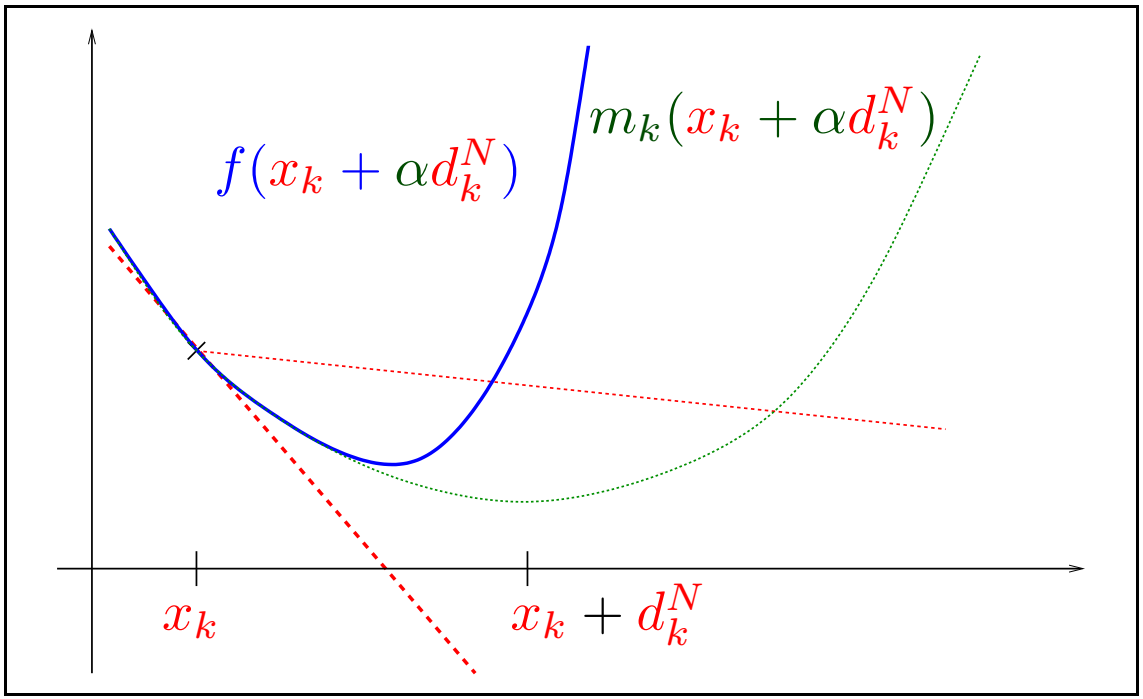

- We have linearization $f(x_k + \alpha d_k^N) \approx f(x_k) + \alpha \nabla f(x_k)^T d_k^N$
- Relax slope, and ask for decrease w.r.t. "relaxed linearization"

$$\boxed{f(x_k + \alpha_k d_k^N) \leq f(x_k) + \eta \alpha_k \nabla f(x_k)^T d_k^N} \qquad \eta \in (0, 1)$$

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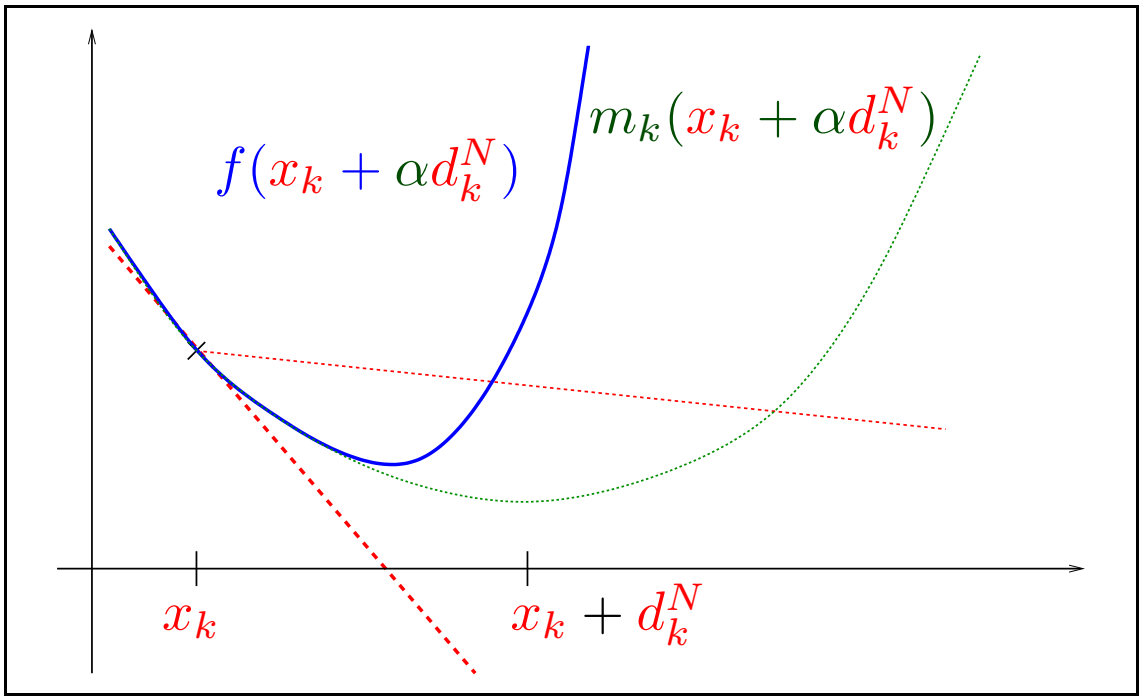

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- Backtracking line search:
  - Try $\alpha_k^l = \left(\frac{1}{2}\right)^l$ for $l = 0, 1, 2, \ldots$, until Armijo condition holds

Nonconvex Problems

- We need that $d_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$ is a descent direction, i.e.,

$$\Phi_k(\alpha)' = -\nabla f(x_k)^T [\nabla^2 f(x_k)]^{-1} \nabla f(x_k) < 0$$

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1. Choose $\delta \geq 0$ so that

$$W_k = \nabla^2 f(x_k) + \delta I \succ 0$$

and perform "trial factorizations" (e.g. Cholesky) until $W_k \succ 0$. ("Bend into directions of steepest descent.")

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- Important alternative approach: Trust region methods (not covered)

Global Convergence Proof (1)

Method:

$$d_k = -W_k^{-1} \nabla f(x_k) \qquad f(x_{k+1}) - f(x_k) \leq \eta \alpha_k \nabla f(x_k)^T d_k$$

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Assume:

$$\exists \epsilon_1, \epsilon_2 > 0,\ f_{\text{low}},\ M : \epsilon_1 I \prec W_k \prec \epsilon_2 I,\ f(x) \geq f_{\text{low}},\ \|\nabla^2 f(x)\| \leq M$$

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Have:

$$\begin{aligned}
\|d_k\| &\leq \epsilon_1^{-1}\|\nabla f(x_k)\| && (\xi^{\alpha_k} \in [x_k, x_k + d_k]) \\
f(x_k + \alpha d_k) - f(x_k) &= \alpha \nabla f(x_k)^T d_k + \alpha^2 {d_k}^T \nabla^2 f(\xi^{\alpha_k}) d_k \\
&\leq \alpha \nabla f(x_k)^T d_k + \alpha^2 M \|d_k\|^2 \\
\nabla f(x_k)^T d_k &= -\nabla f(x_k)^T W_k^{-1} \nabla f(x_k) \leq -\epsilon_2^{-1}\|\nabla f(x_k)\|^2
\end{aligned}$$

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Have:

$$\begin{aligned} \|d_k\| &\leq \epsilon_1^{-1}\|\nabla f(x_k)\| && (\xi^{\alpha_k} \in [x_k, x_k + d_k]) \\ f(x_k + \alpha d_k) - f(x_k) &= \alpha \nabla f(x_k)^T d_k + \alpha^2 {d_k}^T \nabla^2 f(\xi^{\alpha_k}) d_k \\ &\leq \alpha \nabla f(x_k)^T d_k + \alpha^2 M \|d_k\|^2 \\ \nabla f(x_k)^T d_k &= -\nabla f(x_k)^T W_k^{-1} \nabla f(x_k) \leq -\epsilon_2^{-1}\|\nabla f(x_k)\|^2 \end{aligned}$$

Therefore:

$$\begin{aligned} & f(x_k + \alpha d_k) - f(x_k) - \eta\alpha \nabla f(x_k)^T d_k \\ \leq\ & \alpha(1-\eta)\nabla f(x_k)^T d_k + \alpha^2 M \epsilon_1^{-2}\|\nabla f(x_k)\|^2 \\ \leq\ & -\alpha(1-\eta)\epsilon_2^{-1}\|\nabla f(x_k)\|^2 + \alpha^2 M \epsilon_1^{-2}\|\nabla f(x_k)\|^2 \end{aligned}$$

Global Convergence Proof (1)

Method: $\boxed{d_k = -W_k^{-1}\nabla f(x_k) \qquad f(x_{k+1}) - f(x_k) \leq \eta\alpha_k \nabla f(x_k)^T d_k}$

Assume:

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for $\alpha < \frac{\epsilon_1(1-\eta)}{\epsilon_2 M} =: \bar{\alpha}$. Hence $\alpha_k \geq \frac{1}{2}\bar{\alpha} > 0$ from backtracking line search.

Global Convergence Proof (2)

Method: $\boxed{d_k = -W_k^{-1}\nabla f(x_k) \qquad f(x_{k+1}) - f(x_k) \leq \eta\alpha_k \nabla f(x_k)^T d_k}$

Have: $\alpha_k \geq \frac{1}{2}\bar{\alpha} > 0$ and $\nabla f(x_k)^T d_k \leq -\epsilon_2^{-1}\|\nabla f(x_k)\|^2$.

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Since $f(x_k) \geq f_{\text{low}}$, we have global convergence result:

$$\boxed{\lim_{k\to\infty} \|\nabla f(x_k)\| = 0}$$

Local Convergence Of Globalized Method

Assume:

- x_* satisfies sufficient second order optimality conditions.
- x_k gets close to x_*.
- No Hessian modification takes place for large k.
  (Remember: $\nabla^2 f(x_*) \succ 0$)

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- x_* satisfies sufficient second order optimality conditions.
- x_k gets close to x_*.
- No Hessian modification takes place for large k.
  (Remember: $\nabla^2 f(x_*) \succ 0$)

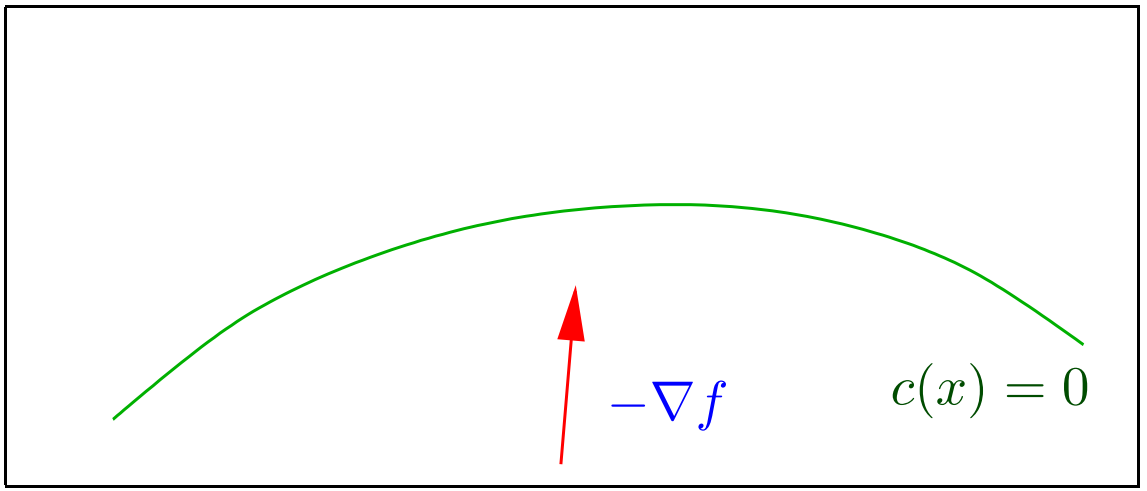
Then, using Taylor's theorem, one can show:

- $\alpha_k = 1$ for large k.
  (i.e., eventually, we take full Newton steps)
- $\{x_k\}$ converges quadratically to x_*.

Equality-Constrained Optimization

First Order Optimality Conditions Motivation

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



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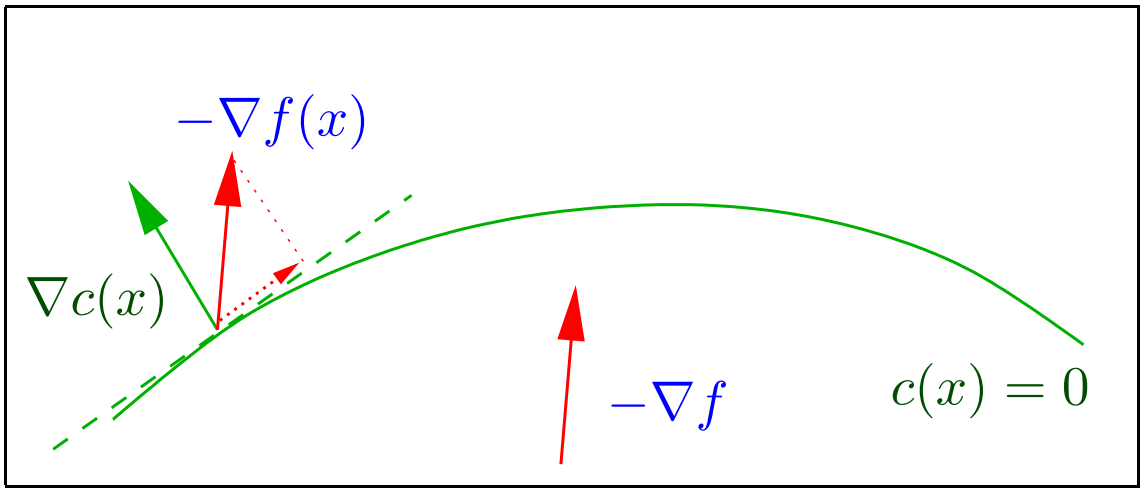

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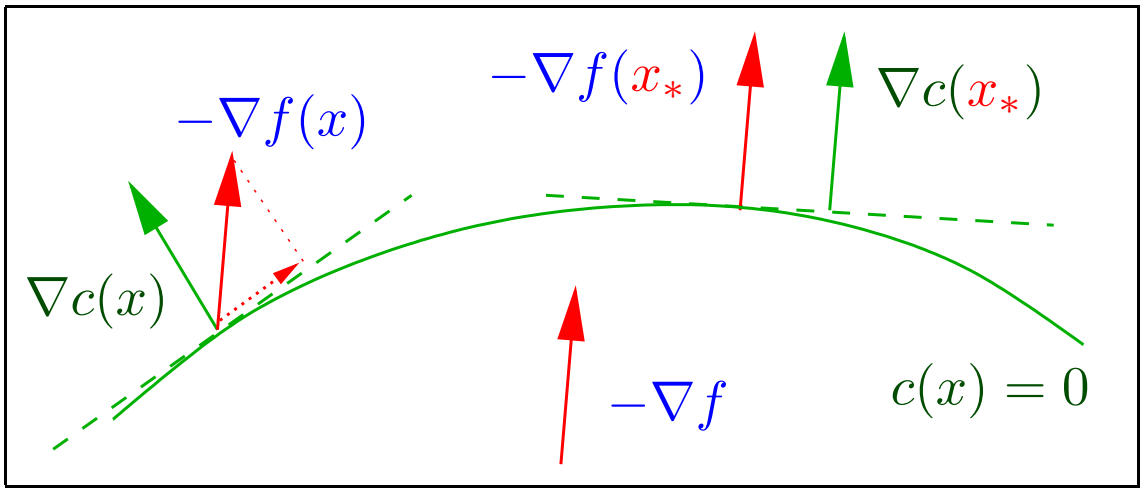

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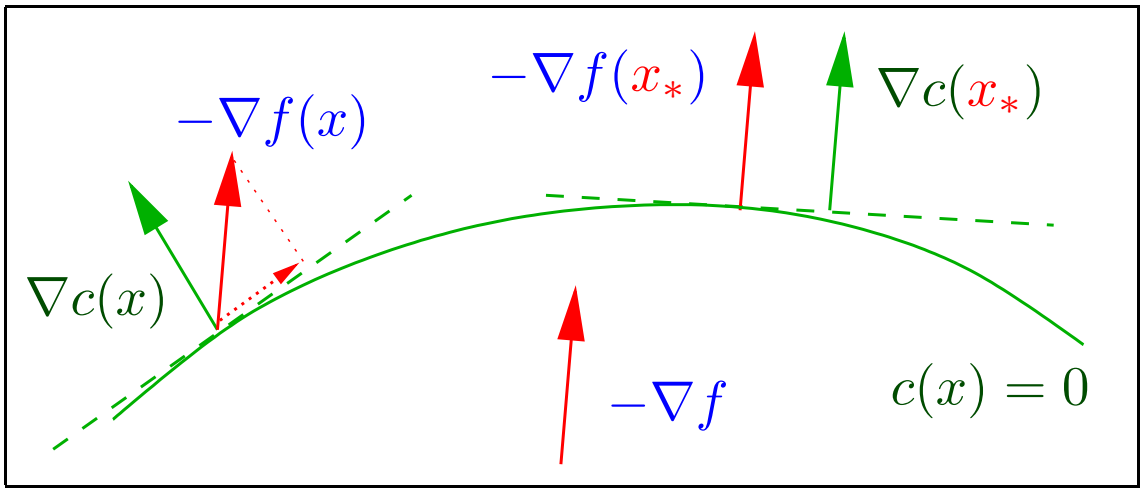

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$$\begin{aligned} \nabla f(x_*) + \nabla c(x_*)\lambda_* &= 0 \\ c(x_*) &= 0 \end{aligned}$$

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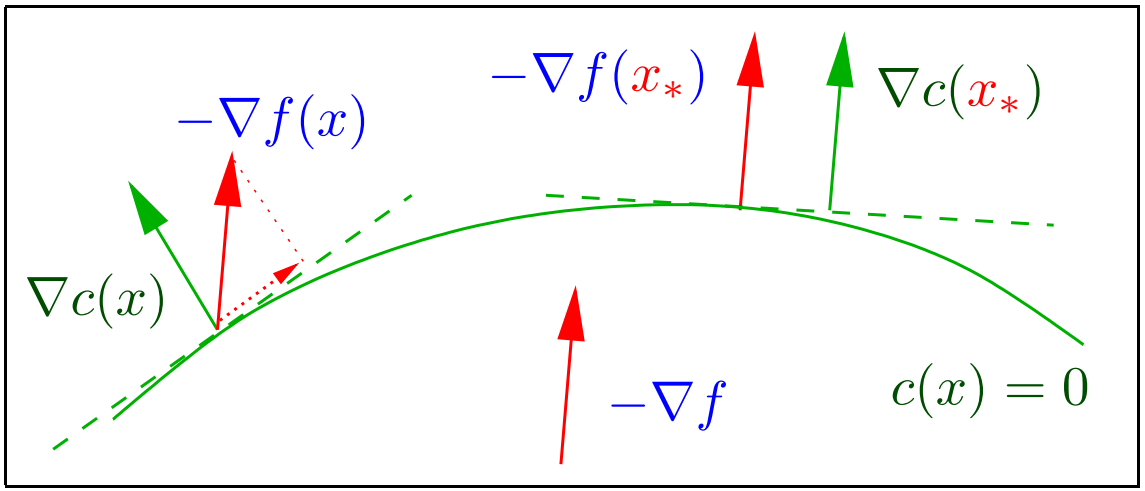

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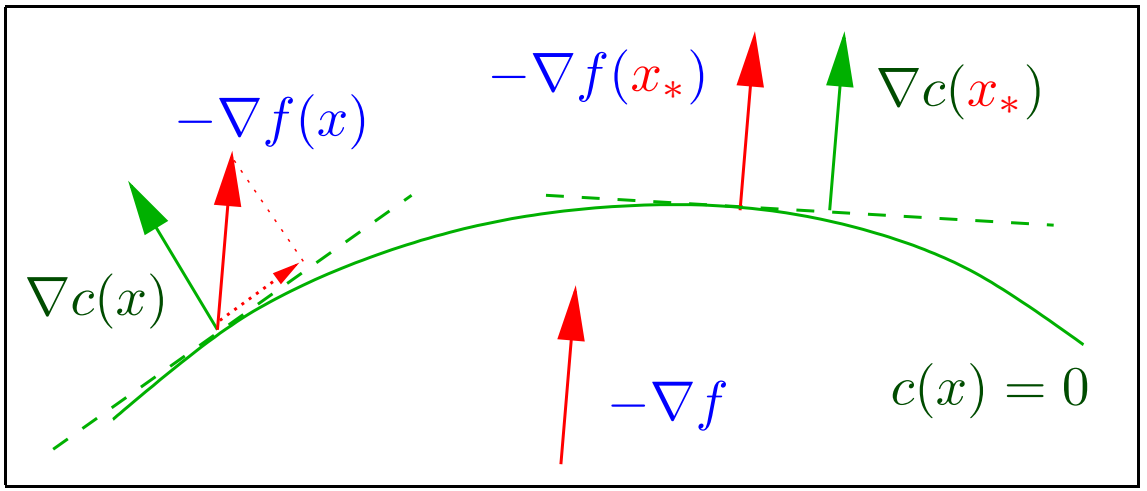

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Lagrangian function:

$$\mathcal{L}(x, \lambda) = f(x) + c(x)^T \lambda$$

λ_* are called optimal (Lagrangian) multipliers.

First Order Optimality Conditions (1)

- Assume:
  - x_* is a local solution, i.e., there exists neighborhood $\mathcal{N}_*$ of x_* with

    $$f(x) \geq f(x_*) \qquad \text{for all } x \in \mathcal{N}_* \text{ with } c(x) = 0$$

  - $\nabla c(x_*)$ has full rank

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has $x_* = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, but $\nabla f(x_*) = \begin{pmatrix} 2 \\ 0 \end{pmatrix}$, $\nabla c(x_*) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

First Order Optimality Conditions (2)

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

x	Variables
$f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$	Objective function
$c(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^m$	Equality constraints

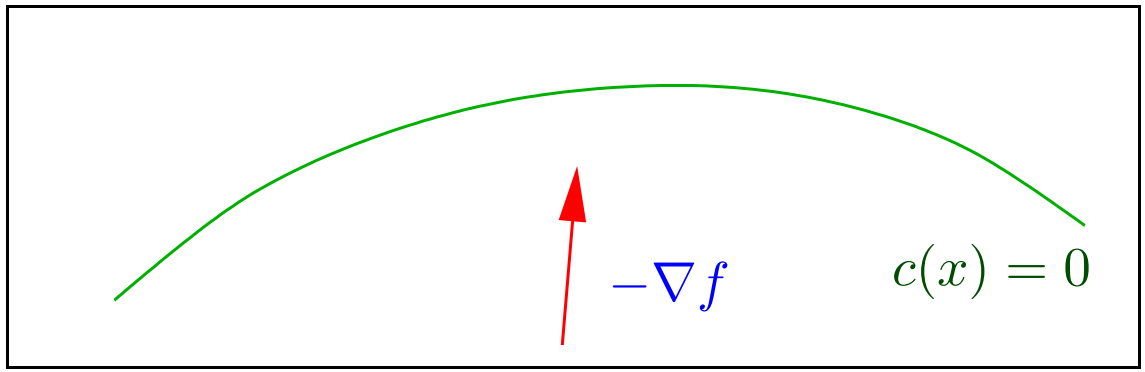
From implicit function theorem:

- Can partition $x = (y, z)$ with
  - $y \in \mathbb{R}^{n-m}$ (independent variables)
  - $z \in \mathbb{R}^m$ (dependent variables)
- Find C^2 function $\Phi(y) : \mathbb{R}^{n-m} \longrightarrow \mathbb{R}^m$, so that

$$\Phi(y_*) = z_* \quad \text{and} \quad c(y, \Phi(y)) = 0 \text{ for all } (y, \Phi(y)) \in \mathcal{N}_*$$

i.e., z is determined by y if variables should satisfy $c(x) = 0$

First Order Optimality Conditions (3)



$\Phi(y_*) = z_*$ and $c(y, \Phi(y)) = 0$ for all $(y, \Phi(y)) \in \mathcal{N}_*$

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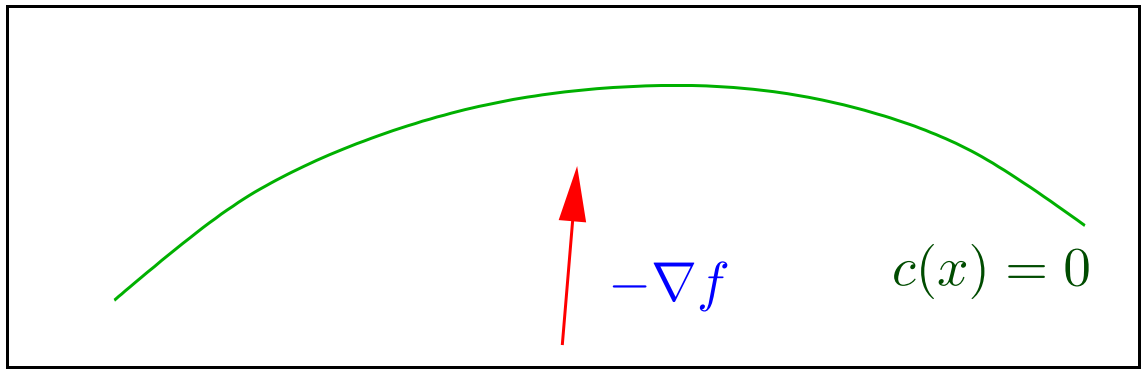

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- Then: x_* is local minimizer of

$$\min f(x), \text{ s.t. } c(x) = 0$$

is equivalent to: $x_* = (y_*, \Phi(y_*))$, where y_* is local minimizer of unconstrained problem

$$\min \Psi(y) := f(y, \Phi(y))$$

First Order Optimality Conditions (4)

Optimality of y_* for

$$\boxed{\min \Psi(y) := f(y, \Phi(y))}$$

implies

$$\begin{aligned} 0 &= \nabla_y \Psi(y_*) = \nabla_y [f(y_*, \Phi(y_*))] \\ &= \nabla_y f(y_*, z_*) + \nabla_y \Phi(y_*) \nabla_z f(y_*, z_*) \end{aligned}$$

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since from $c(y, \Phi(y)) = 0$

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$$0 = \nabla_y [c(y_*, \Phi(y_*))] = \nabla_y c(y_*, z_*) + \nabla_z c(y_*, z_*) \nabla_y \Phi(y_*)$$

Define $\lambda_* := -\left[\nabla_z c(x_*)\right]^{-1} \nabla_z f(x_*)$, then

$$\begin{aligned} 0 &= \nabla_y f(x_*) + \nabla_y c(x_*) \lambda_* \\ 0 &= \nabla_z f(x_*) + \nabla_z c(x_*) \lambda_* \end{aligned}$$

Second Order Optimality Conditions

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

x	Variables
$f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$	Objective function
$c(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^m$	Equality constraints

Lagrangian $\mathcal{L}(x, \lambda) = f(x) + \lambda^T c(x)$; Assumptions as before.

- 2nd order necessary conditions: If x_* is local minimum, then

  for all $d \in \mathbb{R}^n$ with $\nabla c(x_*)^T d = 0$: $\quad d^T \nabla^2_{xx} \mathcal{L}(x_*, \lambda_*)^T d \geq 0$

"Projection of $\nabla^2_{xx} \mathcal{L}(x_*, \lambda_*)$ onto manifold $\mathcal{M}$ is positive semi- definite"

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- 2nd order sufficient conditions:

  If x_* satisfies 1st order necessary conditions and
  for all $d \in \mathbb{R}^n \setminus \{0\}$ with $\nabla c(x_*)^T d = 0$: $\quad d^T \nabla^2_{xx} \mathcal{L}(x_*, \lambda_*)^T d > 0,$

  then x_* is local a solution.

"Projection of $\nabla^2_{xx} \mathcal{L}(x_*, \lambda_*)$ onto manifold $\mathcal{M}$ is positive (semi-)definite"

Newton's Method (again)

- Idea of many algorithms: Apply Newton's method to

$$\begin{aligned} \nabla f(x_*) + \nabla c(x_*)\lambda_* &= 0 \\ c(x_*) &= 0 \end{aligned}$$

- Nonlinear system of equations in (x, λ).
- Fast local convergence for 2nd order sufficient (x_*, λ_*)

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- "Infeasible" algorithm, since $c(x_k) = 0$ can be violated

Interpretation As Quadratic Program

- Newton step:

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- These are the optimality conditions for quadratic program (QP)

$$\begin{aligned} \min_{d \in \mathbb{R}^n} \quad & f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T W_k d \\ s.t. \quad & c(x_k) + \nabla c(x_k)^T d = 0 \end{aligned}$$

- Therefore: We can alternatively solve QP to obtain (d_k^x, λ_k^+)
- Can interpret Newton step as solution of “local model” of NLP

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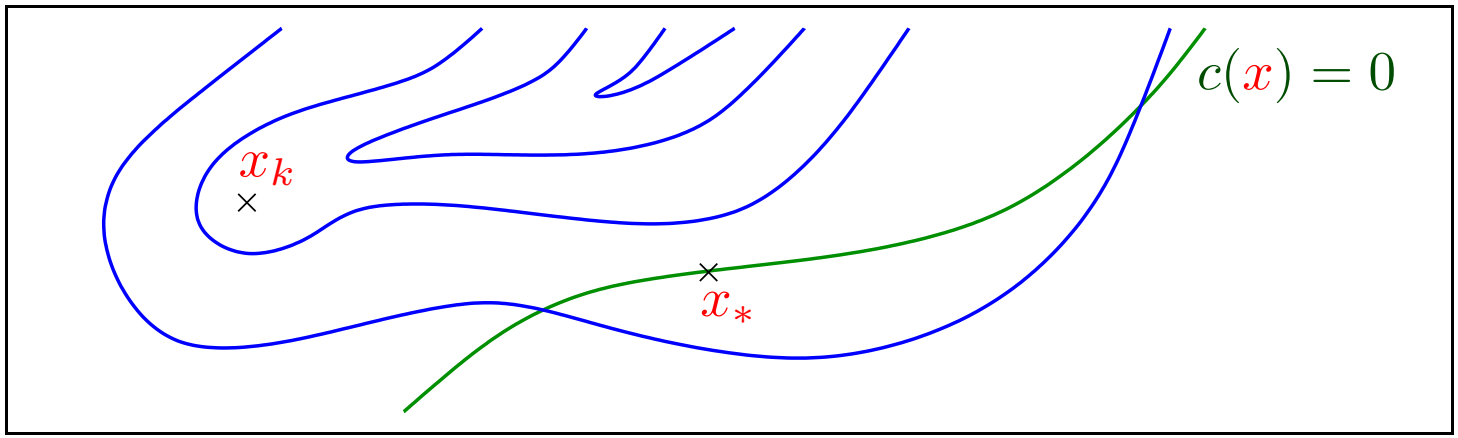
- Implicitly assumed projection of W_k onto null space of $\nabla c(x_k)^T$ is positive definite; otherwise QP is unbounded.

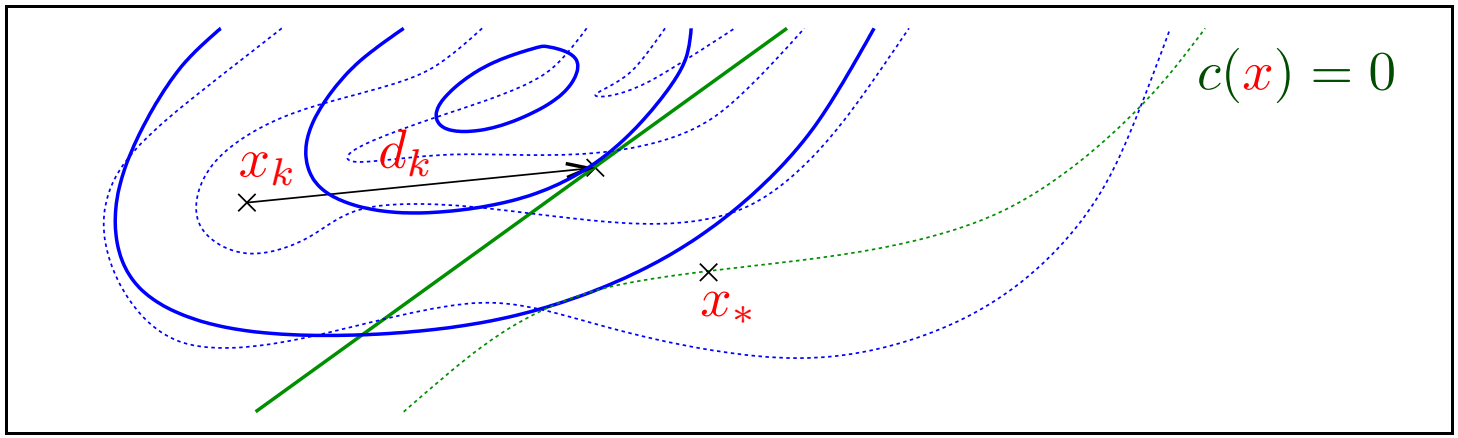
Sequential Quadratic Programming (SQP)



Original Problem

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

Sequential Quadratic Programming (SQP)



Quadratic Model

$$\begin{aligned} \min_{d \in \mathbb{R}^n} \quad & f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T W_k d \\ s.t. \quad & c(x_k) + \nabla c(x_k)^T d = 0 \end{aligned}$$

- At each iteration, compute d_k as solution of QP, and $\lambda_{k+1} = \lambda_k^+$
- Nonconvexity: Ensure that W_k pos. def. in null space of $\nabla c(x_k)^T$
- If $W_k = \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k)$, this is equivalent to Newton's method (fast)

Handling Nonconvexities in SQP

- Want: Projection $(P_k^c)^T W_k P_k^c \succ 0$ (with projection $(P_k^c)^T \nabla c(x_k) = 0$)
- Could compute eigenvalues of $(P_k^c)^T W_k P_k^c$ explicitly (expensive!)

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$$\begin{matrix} n \\ m \end{matrix} \begin{bmatrix} W_k & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix}$$ has n positive, and m negative eigenvalues ("has inertia $(n, m, 0)$")

- Many direct symmetric indefinite linear solvers can easily return inertia
- One way: Perform trial factorizations of $\begin{bmatrix} \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k) + \delta I & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix}$ for increasing values of $\delta \geq 0$, until inertia is correct

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- Other option: "Inertia-controlling" factorization (usually expensive)

Line Search With Merit Function

- Want to ensure convergence to stationary point from any (x_0, λ_0).
- Two (usually conflicting) goals:

$$\boxed{\min f(x)} \qquad \boxed{\min \|c(x)\|}$$

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- Exact penality function: $\Phi_\rho(x) = f(x) + \rho\|c(x)\|$
- If (x_*, λ_*) local solution: $\rho > \|\lambda_*\|^{\text{dual}} \implies x_*$ is local minimizer of $\Phi_\rho(x)$
- Idea: Minimize $\Phi_\rho(x)$ (non-differentiable)

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- Idea: Minimize $\Phi_\rho(x)$ (non-differentiable)
- Basic algorithm (simplified):
  - Compute d_k (ensure correct inertia)
  - Update $\rho_k \geq \rho_{k-1}$, so that directional derivative $D\Phi_{\rho_k}(x_k; d_k) < 0$
  - Backtracking line search $\alpha_k^l = 2^{-l}$, until Armijo condition satisfied:

$$\Phi_{\rho_k}(x_k + \alpha_k d_k) - \Phi_{\rho_k}(x_k) \leq \eta\alpha_k D\Phi_{\rho_k}(x_k; d_k)$$

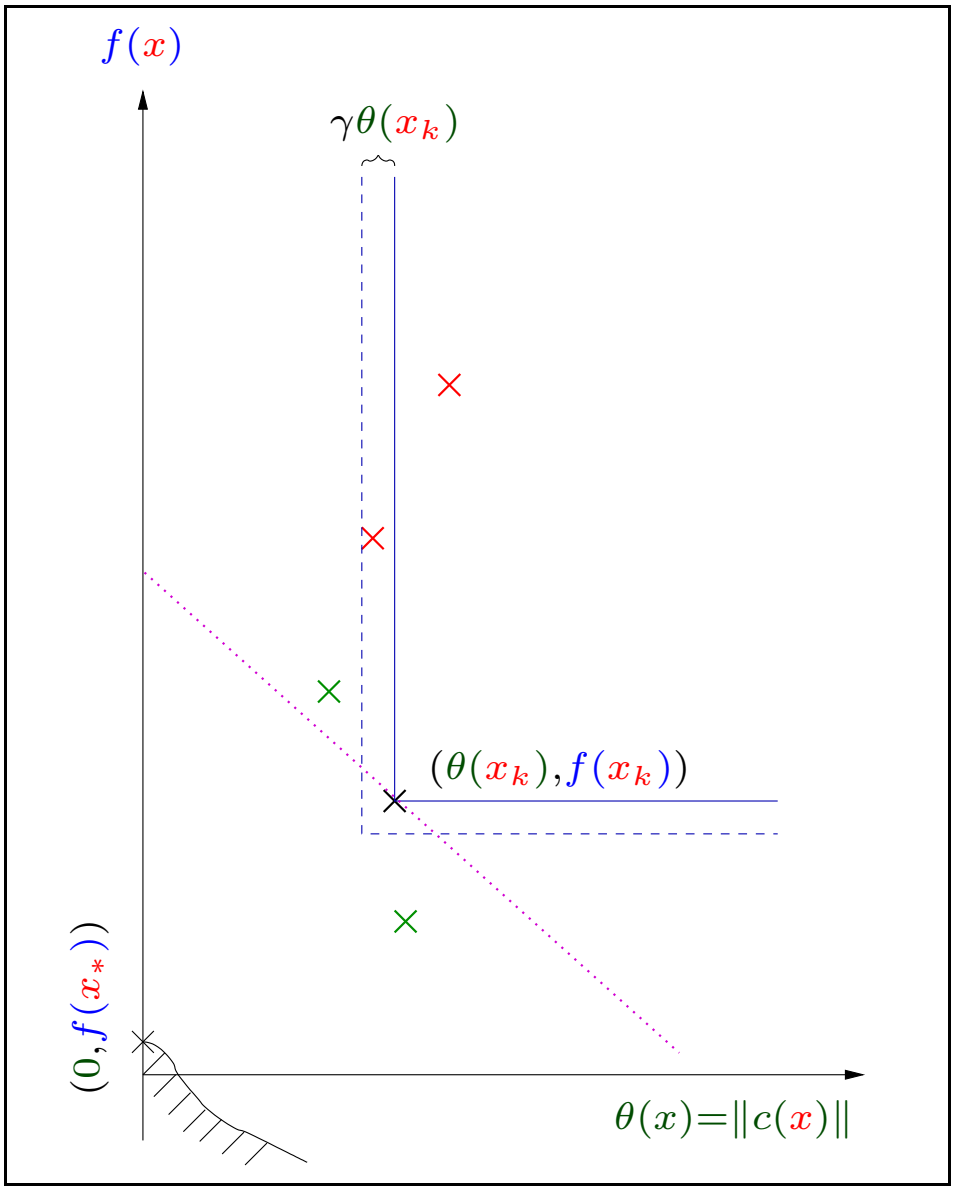
  - Set $x_{k+1} = x_k + \alpha_k d_k$ and $k \leftarrow k + 1$

A Filter Line Search Method

Filter: Alternative to merit function

(Fletcher, Leyffer; 1998)

A Filter Line Search Method



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Idea: Bi-objective optimization

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

$\min \ \theta(x)$ $\qquad$ $\min \ f(x)$

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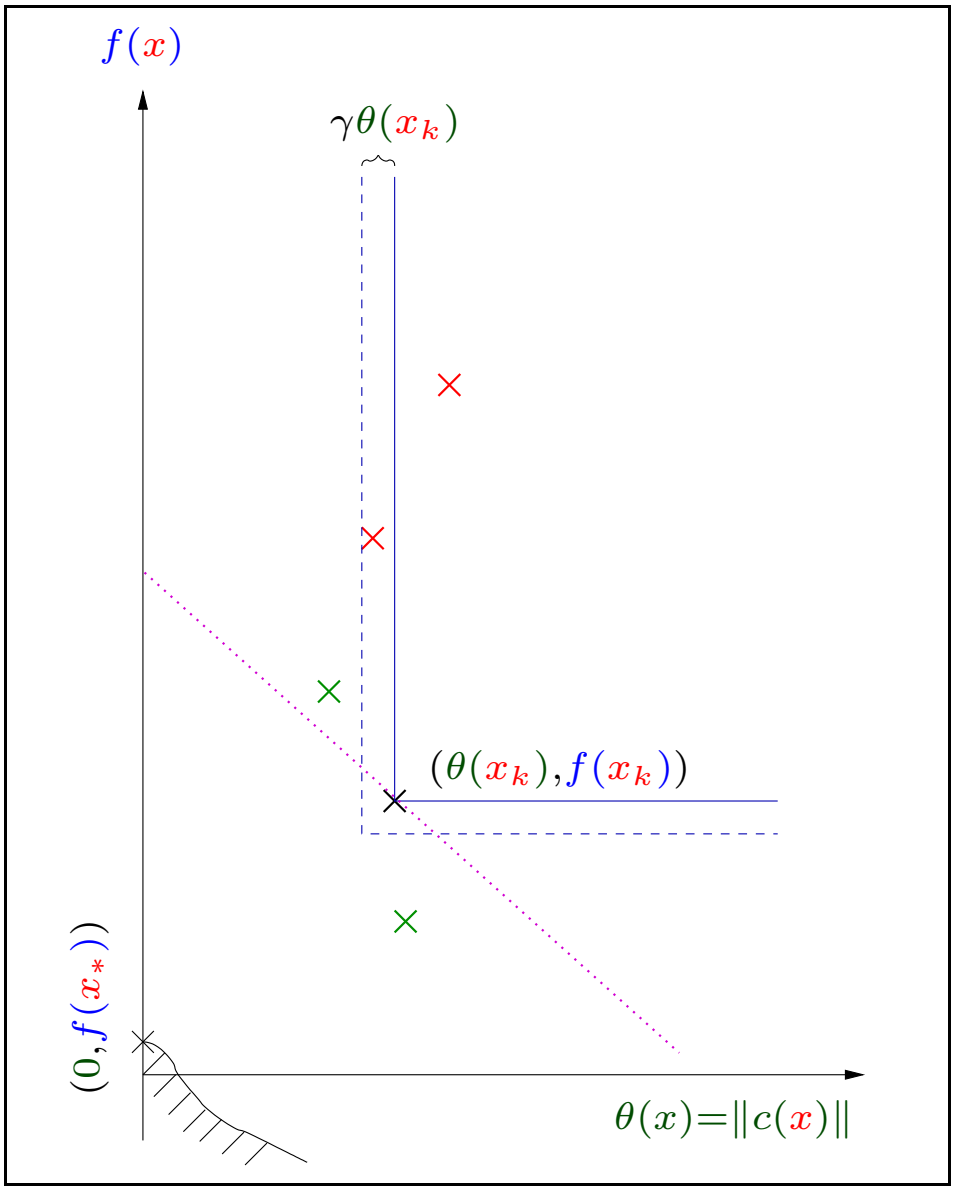

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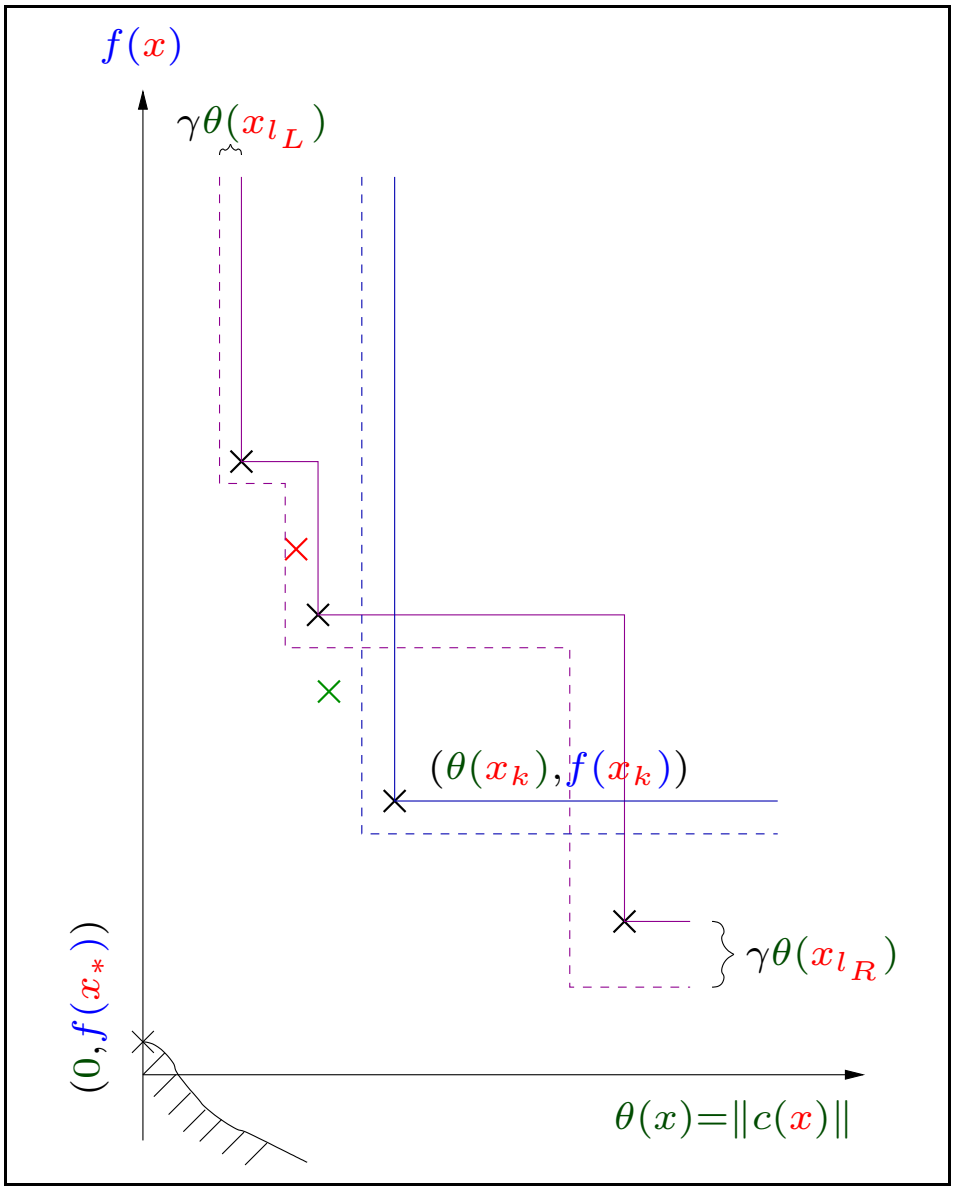
$$\min \quad \theta(x) \qquad\qquad \min \quad f(x)$$

$$x_{\text{tr}} = x_k + \alpha d_k^x$$

Sufficient progress w.r.t. x_k:

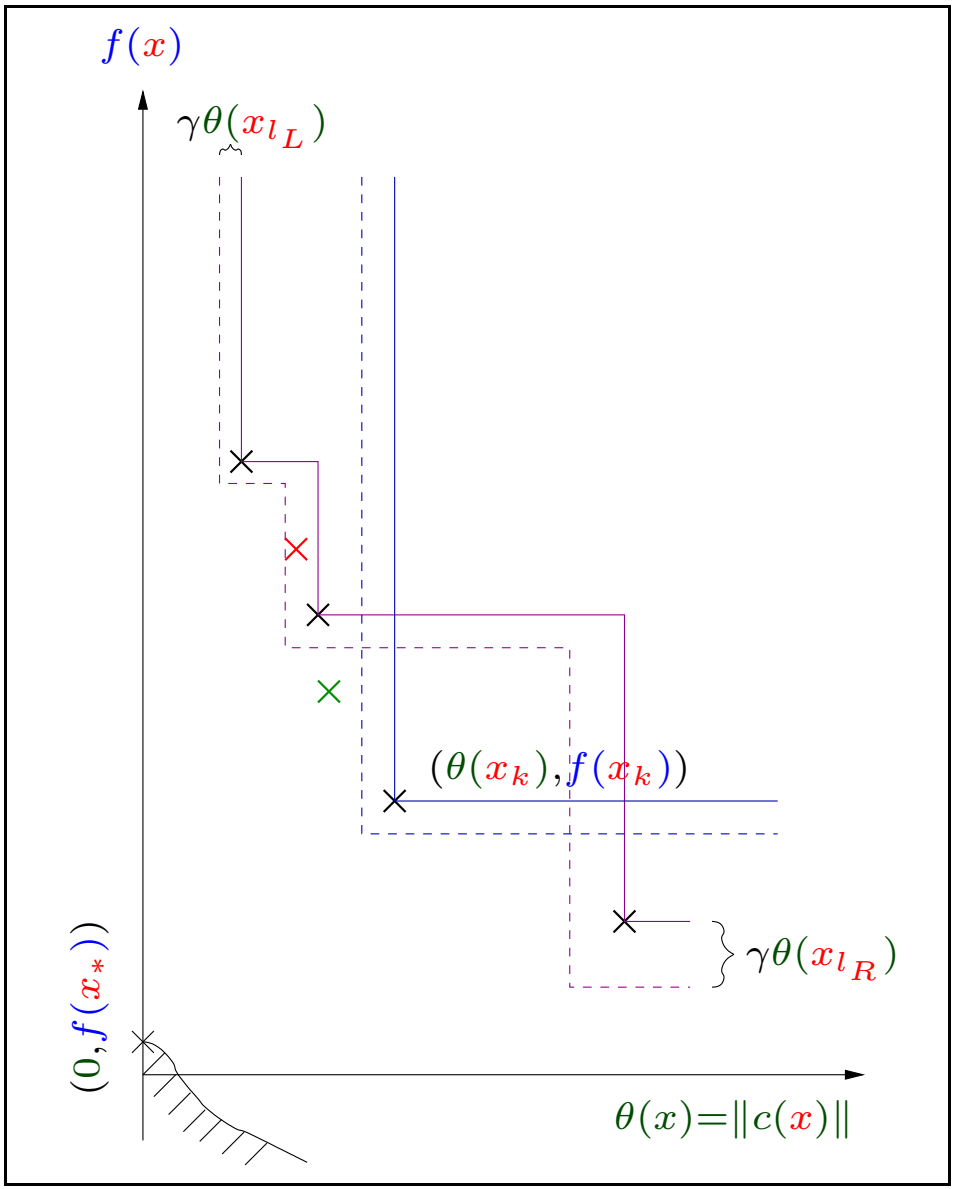
$$\begin{aligned} f(x_{\text{tr}}) &\leq f(x_k) - \gamma_f \theta(x_k) \\ \theta(x_{\text{tr}}) &\leq \theta(x_k) - \gamma_\theta \theta(x_k) \end{aligned}$$

A Filter Line Search Method (Filter)



Need to avoid cycling

A Filter Line Search Method (Filter)



Need to avoid cycling

$\Downarrow$

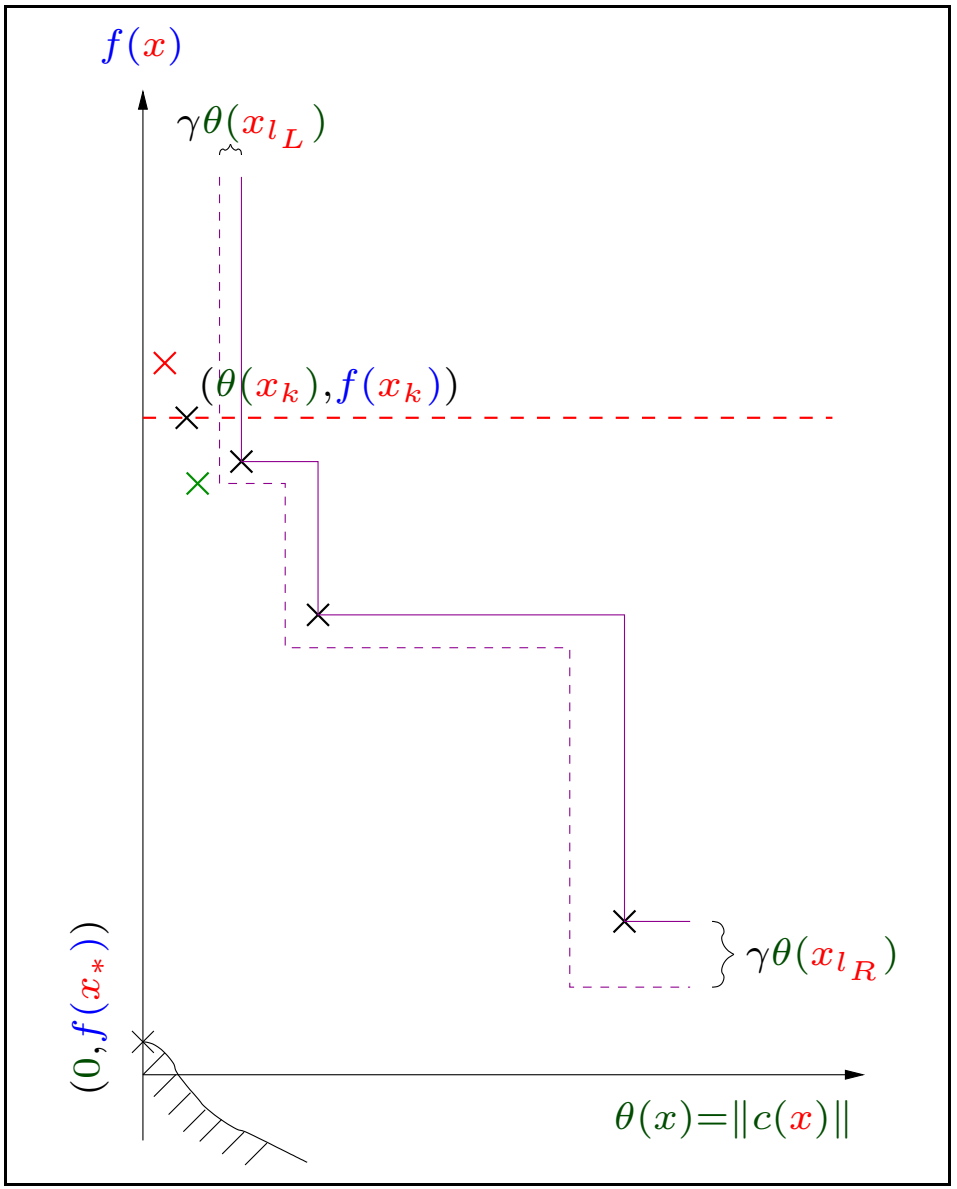
Store some previous $(\theta(x_l), f(x_l))$ pairs in *filter* $\mathcal{F}_k$

Sufficient progress w.r.t. filter:

$$\begin{aligned} f(x_{\text{tr}}) &\leq f(x_l) - \gamma_f \theta(x_l) \\ \theta(x_{\text{tr}}) &\leq \theta(x_l) - \gamma_\theta \theta(x_l) \end{aligned}$$

for $(\theta(x_l), f(x_l)) \in \mathcal{F}_k$

A Filter Line Search Method ("f-type")



If *switching condition*

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

holds ($s_\theta > 1$):

$$\Downarrow$$

Armijo-condition on $f(x)$:

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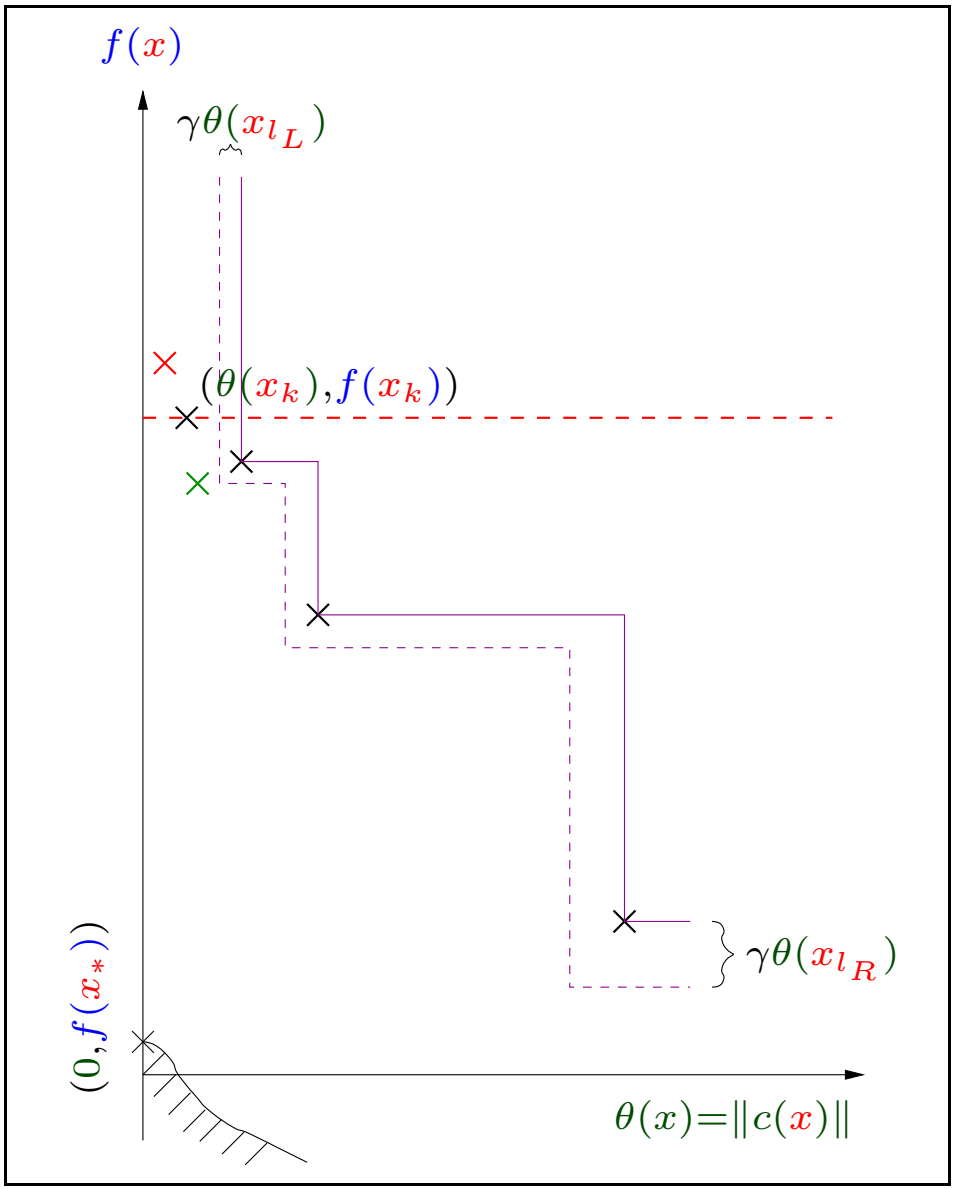

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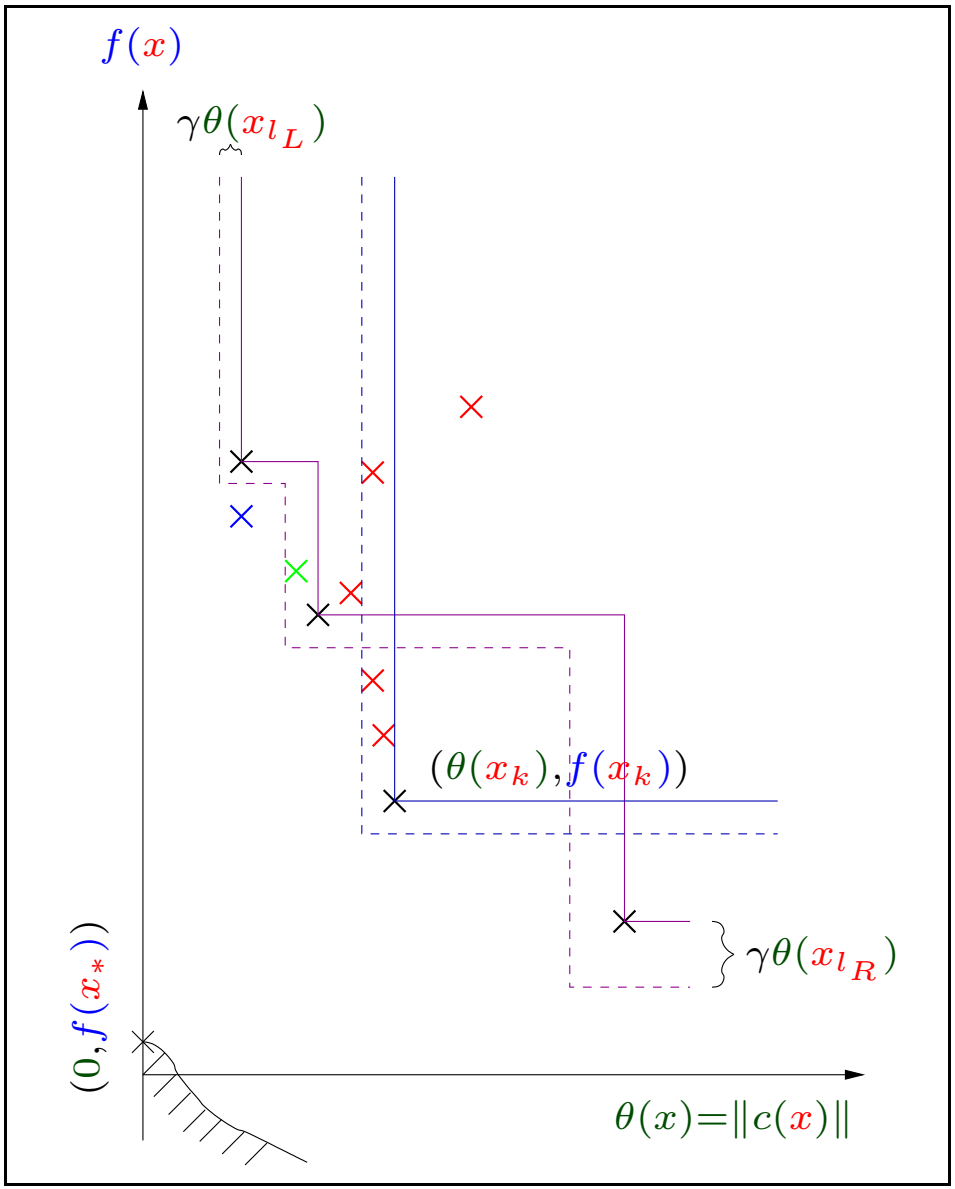
$\Longrightarrow$ Don't augment $\mathcal{F}_k$ in that case

A Filter Line Search Method (Restoration)



If no admissible step size α_k can be found

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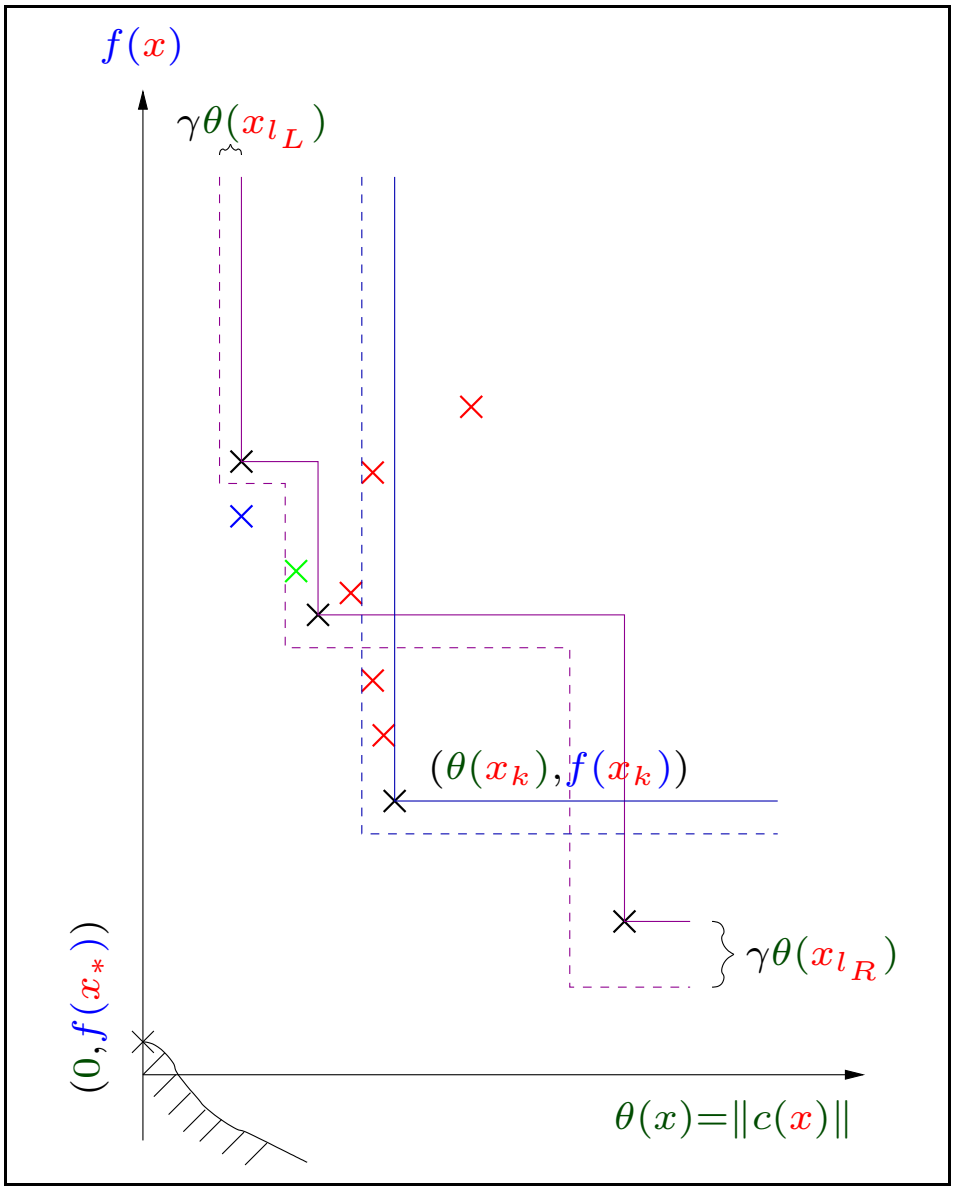

If no admissible step size α_k can be found

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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

Global Convergence Of Filter Method

- Assume
  - Functions and their derivatives are bounded and Lipschitz continuous
  - Singular values of $\nabla c(x_k)$ are bounded away from zero
  - W_k is bounded, and $(P_k^c)^T W_k P^c \succ \epsilon I$ for $\epsilon > 0$

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- Then
  - $\lim_k \|c(x_k)\| = 0$ (feasibility)
  - $\liminf_k \|(P_k^c)^T \nabla f(x_k)\| = 0$ (optimality)

Local Convergence Of Line Search Method

- If $W_k = \nabla^2_{xx}\mathcal{L}(x_k, \lambda_k)$, then (d_k^x, d_k^λ) is Newton step

  $\Longrightarrow$ Fast local convergence if $\alpha_k = 1$ for large k

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  - Even arbitrarily close to nice local solution x_*, we can have

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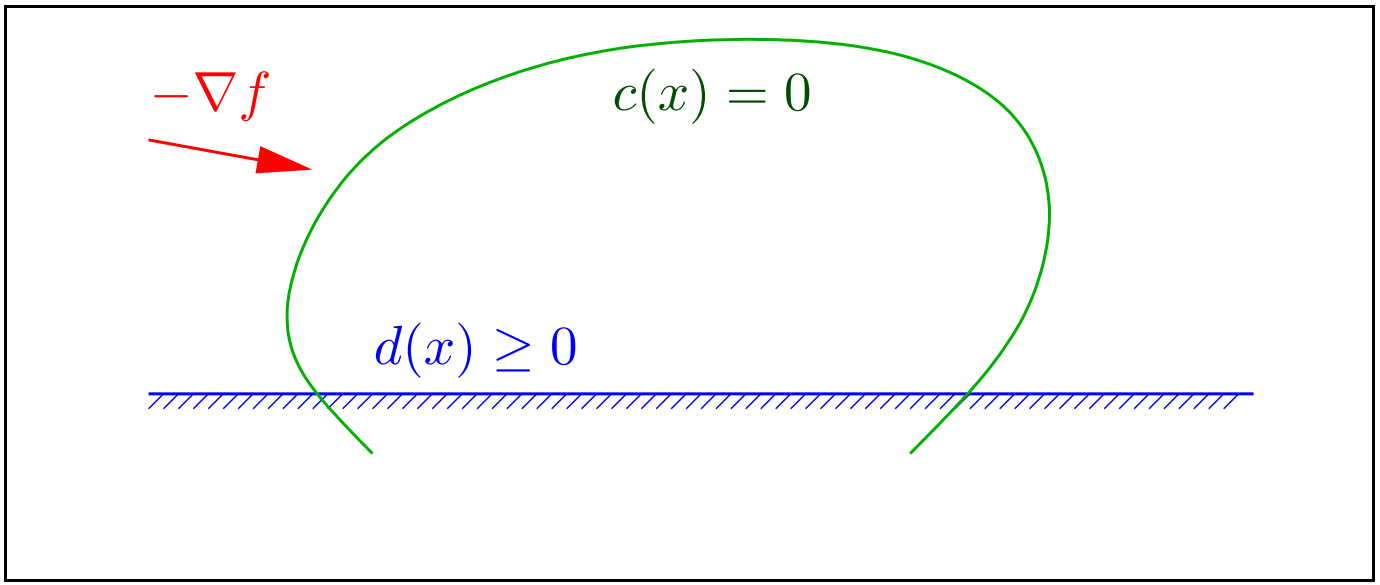
  - Watchdog: Accept d^x_k temporarily and continue. Go back and perform line search with d^x_k if no progress after L iterations

Generally Constrainted Optimization

Optimality Conditions (Motivation)

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



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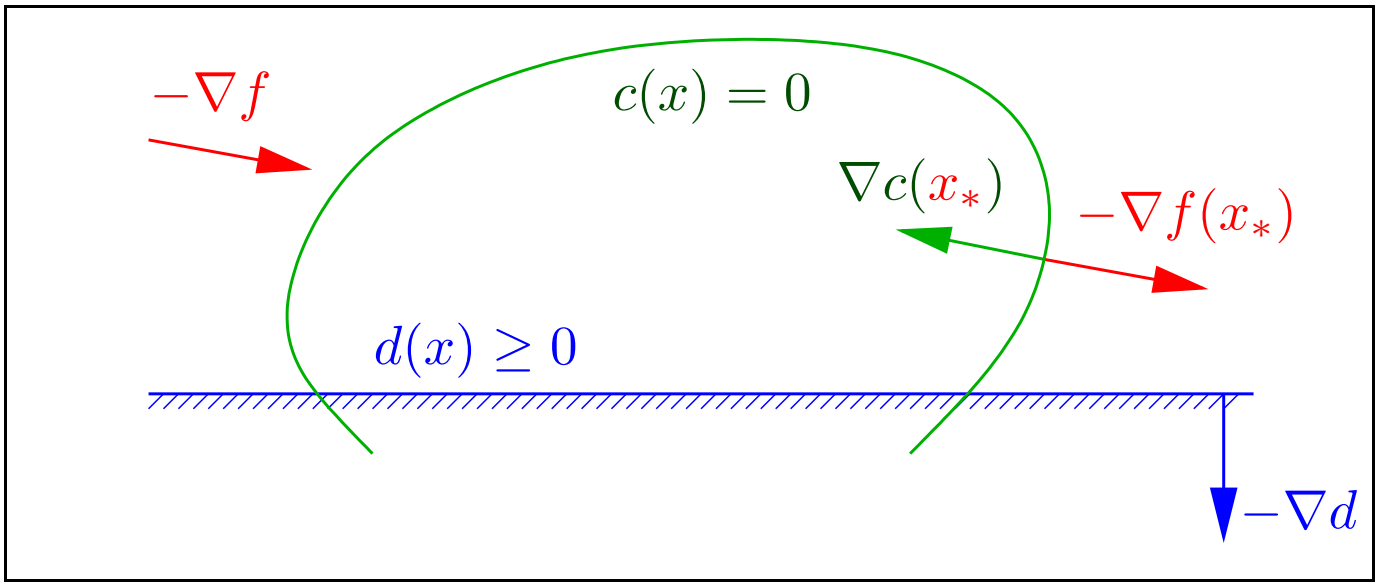

$$\begin{aligned} -\nabla f(x_*) &= \nabla c(x_*)\lambda_* - \nabla d(x_*) z_* \\ c(x_*) &= 0 \\ d(x_*) &> 0 \\ z_* &= 0 \end{aligned}$$

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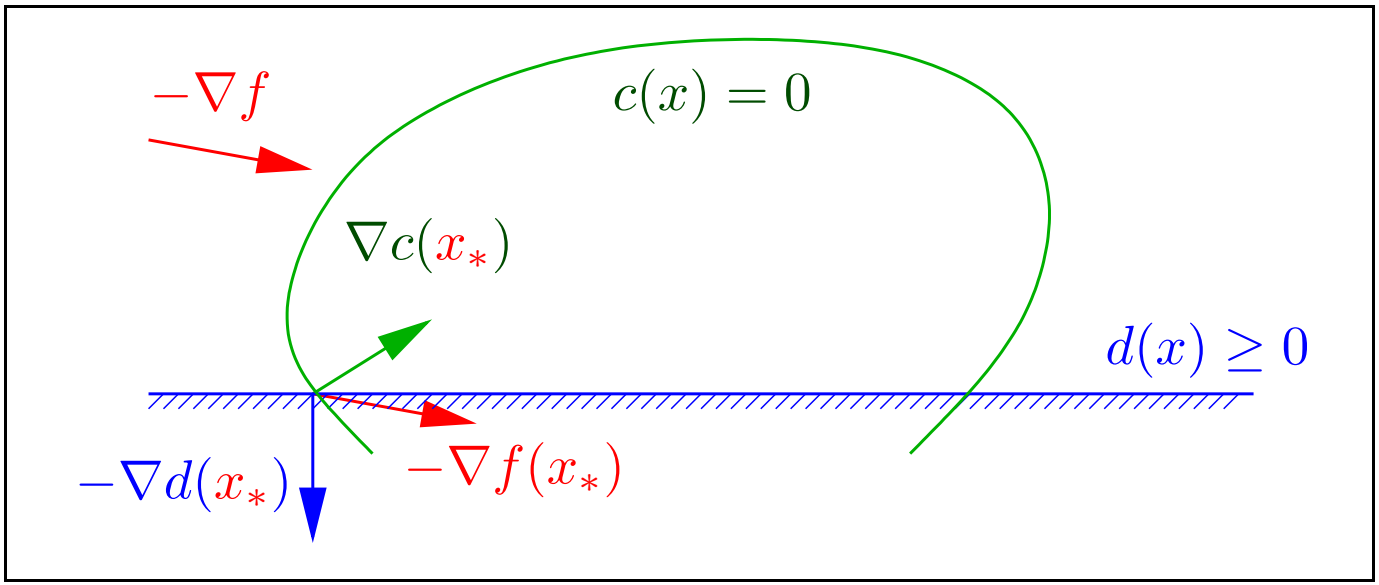

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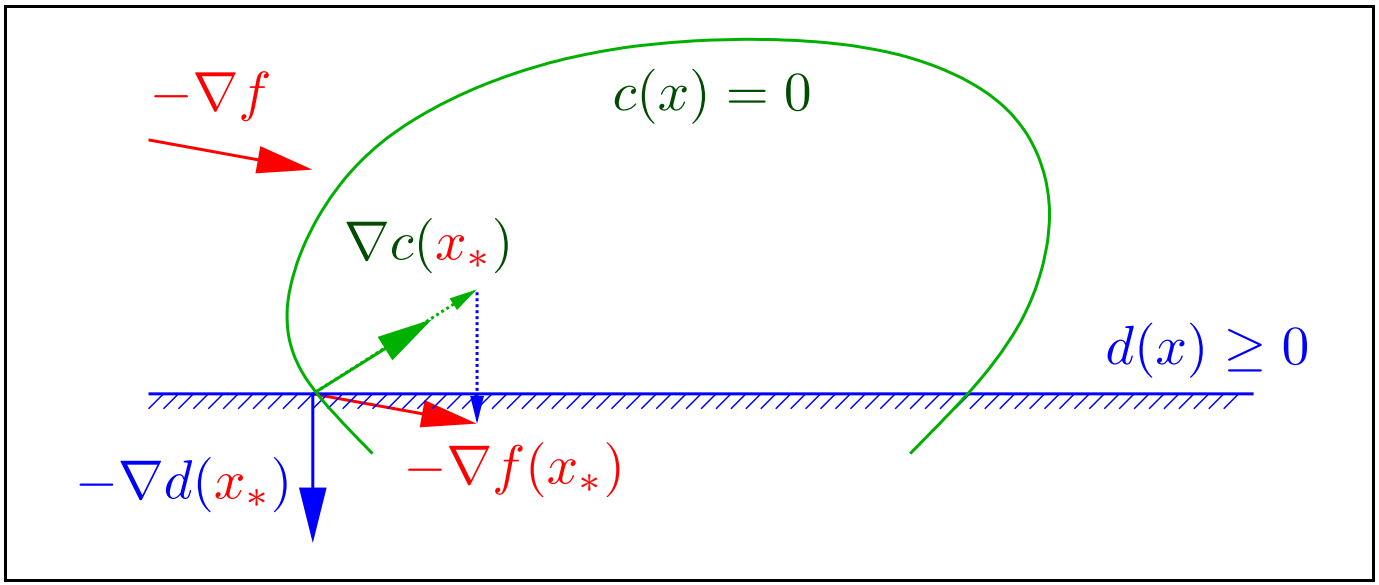

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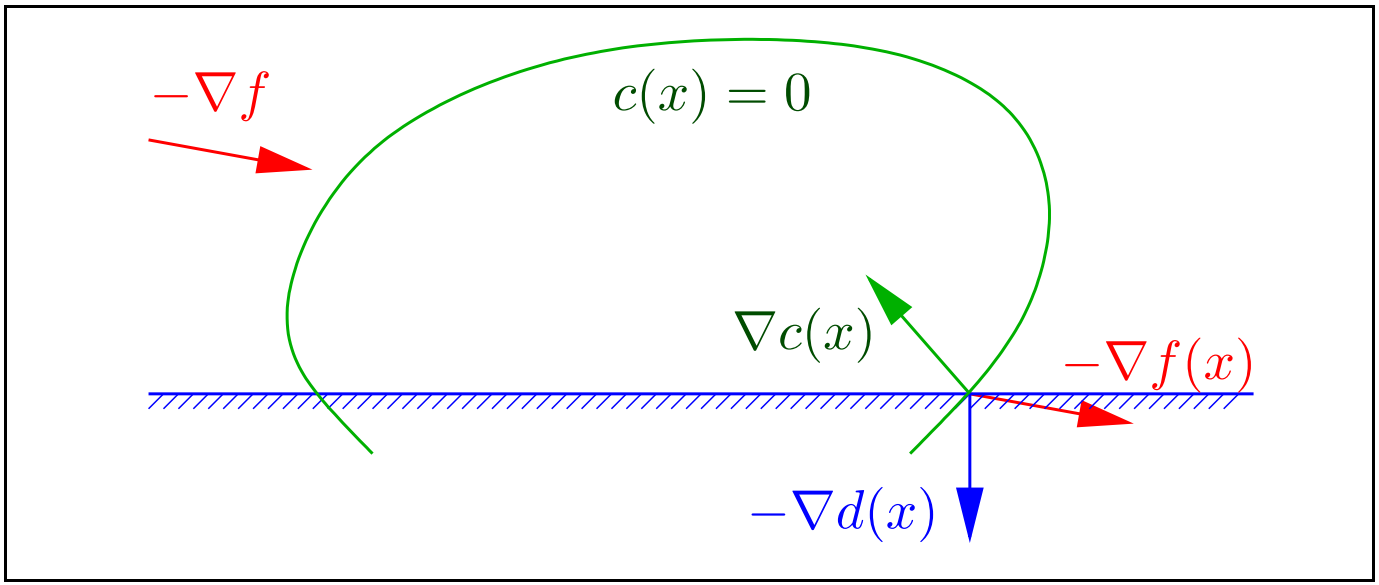

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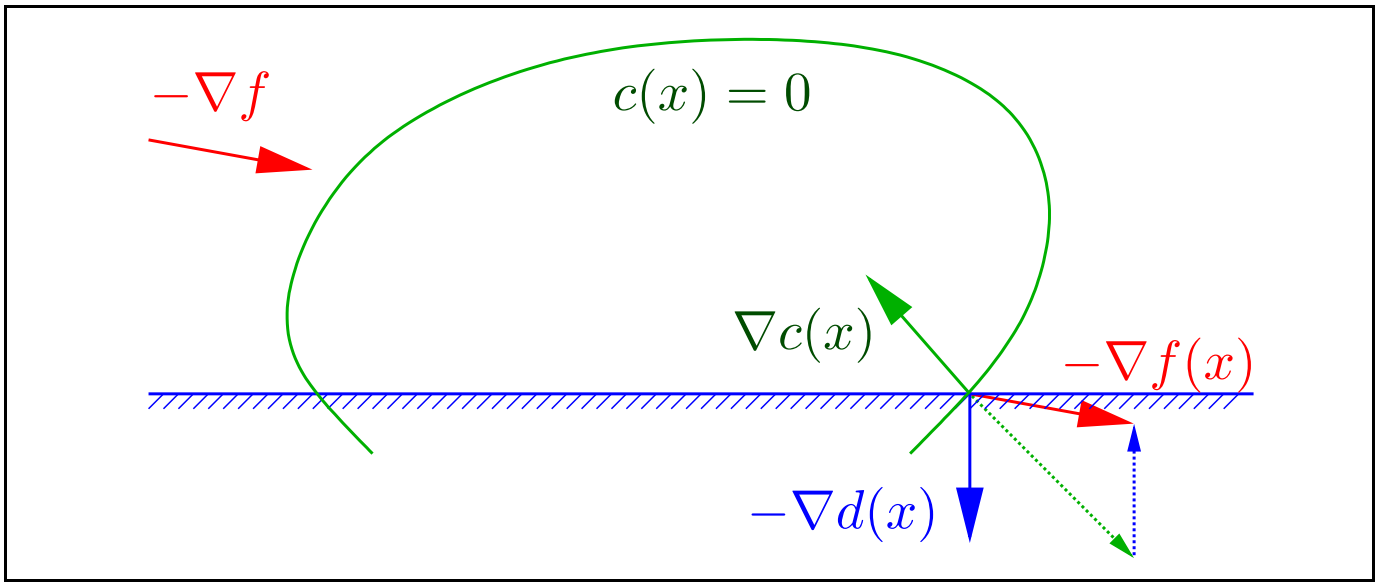

$$\begin{aligned} -\nabla f(x) &= \nabla c(x)\lambda - \nabla d(x) z \\ c(x) &= 0 \\ d(x) &= 0 \\ z &< 0 \quad \text{Wrong sign!} \end{aligned}$$

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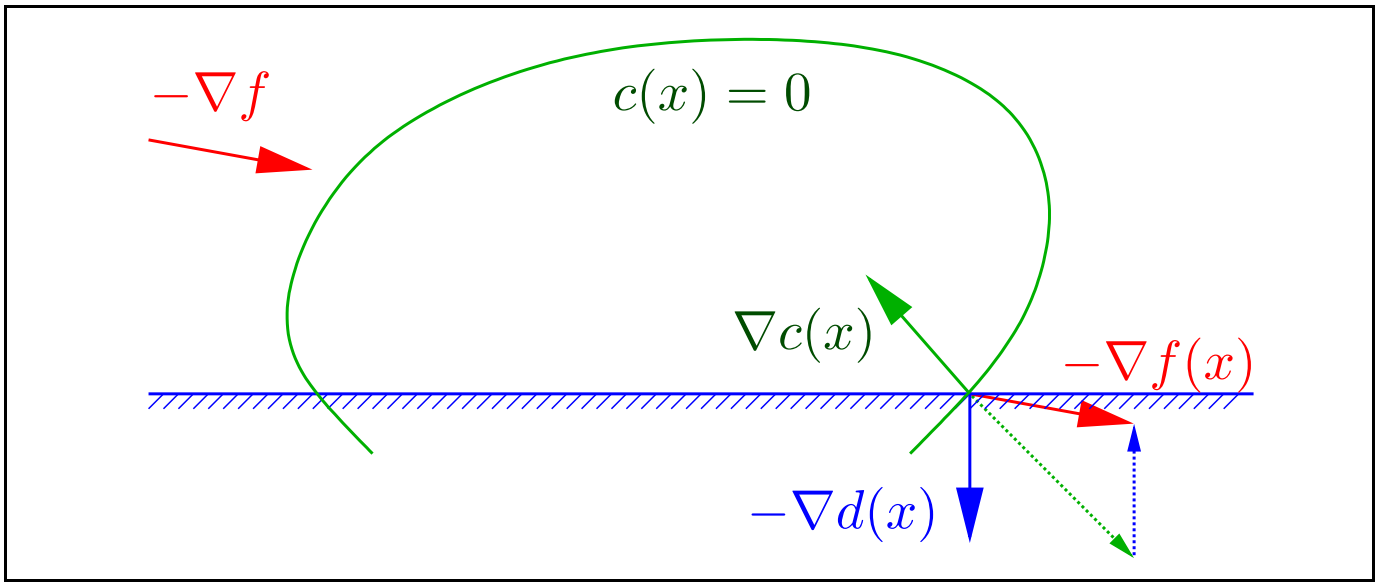

Karush-Kuhn-Tucker (KKT) conditions

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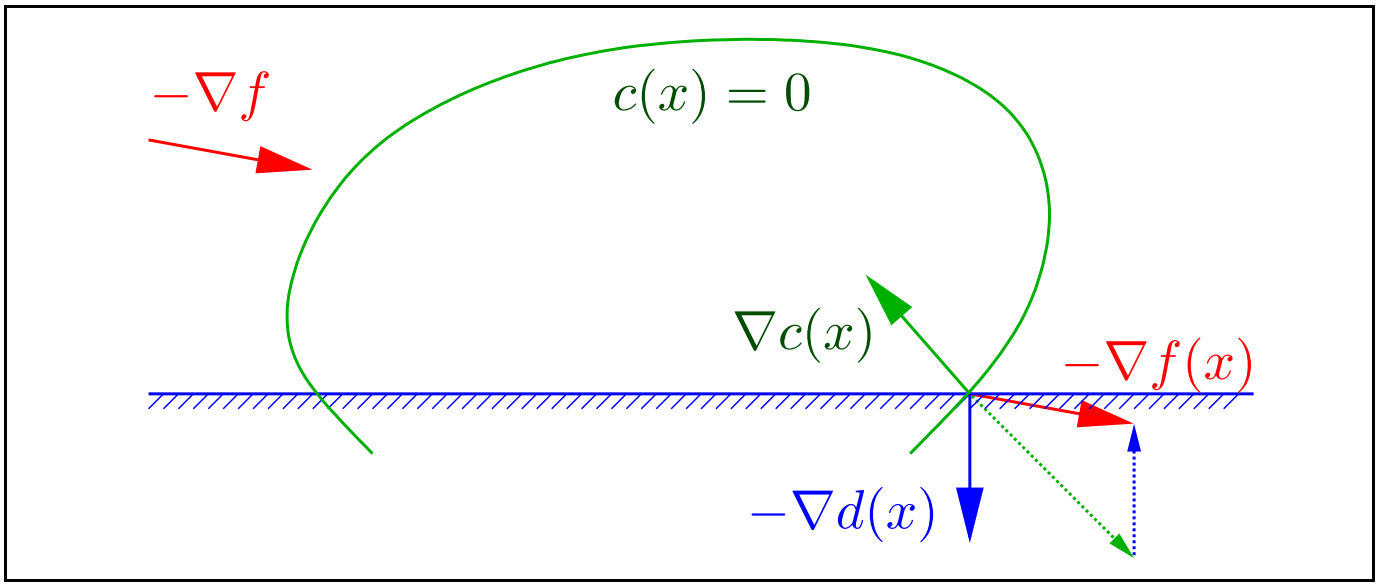

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Necessary Optimality Conditions

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

x	Variables
$f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$	Objective function
$c(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^m$	Equality constraints
	Bound constraints (w.l.o.g)

- If x_* local solution (at which constraint qualification holds), then exist multipliers $\lambda_* \in \mathbb{R}^m$, $z_* \in \mathbb{R}^n$ so that KKT conditions hold:

$$\begin{aligned} \nabla f(x_*) + \nabla c(x_*)\lambda_* - z_* &= 0 && \text{dual feasibily} \\ c(x_*) &= 0 && \text{primal feasibily} \\ X_* z_* &= 0 && \text{complementarity} \\ x_*, z_* &\geq 0 && \text{non-negativity} \end{aligned}$$

- $\nabla^2_{xx} \mathcal{L}(x_*, \lambda_*, z_*)$ positive semi-definite in null space of all *active* constraints (Lagrangian: $\mathcal{L}(x, \lambda, z) = f(x) + \lambda^T c(x) - z$)

Constraint Qualifications

- Conditions that ensure that the KKT conditions hold at local solution
- Linearly-Independent Constraint Qualification (LICQ)
  - The gradients of the active constraints

$$\nabla c^{(1)}(x_*), \ldots, \nabla c^{(m)}(x_*) \quad \text{and} \quad e_i \text{ for } i \in \mathcal{A}(x_*) := \{j : x_*^{(j)} = 0\}$$

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- MFCQ is weaker than LICQ

Sufficient Second Order Conditions

- Assume:
  - LICQ holds at x_*
  - There exist $\lambda_* \in \mathbb{R}^m$ and $z_* \in \mathbb{R}^n$ so that the KKT conditions hold
  - $\nabla^2_{xx}\mathcal{L}(x_*, \lambda_*, z_*)$ is positive definite in null space of all *active* constraints
  - Strict complementarity holds:

$$x_*^{(i)} > 0 \quad \text{or} \quad z_*^{(i)} > 0 \qquad \text{for all } i \in \mathcal{A}(x_*)$$

- Then: x_* is a (strict) local solution

Newton's Method (again...?)

$$\begin{aligned} \nabla f(x) + \nabla c(x) - z &= 0 \\ c(x) &= 0 \\ Xz &= 0 \\ x, z &\geq 0 \end{aligned}$$

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- Complications: Cannot use Newton's method this time because of the non-negativity conditions (might end up at point with wrong sign)
- But we can use the SQP idea (with a "local QP model")

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

$\longrightarrow$

$$\begin{aligned} \min_{d \in \mathbb{R}^n} \quad & f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T W_k d \\ s.t. \quad & c(x_k) + \nabla c(x_k)^T d = 0 \\ & x_k + d \geq 0 \end{aligned}$$

Sequential Quadratic Programming

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- If x_* satisfies sufficient second order conditions and $x_k \to x_*$:
  - For large k: $\mathcal{A}^{\mathrm{QP}}(x_k) = \mathcal{A}^{\mathrm{NLP}}(x_*)$

    (The QP "identifies the correct active set")

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    (The QP "identifies the correct active set")
  - Then, the steps are Newton steps for the equality-constrained NLP

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ s.t. \quad & c(x) = 0 \\ & x^{(j)} = 0 \qquad \text{for } j \in \mathcal{A}^{\mathrm{NLP}}(x_*) \end{aligned}$$

  - Newton's method! $\Longrightarrow$ Quadratic local convergence

Discussion Of SQP

- Originators: Han (1977), Powell (1978)
- Most popular method for NLP (still. . . ?)
- Many different algorithms and implementations:
  - using 2nd derivatives vs. approximating them with quasi-Newton methods
  - line search vs. trust region
  - different merit functions vs. filter
  - Some codes: DONLP2, FilterSQP, FSQP, NPSOL, Sℓ_1QP, SNOPT, and many more. . .
- Crutial question: How do we solve the QP?

QP Solvers in SQP

- Active set solvers:
  - guess which inequalities are active
  - solve corresponding equality constrained QP
    (requires solution of linear equations)
  - correct guess until solution is found
  - towards the end of SQP algorithm, $\mathcal{A}^{\mathrm{QP}}(x_k)$ stays the same
    (if x_* satisfies 2nd order optimality conditions)
  - QP solver can be "warm-started"
  - for large problems: combinatorial complexity to determine $\mathcal{A}^{\mathrm{QP}}(x_k)$ becomes the bottleneck

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  - but no good warm start possibilities (yet?)
- Since early '90s: Apply interior point idea directly to NLP

Interior Point Methods

$$\begin{aligned} \nabla f(x) - \nabla c(x)\lambda - z &= 0 \\ c(x) &= 0 \\ XZe &= 0 \\ (x, z &\geq 0) \end{aligned}$$

- Here: $e = (1, \ldots, 1)^T$

Interior Point Methods

$$\begin{aligned} \nabla f(x) - \nabla c(x)\lambda - z &= 0 \\ c(x) &= 0 \\ XZe &= \mu e \\ (x, z &> 0) \end{aligned}$$

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- Relax complementarity conditions with parameter $\mu > 0$

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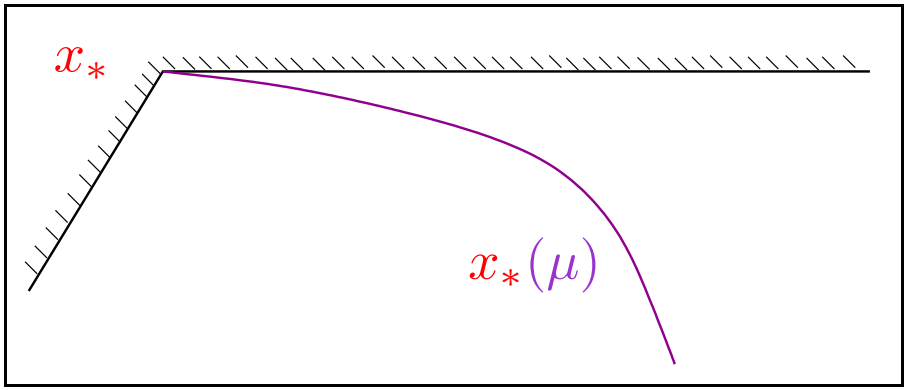

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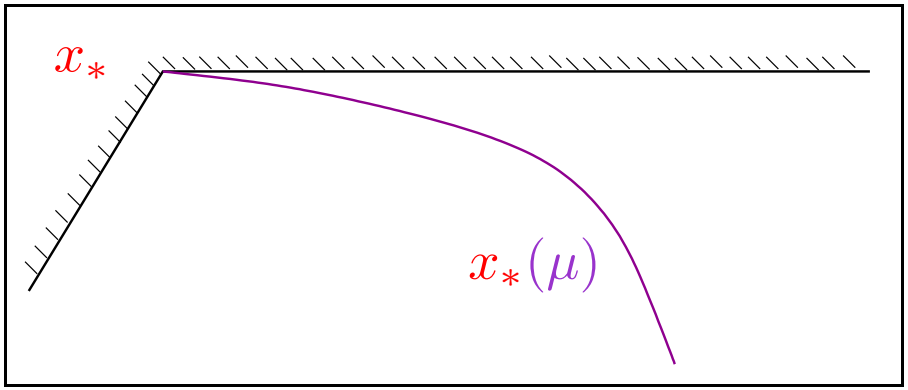

- Here: $e = (1, \ldots, 1)^T$
- Relax complementarity conditions with parameter $\mu > 0$
- Trace solutions $x_*(\mu)$ as function of μ
- If x_* strong local solution: $x_*(\mu) \to x_*$ as $\mu \to 0$
- Homotopy approach: Trace $x_*(\mu_k)$ and drive $\mu_k \to 0$
- Approaching the solution from the interior $x_k > 0$

Newton's Method (yes again!)

$$\begin{aligned} \nabla f(x) - \nabla c(x)\lambda - z &= 0 \\ c(x) &= 0 \\ XZe &= \mu e \\ (x, z &> 0) \end{aligned}$$

Newton steps

$$\begin{bmatrix} W_k & \nabla c(x_k) & -I \\ \nabla c(x_k)^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{pmatrix} d_k^x \\ d_k^\lambda \\ d_k^z \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) + \nabla c(x_k)\lambda_k - z_k \\ c(x_k) \\ X_k Z_k e - \mu e \end{pmatrix}$$

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- If x_* satisfies sufficient 2nd order optimality conditions:
  - Matrix is nonsingular at solution (x_*, λ_*, z_*)
  - $\Longrightarrow$ Can devise superlinearly convergent method if μ_k is updated in particular ways
- Very established for LP, QP, convex problems (e.g. SDP)

Augmented System

$$\begin{bmatrix} W_k & \nabla c(x_k) & -I \\ \nabla c(x_k)^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{pmatrix} d_k^x \\ d_k^\lambda \\ d_k^z \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) + \nabla c(x_k)\lambda_k - z_k \\ c(x_k) \\ X_k Z_k e - \mu e \end{pmatrix}$$

can be solved equivalently by first solving the "augmented system"

$$\begin{bmatrix} W_k + \Sigma_k & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix} \begin{pmatrix} d_k^x \\ d_k^\lambda \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) - \mu X_k^{-1} e + \nabla c(x_k)\lambda_k \\ c(x_k) \end{pmatrix}$$

with $\Sigma_k = X_k^{-1} Z_k$, and then compute

$$d_k^z = \mu X_k^{-1} e - z_k - \Sigma_k d_k^x$$

Barrier Methods

Barrier Problem (fixed μ)

$$\begin{array}{ll} \min\limits_{x\in\mathbb{R}^n} & \varphi_\mu(x) := f(x) - \mu \sum \ln(x^{(i)}) \\ s.t. & c(x) = 0 \end{array} \qquad (B(\mu))$$

- Parameterized by "barrier parameter" $\mu > 0$
- Fiacco-McCormick (1968)
  1. Choose $\mu_0 > 0$, $x_0 > 0$; set $l \leftarrow 0$
  2. Solve $(B(\mu_l))$ from x_l to relaxed tolerance to obtain x_{l+1}
  3. Update $\mu_{l+1} \in (0, \mu_l)$; set $l \leftarrow l + 1$; go back to 2.

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  3. Update $\mu_{l+1} \in (0, \mu_l)$; set $l \leftarrow l + 1$; go back to 2.
- Solve a sequence of barrier problems
  - can use known techniques for equality constrianed optimization
  - know how to globalize and handle non-convexity (almost. . .)
  - fast local convergence? (only for fixed μ_l)

Optimality Conditions For $(B(\mu))$

$$\begin{aligned} \nabla\varphi_\mu(x) + \nabla c(x)\lambda &= 0 \\ c(x) &= 0 \\ (x &> 0) \end{aligned}$$

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Disadvanatges:

- As $\mu_l \to 0$ and $x_l \to x_*$, optimality conditions not defined
- Newton's method for $(B(\mu_l))$ has increasingly smaller "radius of convergence" as $\mu_l \to 0$.

Newton Method For Barrier Problem

$$\begin{bmatrix} W_k + \mu X_k^{-2} & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix} \begin{pmatrix} d_k^x \\ \lambda_k^+ \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) - \mu X_k^{-1} e + \nabla c(x_k) \lambda_k \\ c(x_k) \end{pmatrix}$$

with $W_k = \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k, z_k) = \nabla^2 f(x_k) + \sum_j \lambda_k^{(j)} \nabla^2 c^{(j)}(x_k)$.

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$$\begin{bmatrix} W_k + \Sigma_k & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix} \begin{pmatrix} d_k^x \\ d_k^\lambda \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) - \mu X_k^{-1} e + \nabla c(x_k) \lambda_k \\ c(x_k) \end{pmatrix}$$

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Only difference in "Hessian for barrier term $-\mu \sum_i \log(x^{(i)})$"

- "primal": $\Sigma_k = \mu X_k^{-2}$
- "primal-dual": $\Sigma_k = X_k^{-1} Z_k$
  (maintain iterates for bound multipliers z_k)

Primal-Dual Interior Point Method

$$\begin{bmatrix} W_k + \Sigma_k & \nabla c(x_k) \\ \nabla c(x_k)^T & 0 \end{bmatrix} \begin{pmatrix} d_k^x \\ d_k^\lambda \end{pmatrix} = - \begin{pmatrix} \nabla f(x_k) - \mu X_k^{-1} e + \nabla c(x_k) \lambda_k \\ c(x_k) \end{pmatrix}$$

- Primal method:
  - $\Sigma_k = \mu X_k^{-2}$
  - have good methods for solving $(B(\mu))$ for each μ
  - gives us global convergence
- Primal-dual method:
  - $\Sigma_k = X_k^{-1} Z_k$
  - can achieve fast local convergence, if μ is updated properly
- Primal-dual approach takes advantage of both and is basis for most modern interior point methods for NLP

A Primal-Dual IPM For NLP

1. Given (x_0, λ_0, z_0) with $x_0, z_0 > 0$; $\mu_0 > 0$; set $k \leftarrow 0$
2. Compute primal-dual search direction $(d_k^x, d_k^\lambda, d_k^z)$
3. Determine largest $\alpha_k^\tau, \alpha_k^{z,\tau} \in (0, 1]$ such that (usually $\tau \approx 0.99$)

$$\begin{array}{rcccl} x_k + \alpha_k^\tau d_k^x & \geq & (1-\tau)x_k & > & 0 \\ z_k + \alpha_k^{z,\tau} d_k^z & \geq & (1-\tau)z_k & > & 0 \end{array}$$

4. Perform backtracking line search to find acceptable $\alpha_{k,l} = 2^{-l}\alpha_k^\tau$, using globalization method for $(B(\mu_k))$
5. Accept new iterate

$$\begin{array}{rcl} (x_{k+1}, \lambda_{k+1}) & = & (x_k, \lambda_k) + \alpha_k \left(d_k^x, d_k^\lambda\right) \\ z_{k+1} & = & z_k + \alpha_k^z d_k^z \end{array}$$

6. If $(B(\mu_k))$ is solved sufficiently well, decrease $\mu_{k+1} \in (0, \mu_k)$; otherwise set $\mu_{k+1} \leftarrow \mu_k$
7. Go to step 2.

Example Problem

$$
\begin{aligned}
\min_{x \in \mathbb{R}^3} \quad & x^{(1)} \\
s.t. \quad & (x^{(1)})^2 - x^{(2)} - 1 = 0 \\
& x^{(1)} - x^{(3)} - 0.5 = 0 \\
& x^{(2)}, x^{(3)} \geq 0
\end{aligned}
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- $f(x)$ and $c(x)$ smooth
- $\nabla c(x)$ full rank everywhere
- Only one stationary point:

$$\begin{aligned} x_* &= (1, 0, 0.5)^T \\ \lambda_* &= (-0.5, 0)^T \\ (z_*^{(2)}, z_*^{(3)})^T &= (0.5, 0)^T \end{aligned}$$

- Sufficient 2nd order optimality cond.
- Strict complementarity

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This problem is well–posed!

Let's try starting point $x_0 = (-2, 3, 1)^T \ldots$

But...

ITER	X(1)	X(2)	X(3)
0	-0.20000000D+01	0.30000000D+01	0.10000000D+01
1	-0.18947413D+01	0.25789655D+01	0.10000000D-01
2	-0.12201587D+01	0.25789655D-01	0.23540510D-02
3	-0.12082251D+01	0.25789655D-03	0.93113038D-03
4	-0.12080095D+01	0.25789655D-05	0.15850601D-03
5	-0.12079893D+01	0.14108060D-05	0.15850601D-05
6	-0.12079884D+01	0.14108060D-07	0.10157878D-06
7	-0.12079884D+01	0.14108060D-09	0.22892307D-08
8	-0.12079884D+01	0.21513916D-11	0.22892307D-10
9	-0.12079884D+01	0.21513916D-13	0.25068098D-12
10	-0.12079884D+01	0.21513916D-15	0.25450869D-14

From starting point $x^0 = (-2, 3, 1)^T$, original IPOPT (using line search with primal-dual Newton steps) crashes into bounds!

Different starting points give similar results...

Failure of Global Convergence

$$\begin{aligned} \min_{x \in \mathbb{R}^3} \quad & f(x) \\ s.t. \quad & (x^{(1)})^2 - x^{(2)} - 1 = 0 \\ & x^{(1)} - x^{(3)} - 0.5 = 0 \\ & x^{(2)}, x^{(3)} \geq 0 \end{aligned}$$

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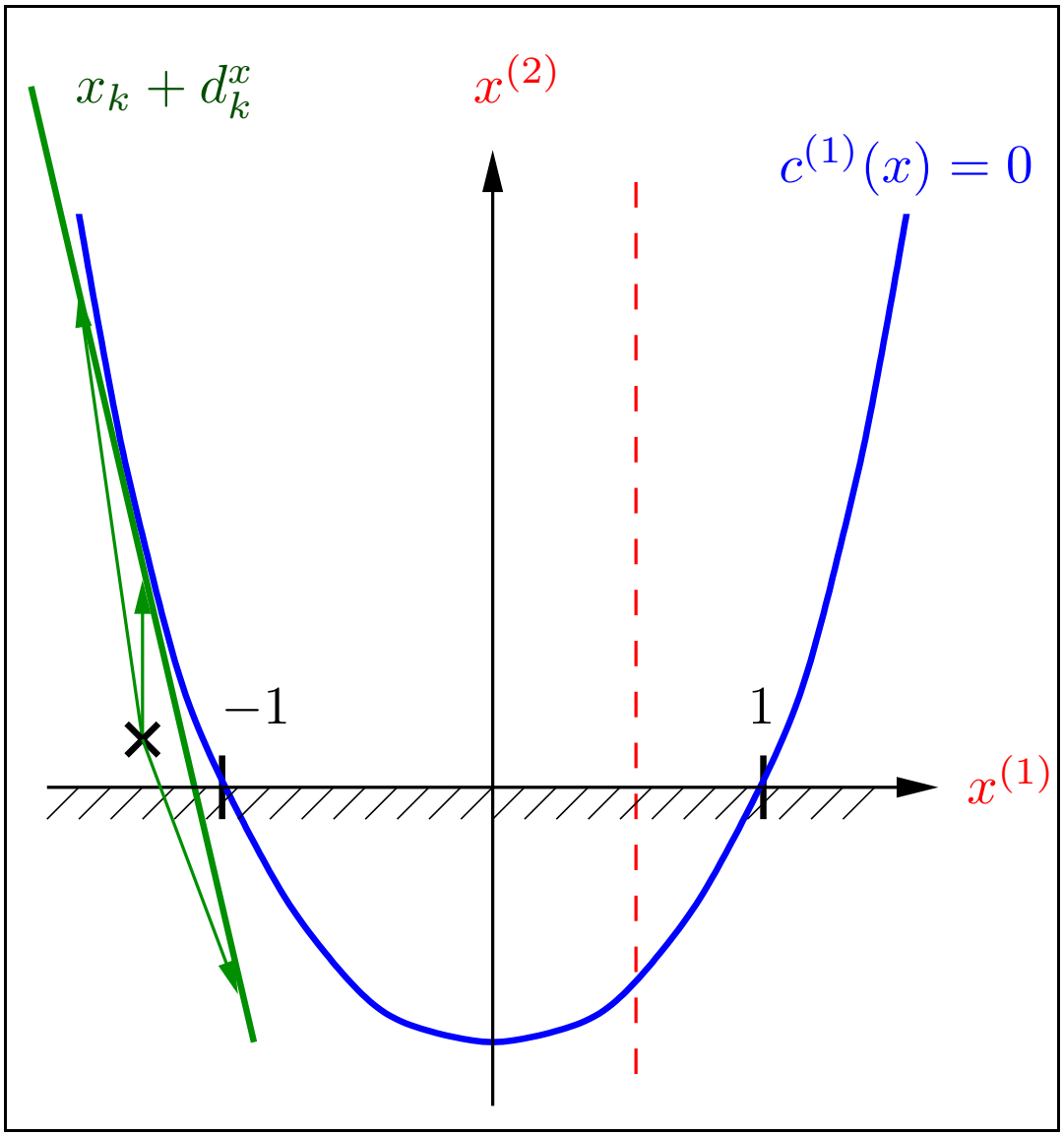
Step computation

1. $\nabla c(x_k)^T d_k^x + c(x_k) = 0$
2. ${x_k}^{(i)} + \alpha_k^x (d_k^x)^{(i)} > 0$



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- Global convergence proofs existed for affected IPM:
  - Implicitly assumed that iterates stay away from bounds for $\mu > 0$.
- In order to overcome convergence problem, we must allow steps that don't satisfy linearization of the constraints

Remedies For Convergence Failure

- Penalizing constraint violation

  Penalty-barrier method:

  - (Fiacco, McCormick)

    (Forsgren, Gill)

$$\min \quad f(x) - \mu \sum_i \ln(x^{(i)}) + \frac{1}{2\mu}\|c(x)\|_2^2$$

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  Splitting equalities:

  - (Tits, W. et al.)
    (Gould, Orban, Toint)

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) + \rho \sum_j c^{(j)}(x) \\ s.t. \quad & c(x) \geq 0 \\ & x \geq 0 \end{aligned}$$

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- Step decomposition in trust region framework
  - e.g., Byrd-Omojokun framework (such as in KNITRO)

Remedies For Convergence Failure

- Penalizing constraint violation

  Penalty-barrier method:

  - (Fiacco, McCormick)
    (Forsgren, Gill)

$$\min \quad f(x) - \mu \sum_i \ln(x^{(i)}) + \frac{1}{2\mu}\|c(x)\|_2^2$$

  Splitting equalities:

  - (Tits, W. et al.)
    (Gould, Orban, Toint)

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- Step decomposition in trust region framework
  - e.g., Byrd-Omojokun framework (such as in KNITRO)

- Filter methods
  - Restoration phase is called when α_k^x becomes very small
  - Steps in restoration phase aim to reduce infeasibility

Ipopt

An algorithm for large-scale nonlinear nonconvex optimization

- Framework: Barrier method (Fiacco-McCormick)
- Steps: Primal-dual interior point method

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- Theoretical convergence properties:
  - Global convergence: From filter method for each $(B(\mu))$
  - Local convergence: If μ_k is updated properly, can achieve superlinear convergence (Gould, Orban, Sartenaer, Toint, 2001))

COIN-OR *http://www.coin-or.org*

- COmputational INfrastructure for Operations Research
- Open source repository for optimization and related software
- Nonprofit foundation (hosted at INFORMS)
- Numerous projects:
  - `Bcp` (parallel framework for Branch, Cut and Pricing algorithms)
  - `Cbc` (COIN Branch and Cut algorithm for MILP)
  - `Cgl` (Cut Generation Library)
  - `Clp` (Coin LP Solver)
  - `Osi` (Open Solver Interface) [`Cplex`, `OSL`, `Xpress MP`, `Clp`, `Glpk`]
  - `Ipopt` (Interior Point NLP solver)
  - `DFO`, `NLP-API`, `GAMSlinks`, `SMI`, `SVM-QP`, `CSPD`, `CppAD`, `...`
- Also models/data sets (for benchmarking, allow recreating results from papers), frameworks
- Contribution are WELCOME!

Implementation Of Ipopt

- Code IPOPT available as open source on COIN-OR
- Written in C++ (replaces earlier Fortran version) (with Carl Laird, CMU)
- Interfaced with AMPL, GAMS, CUTEr, (Matlab?); available on NEOS
- Has been used for
  - Optimization of differential-algebraic systems
  - Nonlinear model predictive control
  - Air traffic resolution (MPECs, (Raghunathan, 2004)) ...
- `coin-ipopt` mailing list with 184 subscribers
- Recent developments
  - Adaptive choice of the barrier parameter (Nocedal, W, Waltz, 2005)
  - Interfaces to a number of linear solvers:
    - Harwell, WSMP, MUMPS, Pardiso (Schenk, W, Hagemann, 2005)
    - This is a crutial part in terms of efficiency and robustness
  - Limited memory quasi-Newton approximation of 2nd derivatives

Adaptive Barrier Parameter

Barrier Methods for NLP

$$\begin{array}{ll} \min & f(x) \\ s.t. & c(x) = 0 \\ & x \geq 0 \end{array} \quad \longrightarrow \quad \begin{array}{ll} \min & f(x) - \mu \sum \ln(x^{(i)}) \\ s.t. & c(x) = 0 \end{array} \qquad \mathrm{BP}(\mu)$$

- Fiacco-McCormick approach:
  Solve barrier problem $\mathrm{BP}(\mu_l)$ (approximately) for monotone sequence of barrier parameters $\{\mu_l\} \to 0$
- Many different variants
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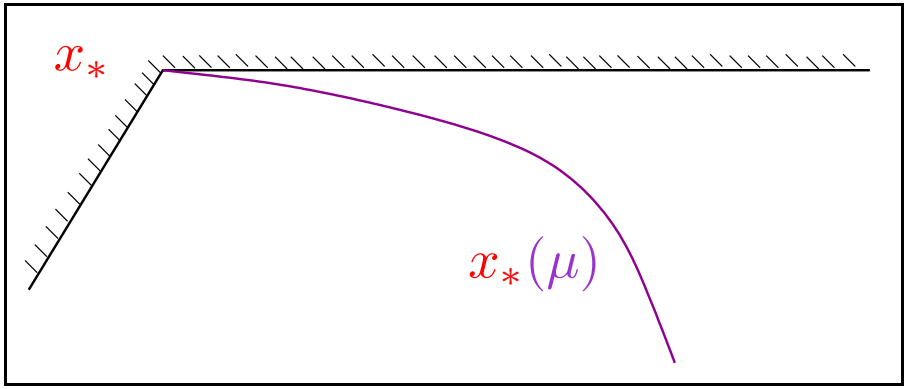
- Many different variants
  (primal-dual, different handling of constraints)
- Global convergence: Ensure global convergence for each $\mathrm{BP}(\mu_l)$
- Possible problems:
  - For given large μ, problem might be unbounded or difficult
  - Difficult to find good starting value μ_0
  - Fixing μ for several iterations might not be most efficient option
    (don't really want to solve $\mathrm{BP}(\mu_l)$)

Solving Primal-Dual Equations

$$\begin{aligned} \nabla f(x) - \nabla c(x)\lambda - z &= 0 \\ c(x) &= 0 \\ XZe &= \mu e \\ x, z &\geq 0 \end{aligned}$$



- Concentrate on solving the primal-dual equations (with $\mu = 0$)
- Follow the central path $x_*(\mu)$ as $\mu \to 0$
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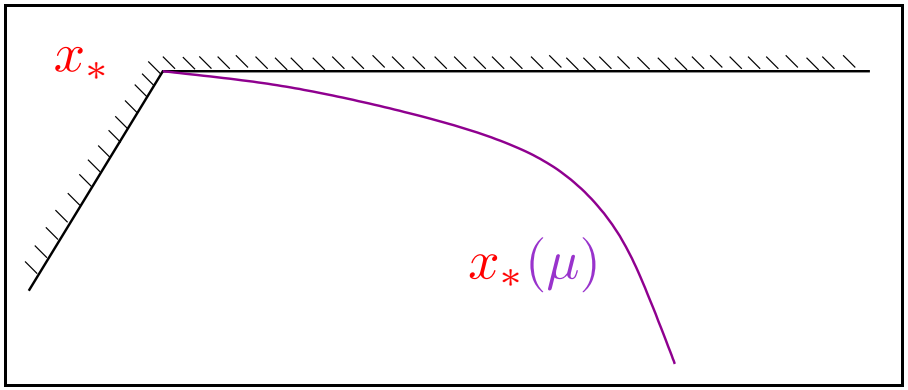

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- Methods adapt μ non-monotonically in every iteration
- Very effective for LP, QP, convex programming
- Global convergence issues:
  - Solving PD equations good enough for convex problems
  - In nonconvex case: Ignoring $f(x)$ can lead more easily to convergence to saddle points or maxima

Our Goal

Want to combine best of both approaches

1. Globalization method for $\mathrm{BP}(\mu)$, e.g.
   - KNITRO (Byrd, Nocedal, Waltz, et al.)
     - Trust region, merit function
   - IPOPT (W, Biegler)
     - Line search, filter method
   - Your favorite method

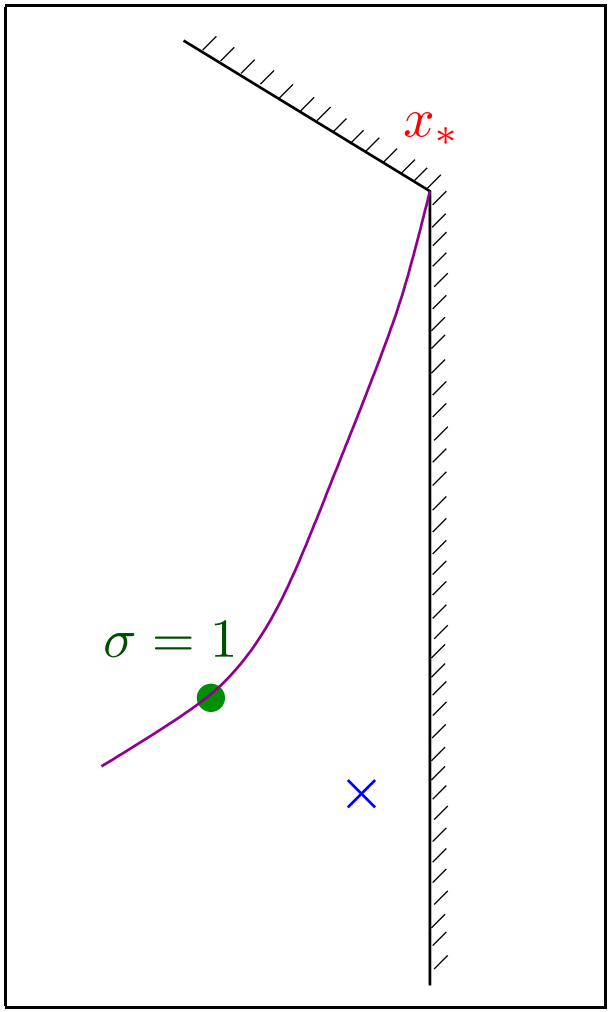
2. Effective adaptive update rules for μ

in an efficient, globally convergent framework

Choosing Adaptive Barrier Parameter

$$\mu = \sigma \frac{x^T z}{n}$$

with centering parameter σ



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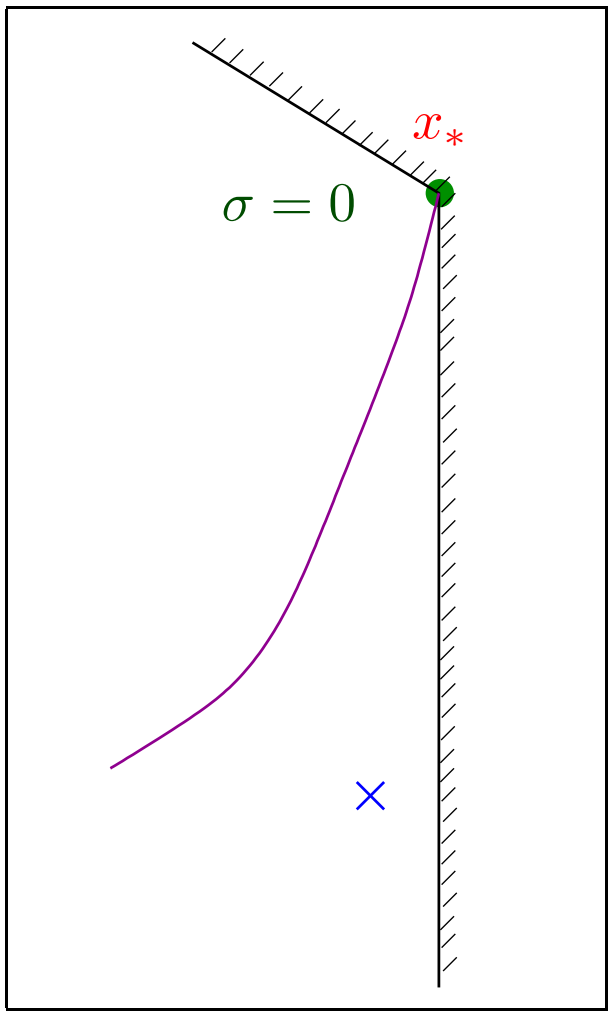

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Methods previously proposed:

1. LOQO centrality rule (formula)
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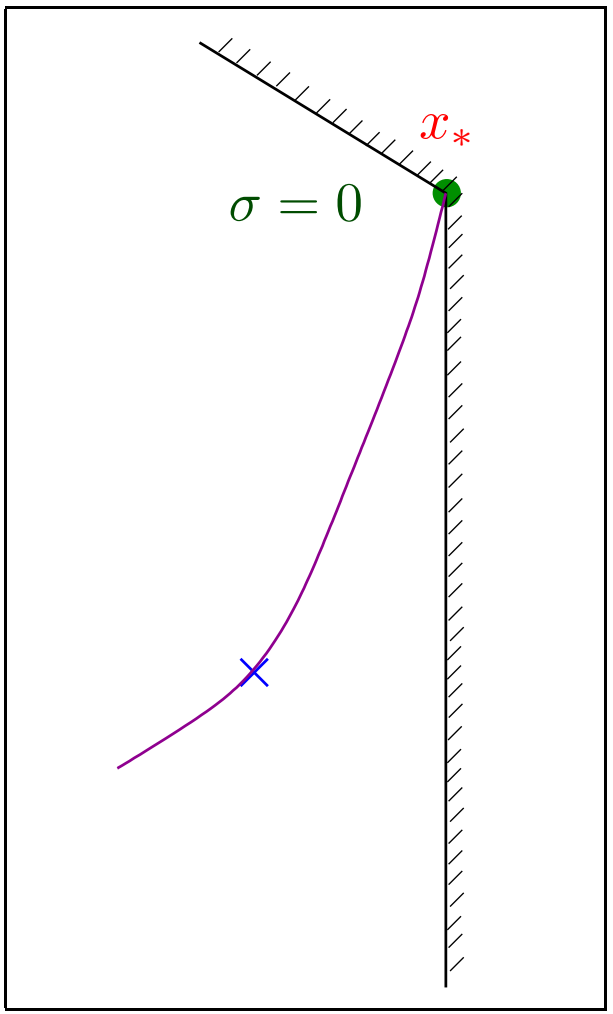

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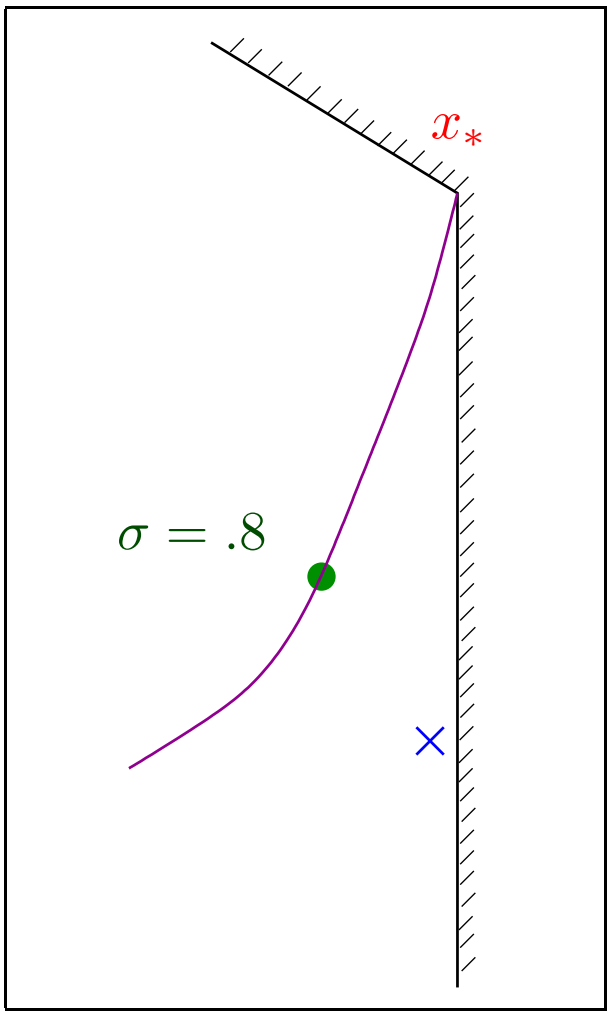

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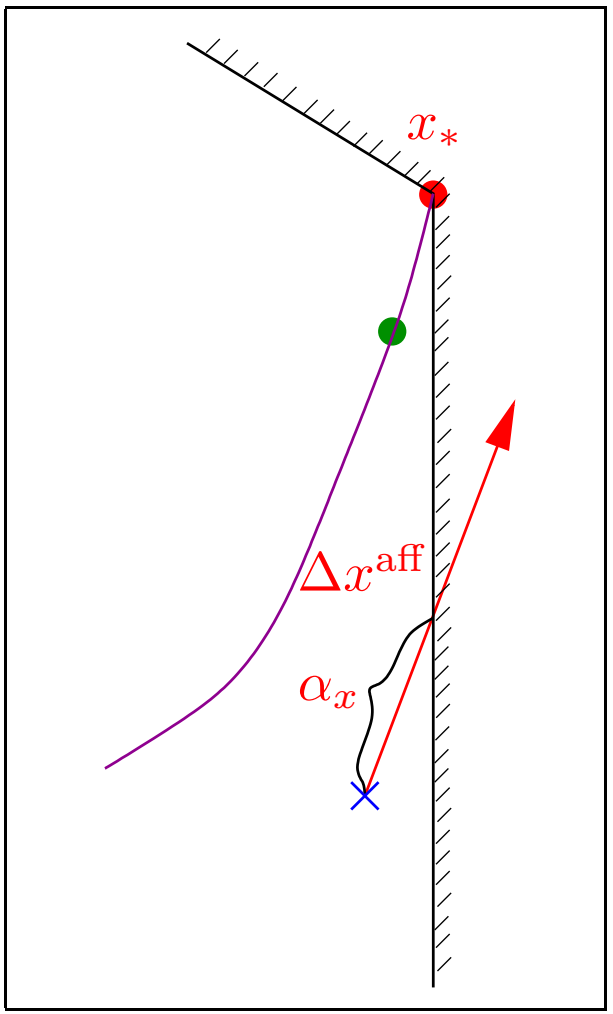
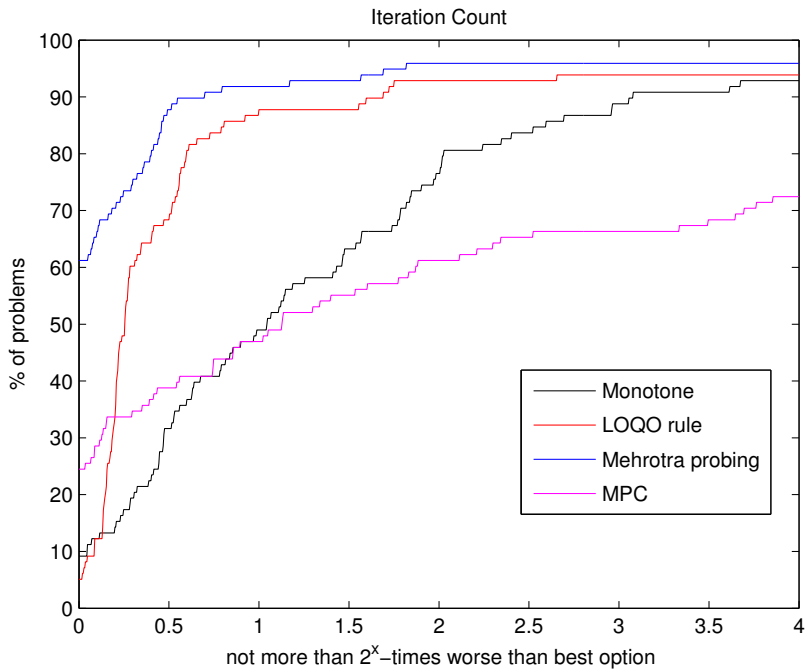
2. Mehrotra's probing rule for LP
   (Mehrotra, 1992)

$$\sigma = \left(\frac{(x + \alpha^x \Delta x^{\text{aff}})^T (z + \alpha^z \Delta z^{\text{aff}})}{x^T z} \right)^3$$

(requires extra step computation)



Adaptive Strategies (Ipopt)



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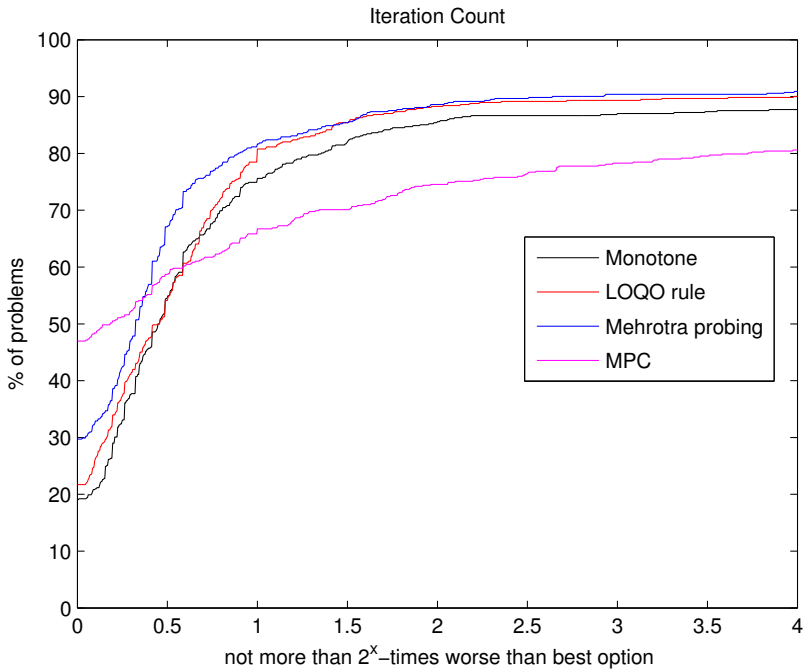
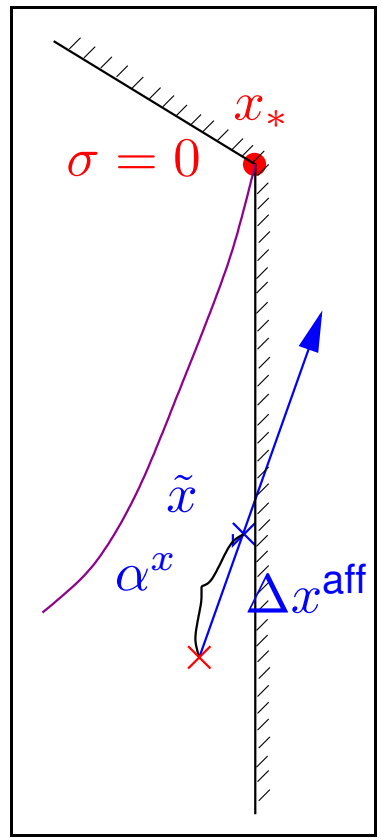


CUTEr

No line search (always fraction-to-the-boundary step size)

Can We Improve The Probing Strategy?

$$\begin{bmatrix} W & A(x) & -I \\ A(x)^T & 0 & 0 \\ Z & 0 & X \end{bmatrix} \begin{pmatrix} \Delta x^{\text{aff}} \\ \Delta \lambda^{\text{aff}} \\ \Delta z^{\text{aff}} \end{pmatrix} = - \begin{pmatrix} \nabla f(x) + A(x)\lambda - z \\ c(x) \\ XZe \end{pmatrix}$$



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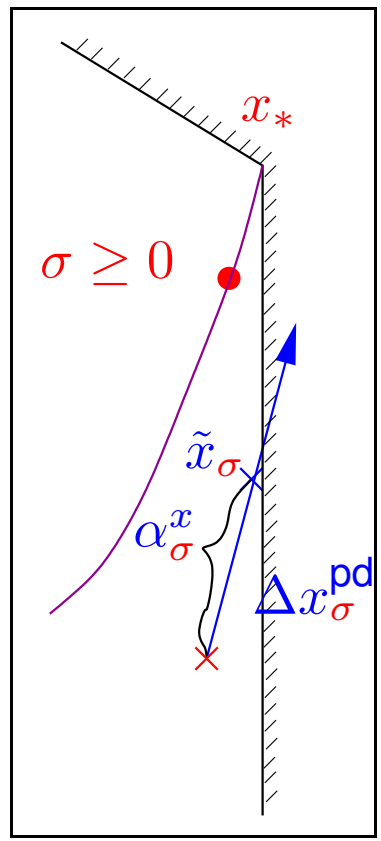

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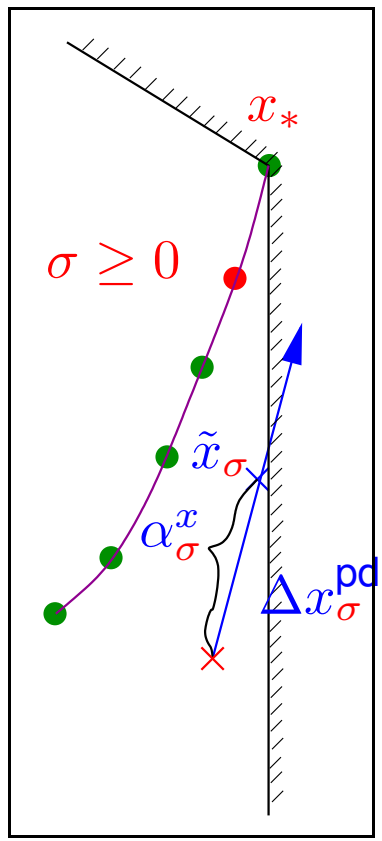

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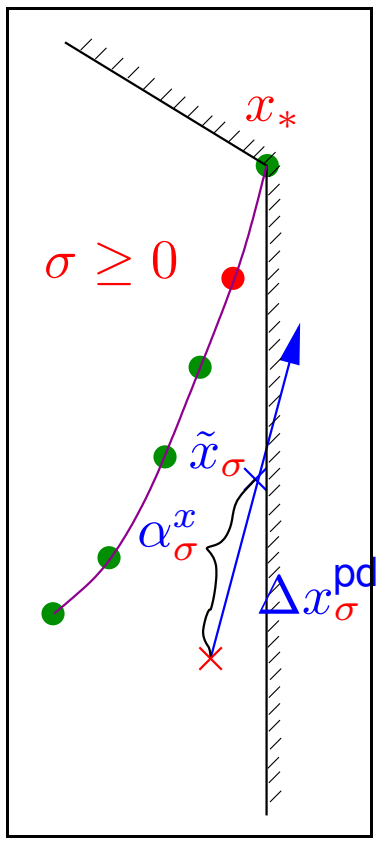
- Then, $\Delta_\sigma^{\text{pd}} = \Delta^{\text{aff}} + \sigma \Delta^{\text{cen}}$ cheaply available for all $\sigma \geq 0$



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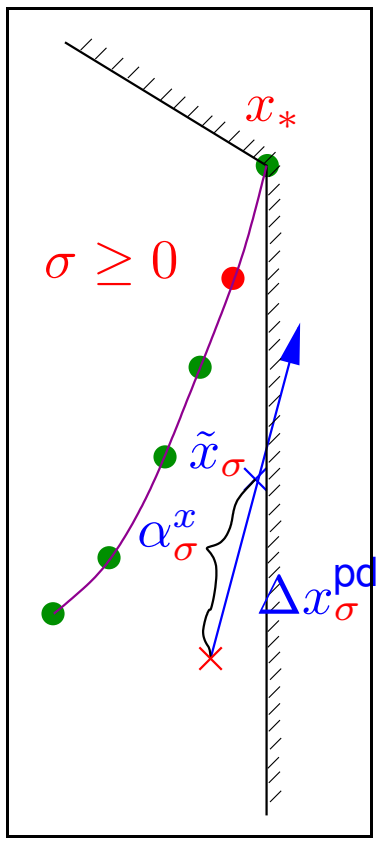
- Given $\sigma \geq 0$, examine probing points

$$\begin{aligned} \tilde{x}_\sigma &= x + \alpha_\sigma^x \Delta x_\sigma^{\text{pd}} \\ \tilde{\lambda}_\sigma &= \lambda + \alpha_\sigma^z \Delta \lambda_\sigma^{\text{pd}} \\ \tilde{z}_\sigma &= z + \alpha_\sigma^z \Delta z_\sigma^{\text{pd}} \end{aligned}$$

where

$$\begin{aligned} \alpha_\sigma^x &= \max\{\alpha \in (0,1] : x + \alpha \Delta x_\sigma^{\text{pd}} \geq (1-\tau)x\} \\ \alpha_\sigma^z &= \max\{\alpha \in (0,1] : z + \alpha \Delta z_\sigma^{\text{pd}} \geq (1-\tau)z\} \end{aligned}$$



Quality Function For Centering Parameter

- Search for the "best" σ that minimizes some "quality function" $\Phi(\sigma)$
  E.g.,

$$\Phi(\sigma) = \left\| \begin{pmatrix} \nabla f(\tilde{x}_\sigma) + A(\tilde{x}_\sigma)\tilde{\lambda}_\sigma - \tilde{z}_\sigma \\ c(\tilde{x}_\sigma) \\ \tilde{X}_\sigma \tilde{Z}_\sigma e \end{pmatrix} \right\|_2^2$$

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- Do not want to evaluate functions and gradients
- "Linear quality function"

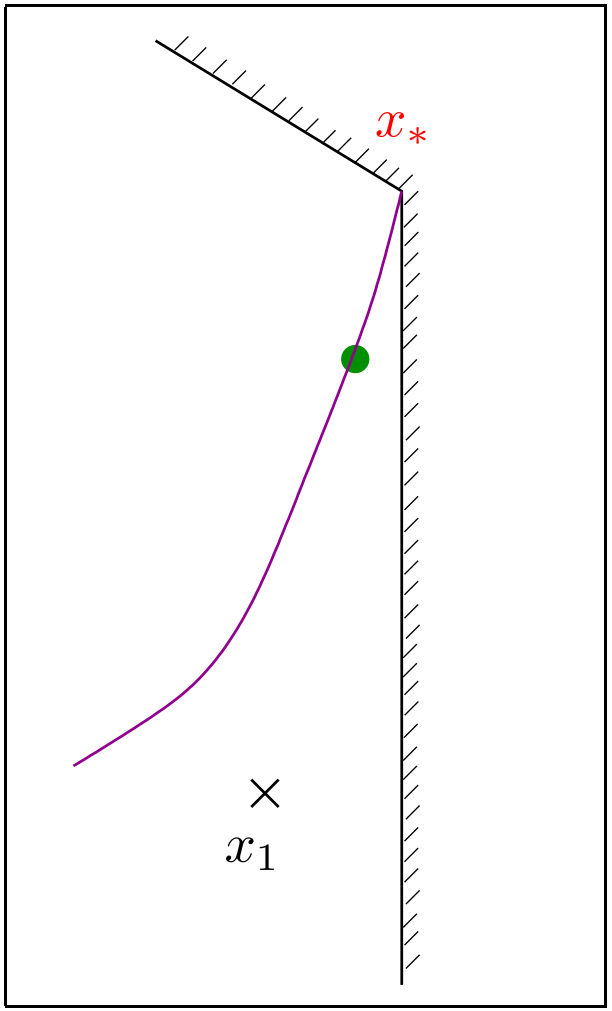
$$\begin{aligned} \Phi(\sigma) \;=\; & (1-\alpha_\sigma^z)^2 \|\nabla f(x_k) + A(x_k)\lambda_k - z_k\|_2^2 + \\ & (1-\alpha_\sigma^x)^2 \|c(x_k)\|_2^2 + \\ & \|\tilde{X}_\sigma \tilde{Z}_\sigma e\|_2^2 \end{aligned}$$

  - Accurately predicts primal-dual error at probing point for LPs
  - Relatively inexpensive to compute (need α_σ^x, α_σ^z, $\tilde{X}_\sigma \tilde{Z}_\sigma e$ for given σ)
  - $\Phi(\sigma)$ is non-smooth, non-convex; use direct search

A General Globalization Framework

For each iteration k:

1. Choose μ_k by adaptive rule (*free mode*)



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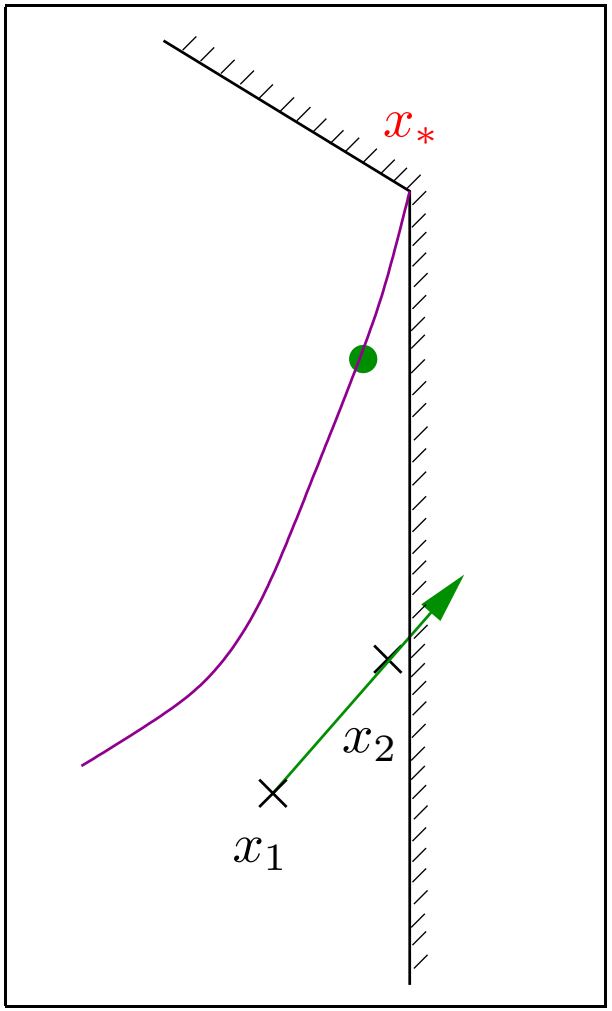

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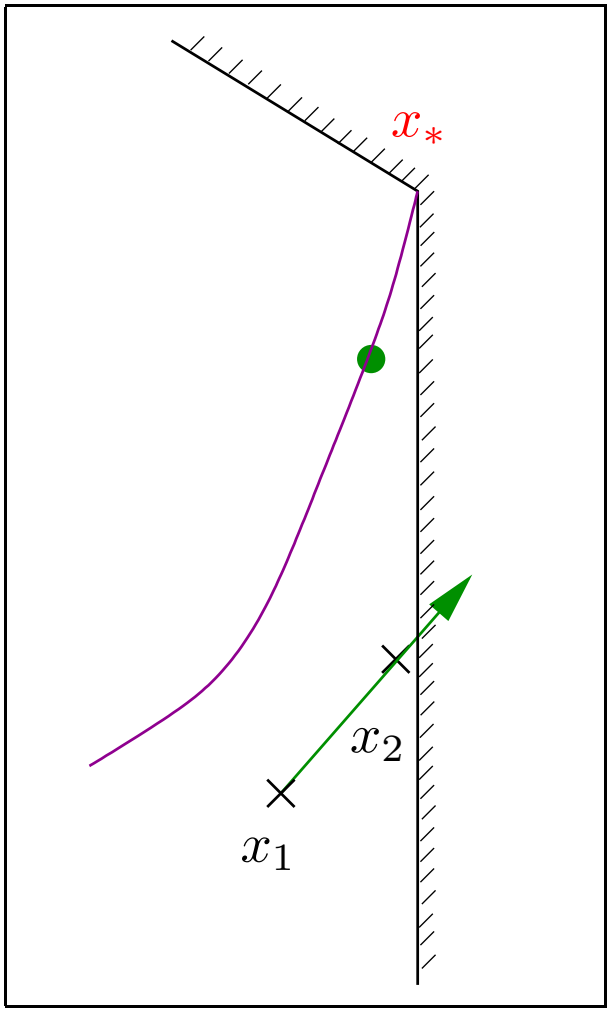

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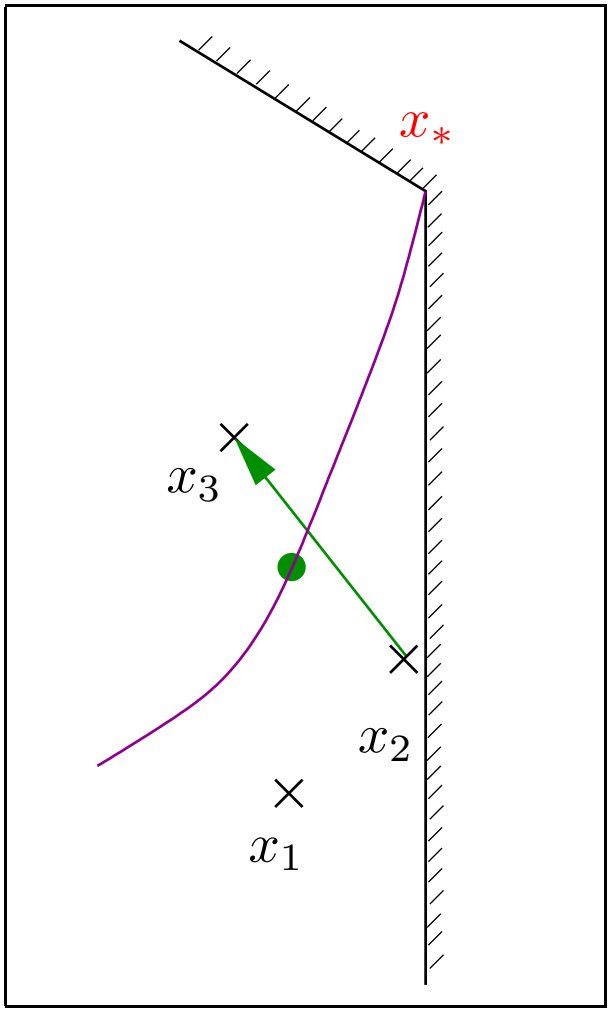
   - Yes: Continue with next iteration



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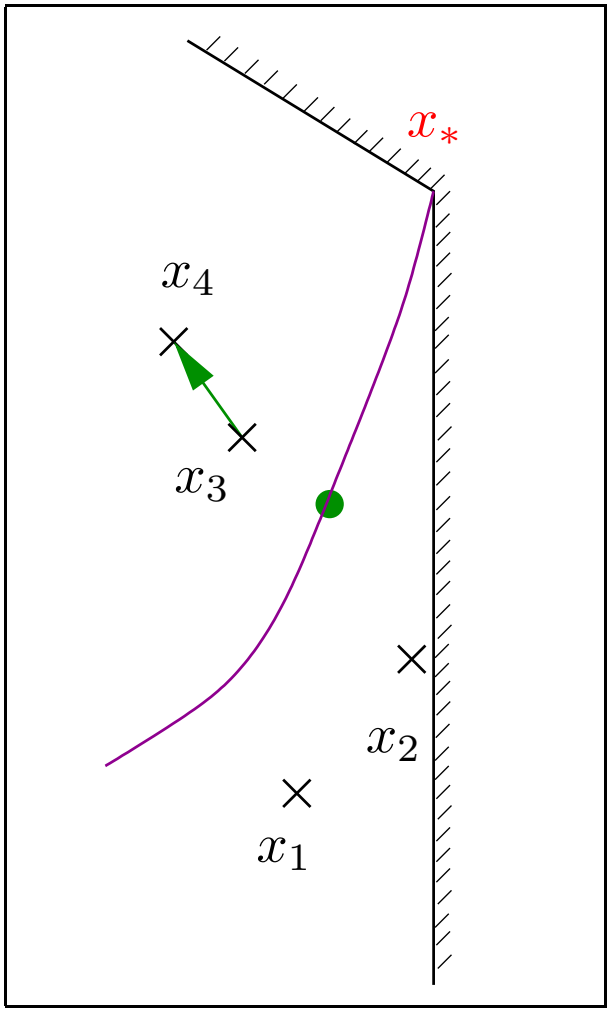

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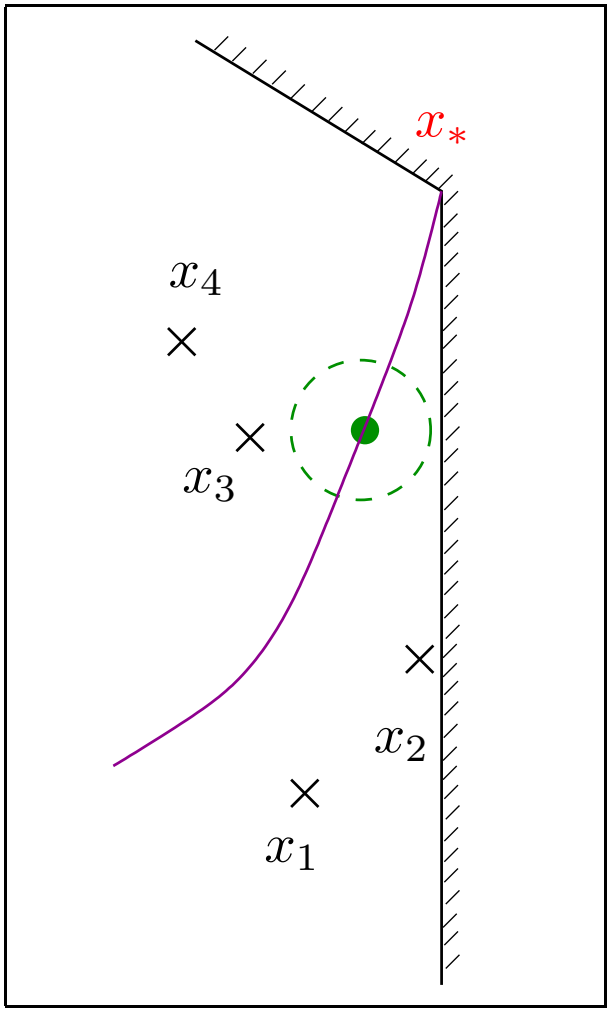
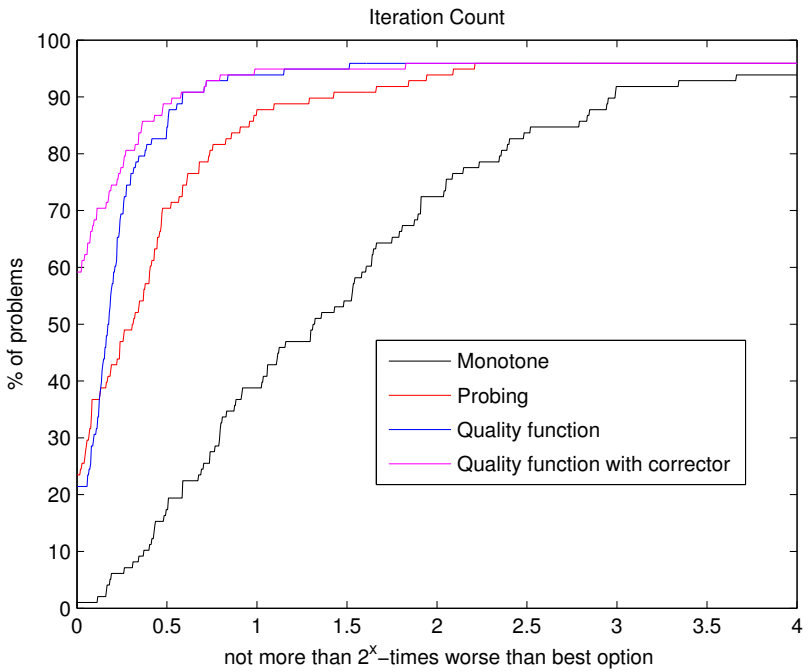
3. Progress for original NLP? (suff. progress in $\|\mathsf{PD_error}_k\|_2^2$?)
   - Yes: Continue with next iteration
   - No: (*monotone mode*)
     (a) execute robust, monotone Fiacco-McCormick algorithm (approx. solve $\mathrm{BP}(\bar{\mu})$ problems)
     (b) if suff. progress for original NLP, return to *free mode*



Globalization Strategy (Ipopt)



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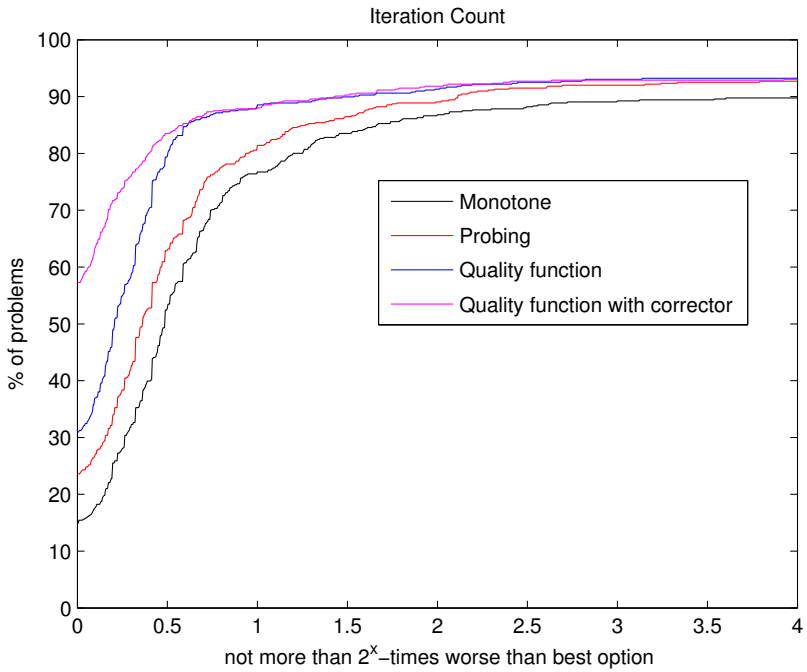
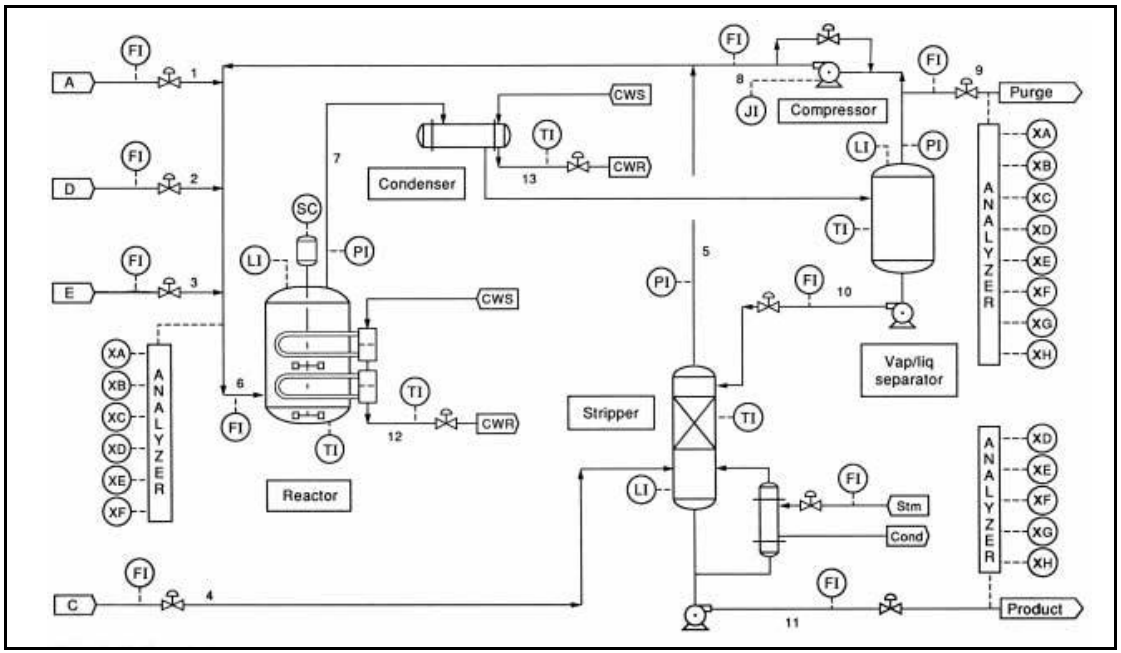


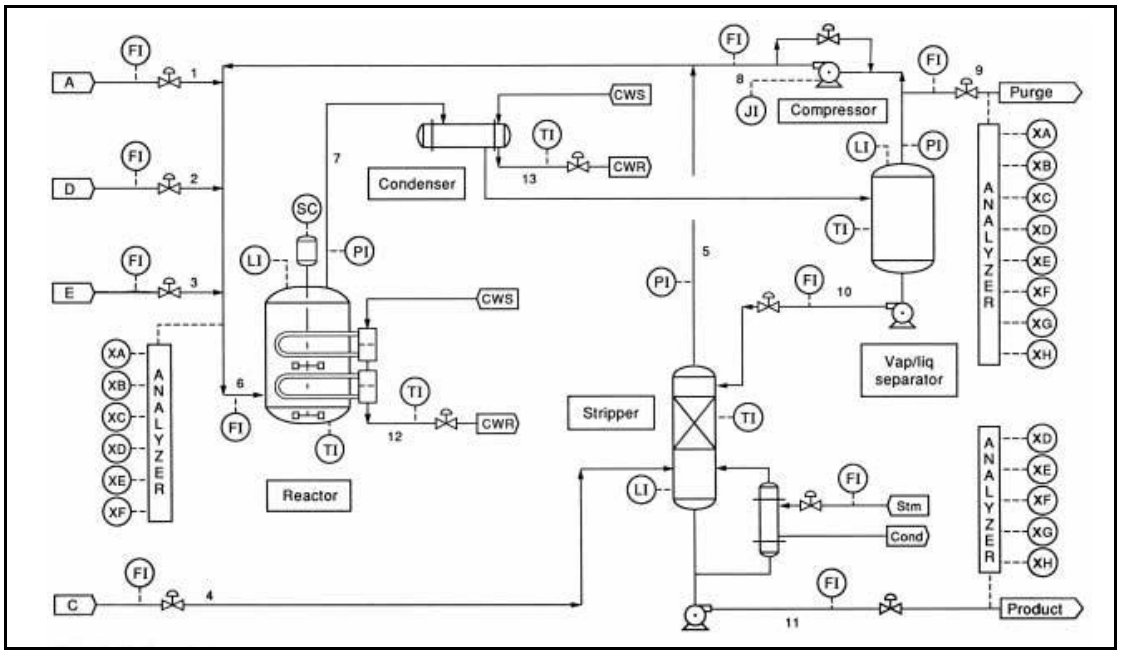
CUTEr

Nonlinear Optimization Applications

Design and Operation of Chemical Plant

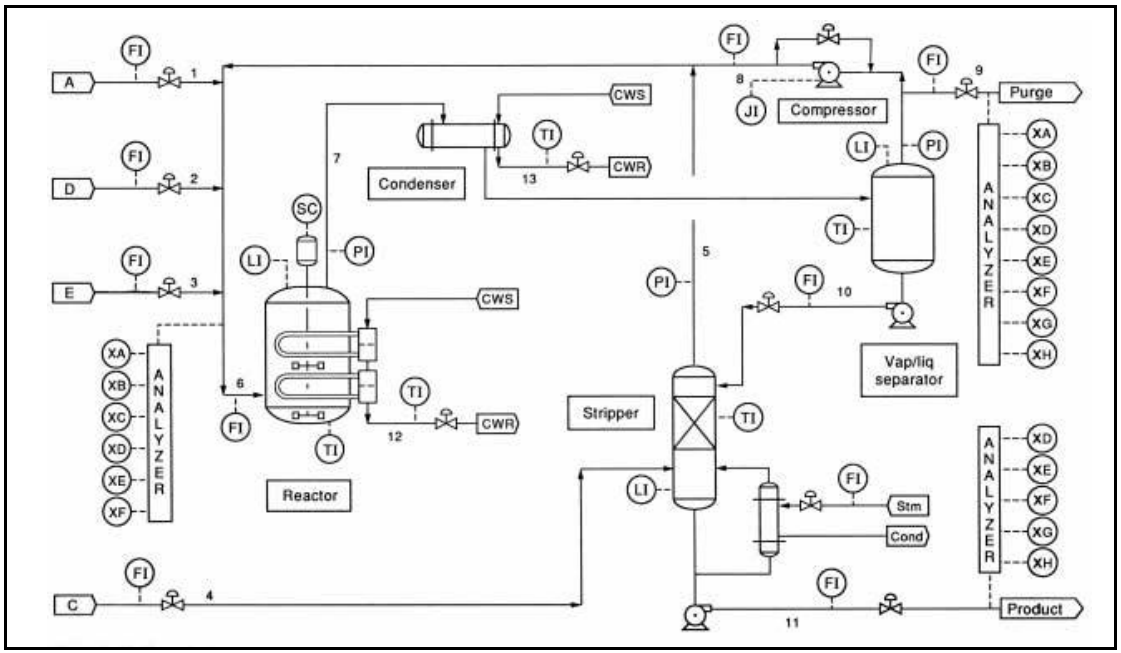


Design and Operation of Chemical Plant



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

Design and Operation of Chemical Plant



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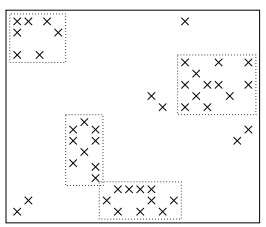
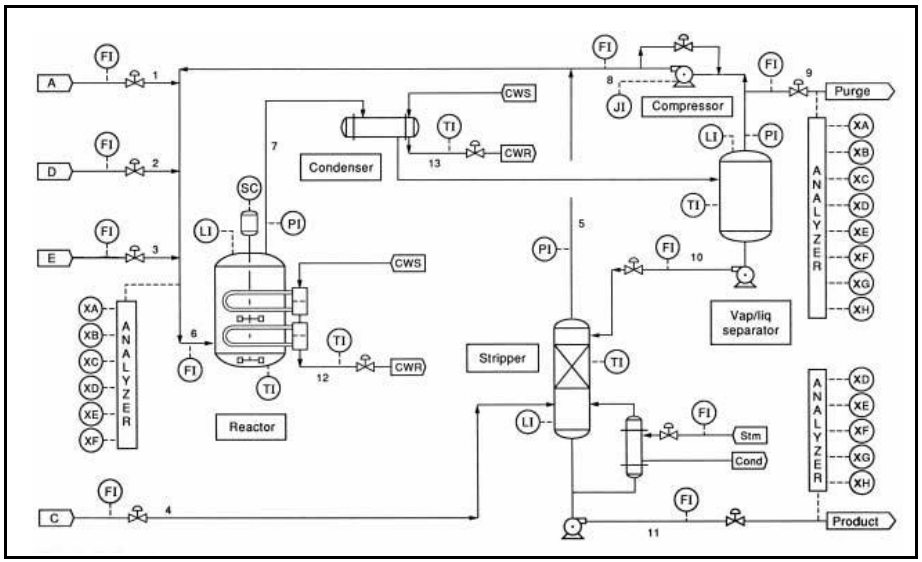
Constraint Jacobian

$$\nabla c(x)^T =$$



is sparse and structured

Design Under Uncertainty



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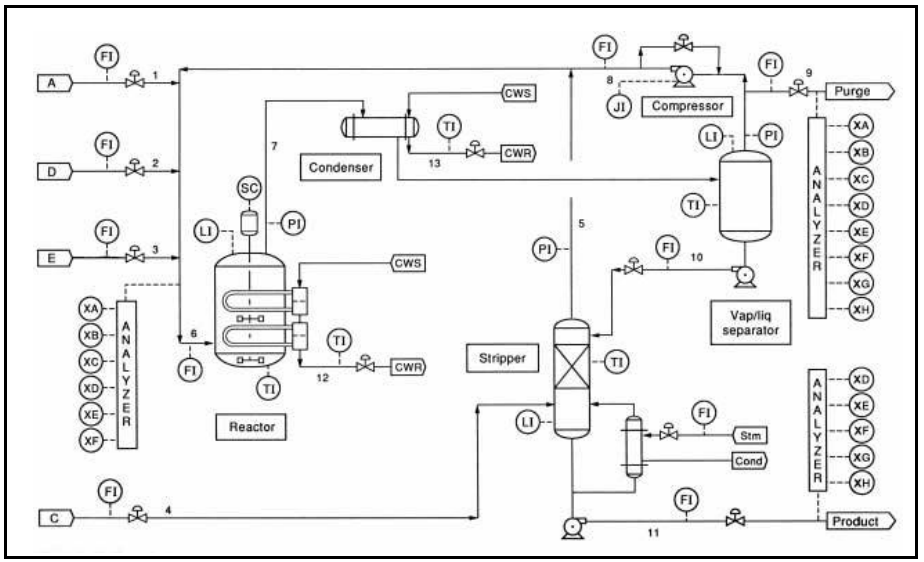

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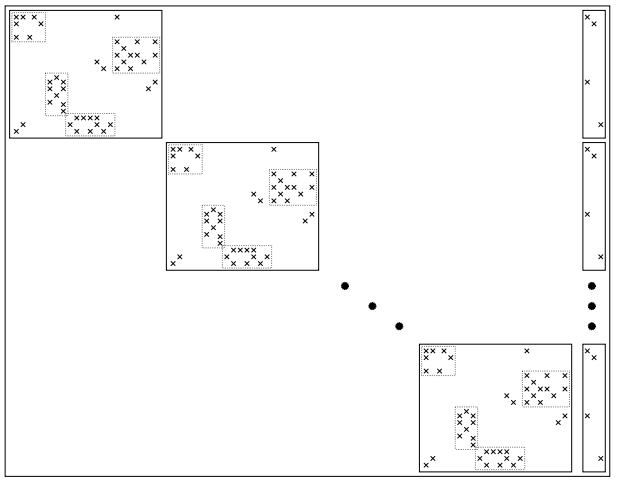
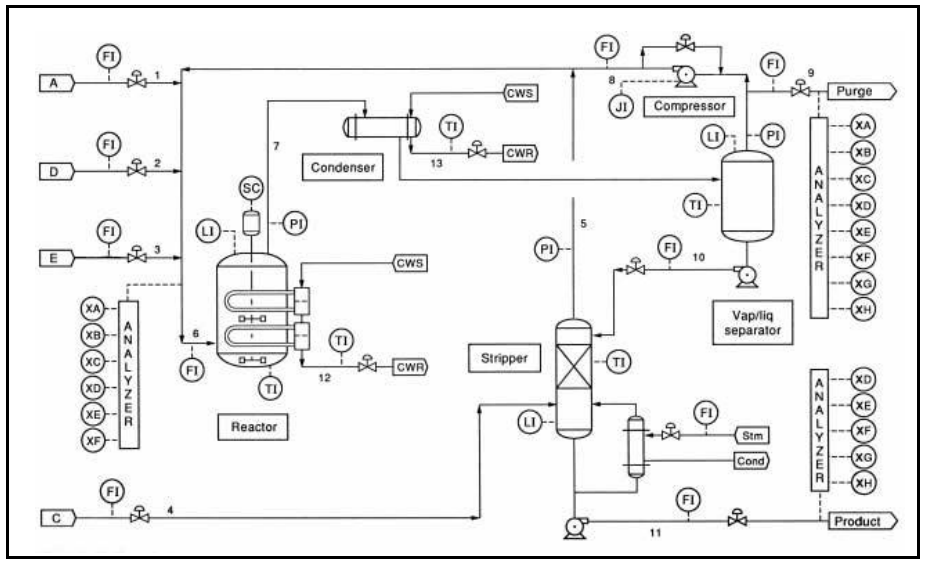


- Scenario parameters: $F^l_{in}, x^l_{in}, T^l_{env}, p^l_{env}, \ldots$ (given)
  (defining scenarios $l = 1, \ldots, L$)
- Design variables: $V_{react}, D_{dist}, h_{tank}, \ldots$
- Control variables: $Q^l_{heat}, r^l_{refl}, v^l_{valve}, \ldots$
- State variables: $x^l_{str}, F^l_{str}, L^l_{tank}, T^l, p^l, \ldots$

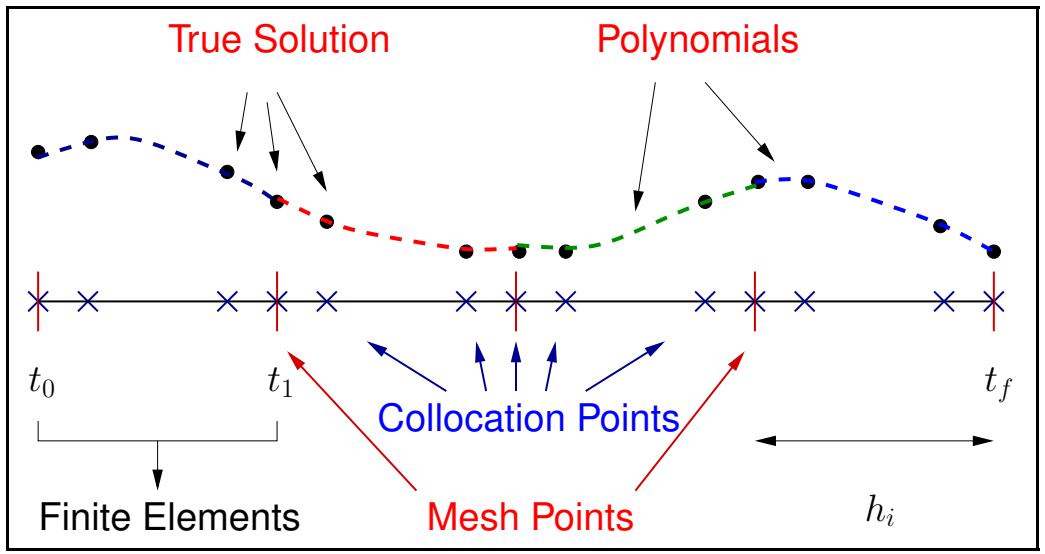
Optimal Control / Dynamic Optimization

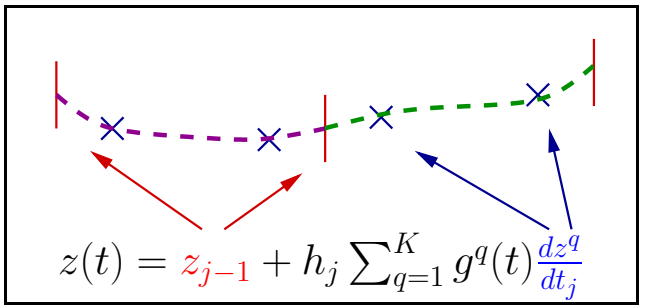


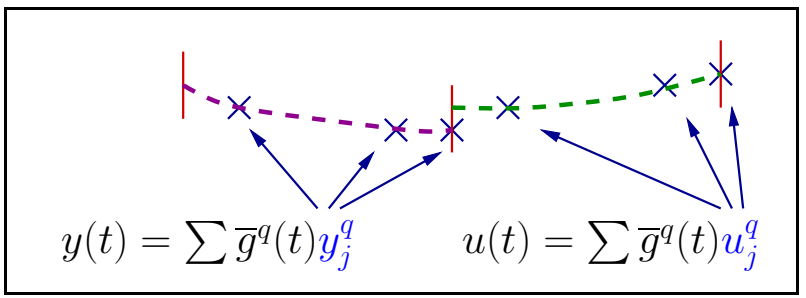
$$\begin{aligned} \min_{z,y,u,p} \quad & f(z(t_f), y(t_f), u(t_f), p) \\ s.t. \quad & F(\dot{z}(t), z(t), y(t), u(t), p) = 0 \\ & G(z(t), y(t), u(t), p) = 0 \\ & z(0) = z_{init} \\ & \textit{bound constraints} \end{aligned}$$

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

Discretization of DAEs



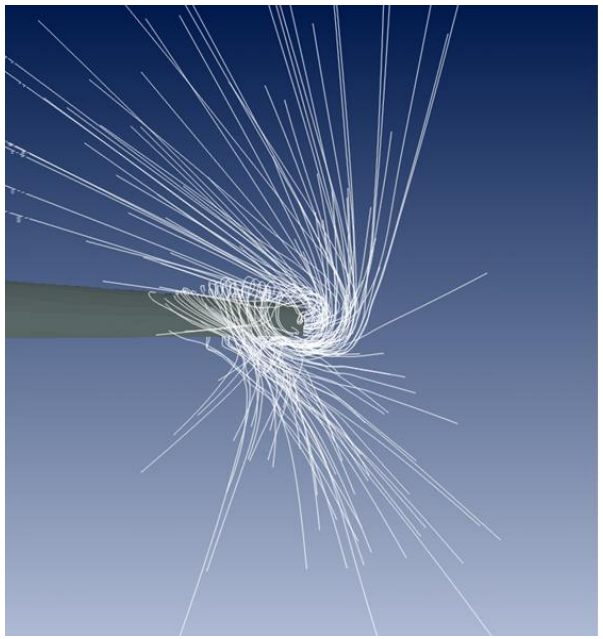




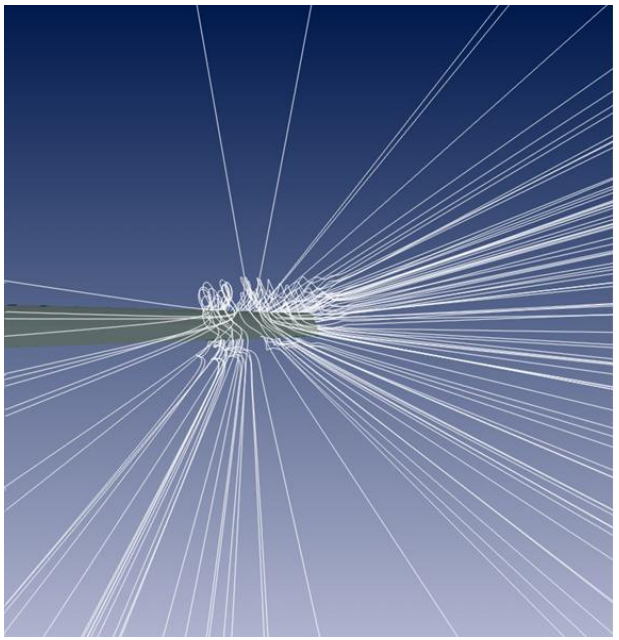
- x: Coefficients in polynomial representation
- c: DAE at collocation points / continuity equations
- Many variables $n = 1,000 - 10,000,000$
- Relatively few degrees of freedom ($n - m = 10 - 10,000$)
- Jacobian sparse and structured (almost block-diagonal)
- Finer discretization gives better approximation

Problems with PDEs

Uncontrolled



Controlled



- Constraints: discretized PDEs
- Very large problems
- Iterative linear solvers (preconditioners)
- Require parallel computing

- Applications:
  - Design (plains, cars)
  - Inverse Problems (geological data)
  - Hypothermia cancer treatment

Computationally Challenging Problems

- Large-Scale NLPs

Analytic functions

- e.g. discretized DAEs/PDEs
- 1st derivatives available
- 2nd deriv. available or approx.

Many variables (n up to $10,000,000$)

Exploit structure

- Sparse, structured $\nabla c(x)^T$
- PDE preconditioners
- Few vs. many degrees of freedom

The Other Extreme

- Computation of functions very expensive
- Function evaluation might include
  - Simulation of complicated system
  - Laboratory experiment (car crash test)
- Functions might be “noisy”
- Computation of gradients impossible or difficult
- Applications
  - Design of cars/planes (helicopter blades; jet engines)
  - Energy network optimization
- Solution methods:
  - Surrogate models (derivative-free optimization)
  - Pattern search (PDS, Nelder-Meade)
- Number of variables usually very small (n up few 100)
  (the relevant quantities determined by statisticians)

Computationally Challenging Problems

Large-Scale NLPs	Small NLPs
Analytic functions	Expensive function evaluations
– e.g. discretized DAEs/PDEs	– e.g. simulation/experiments
– 1st derivatives available	– no derivatives available
– 2nd deriv. available or approx.	– numerical noise
Many variables (n up to $10,000,000$)	Few variables (n up to 100)
Exploit structure	Methods
– Sparse, structured $\nabla c(x)^T$	– Surrogate models (DFO)
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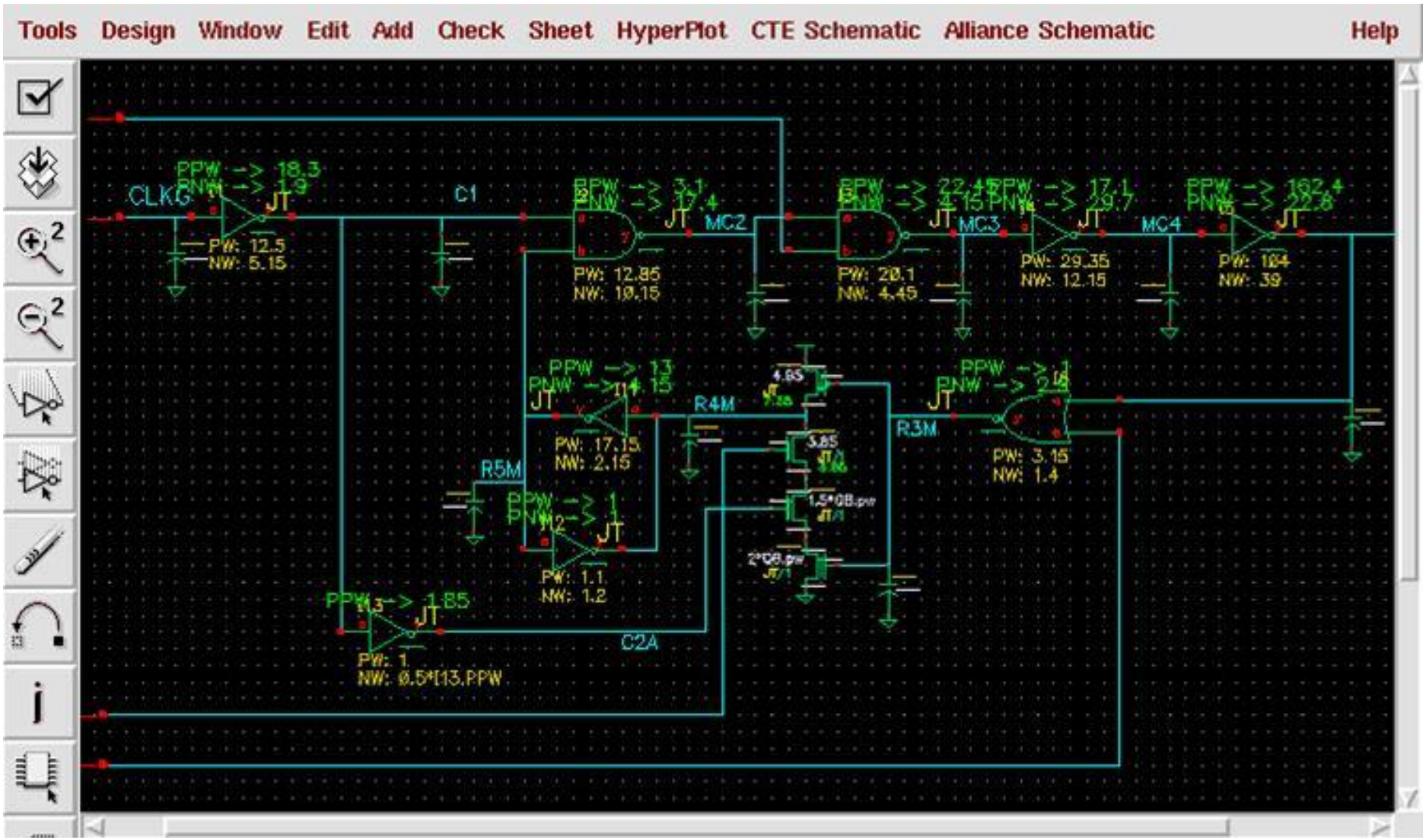
Circuit Tuning

Circuit Tuning: Basic Concepts



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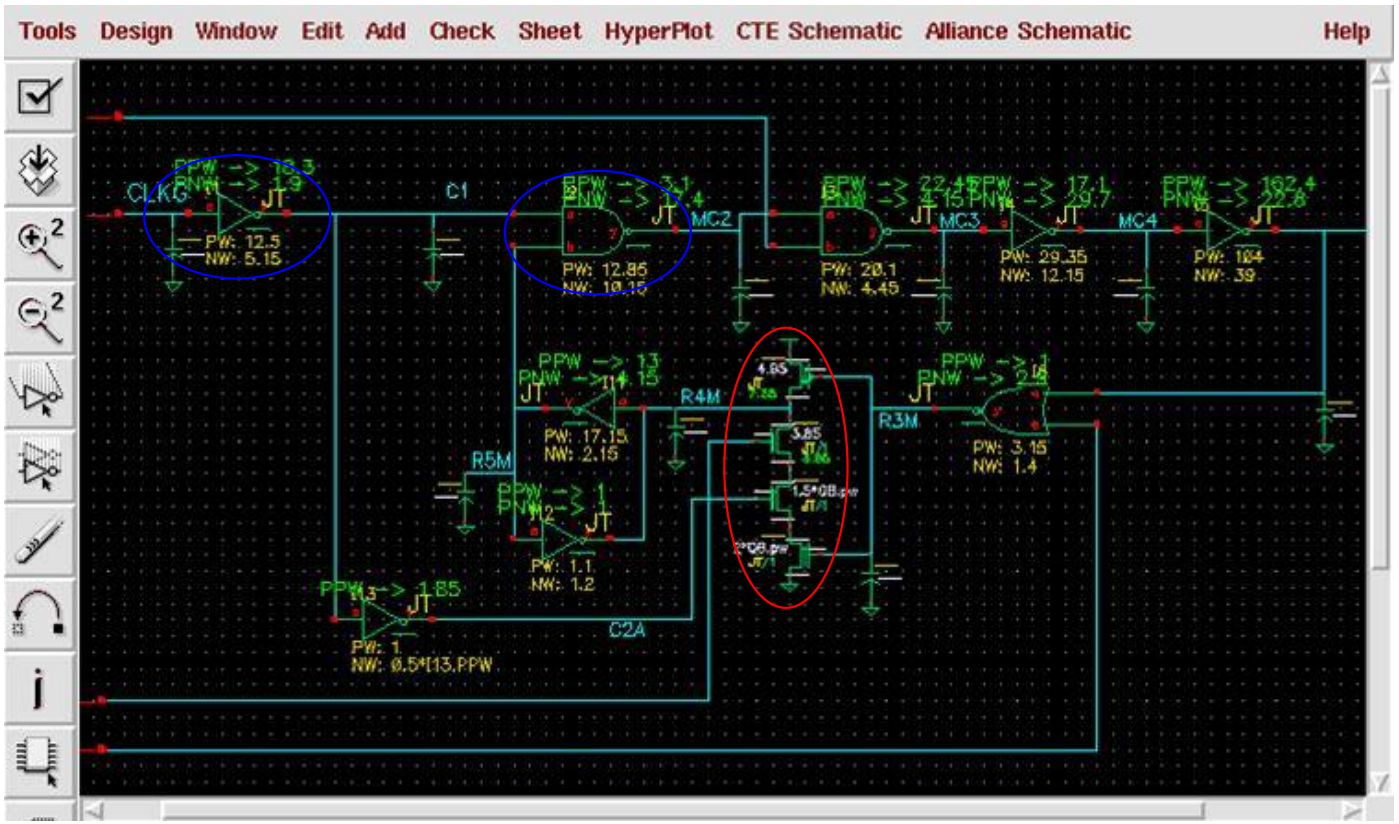
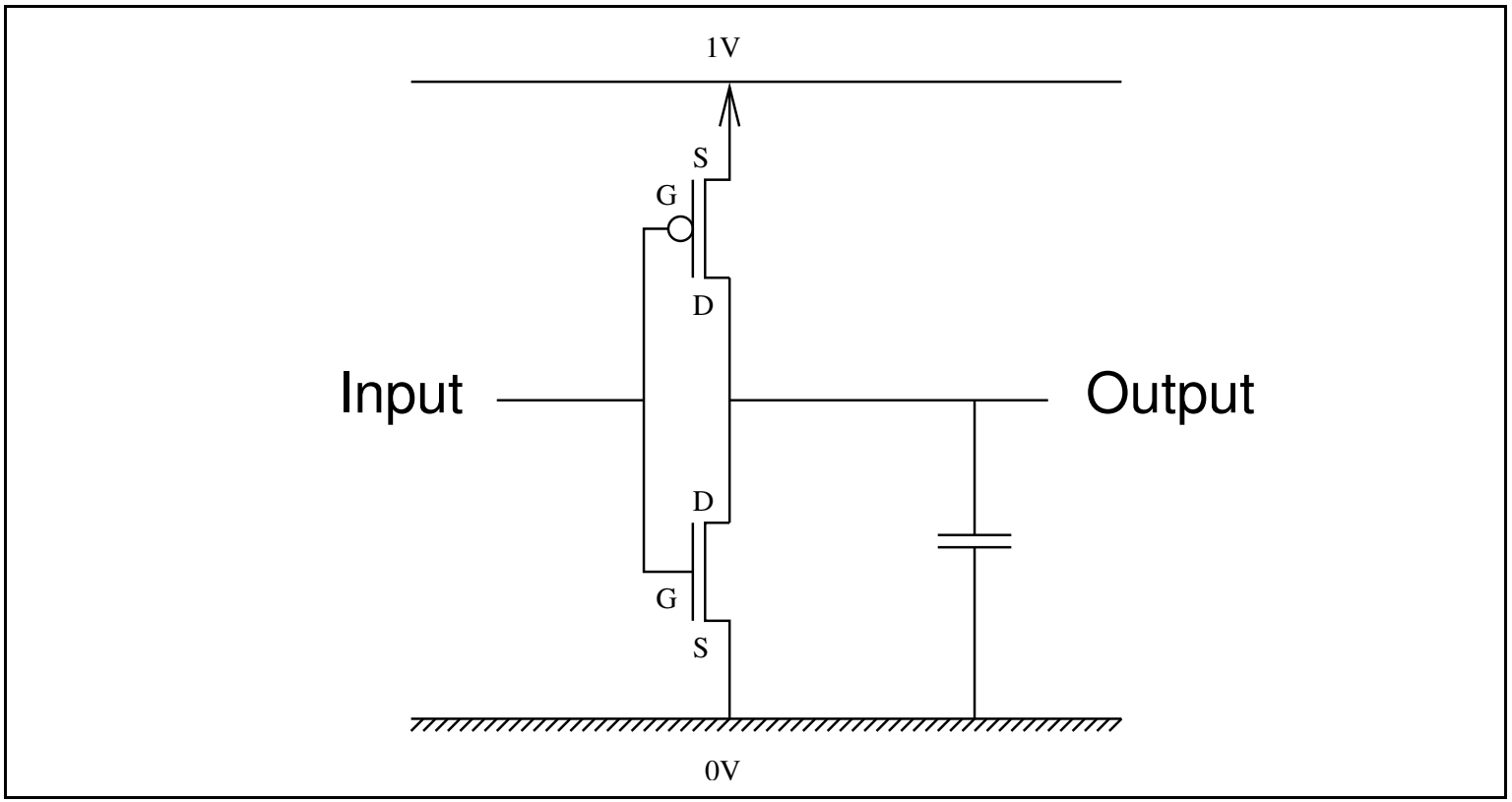


- Basic building blocks:
  - Transistors (switches); Gates (logical units)
- Connected by wires

A Simple Example: Inverter (NOT-Gate)



- Two transistors (P-FET and N-FET)

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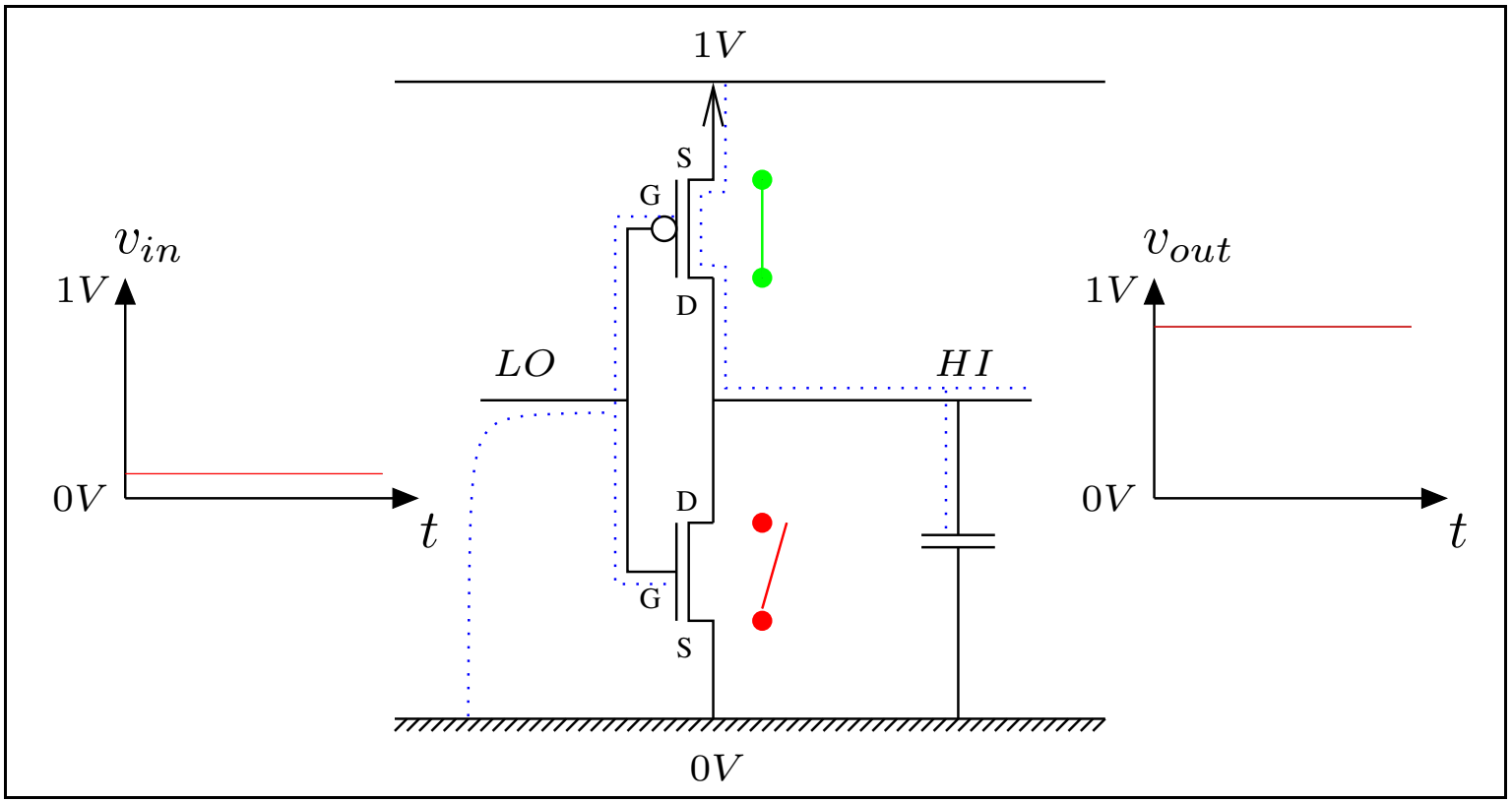

- Two transistors (P-FET and N-FET)
  - Input Lo $\longrightarrow$ Output Hi

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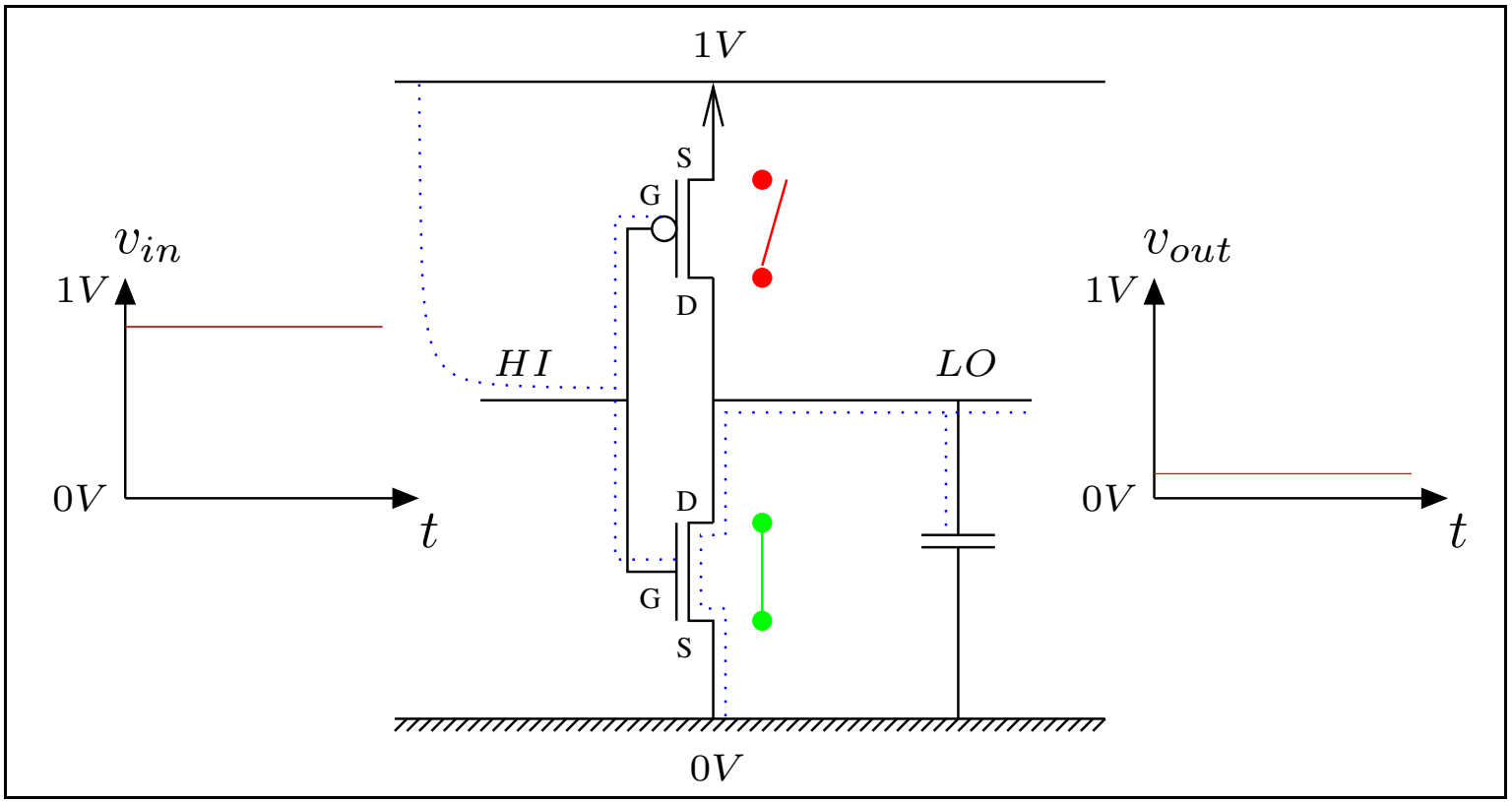
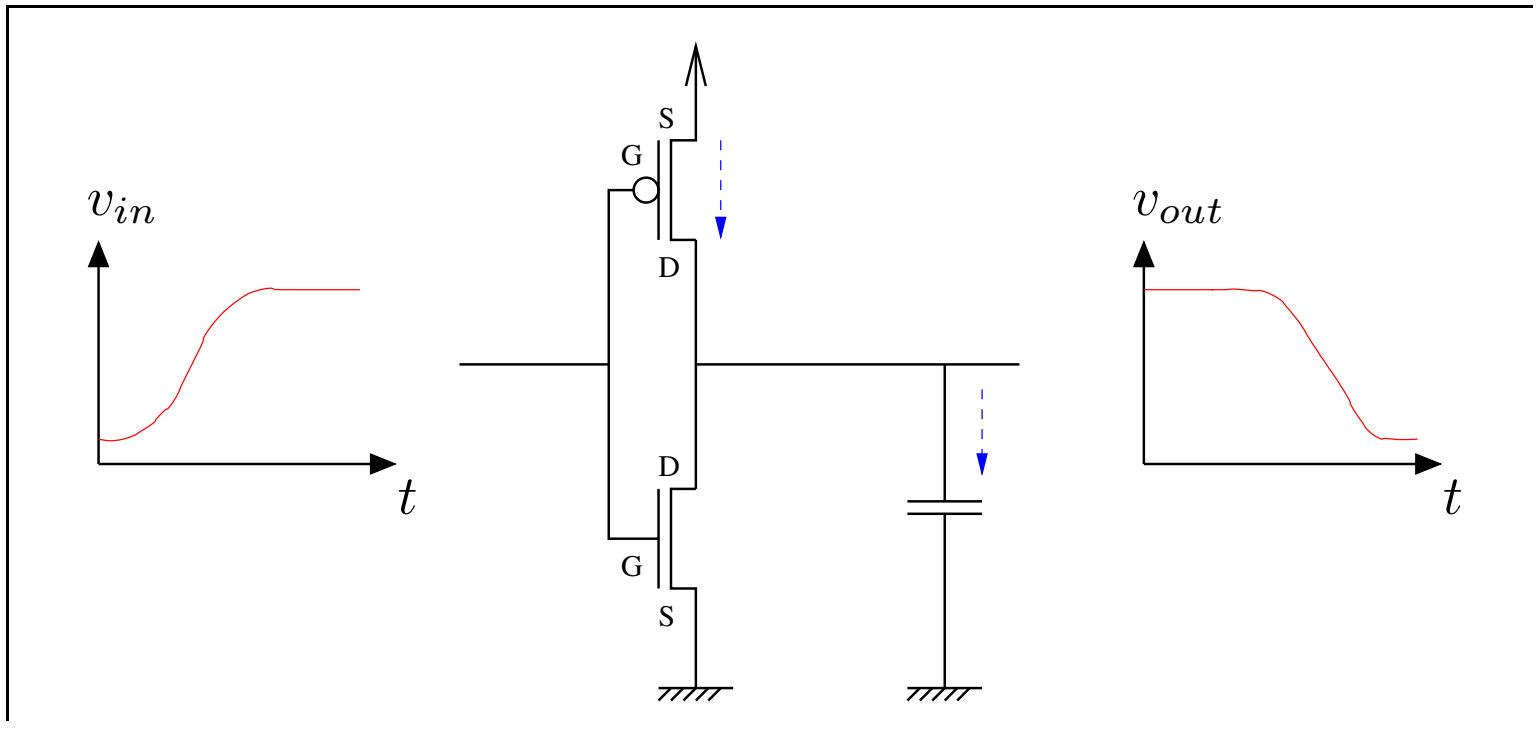
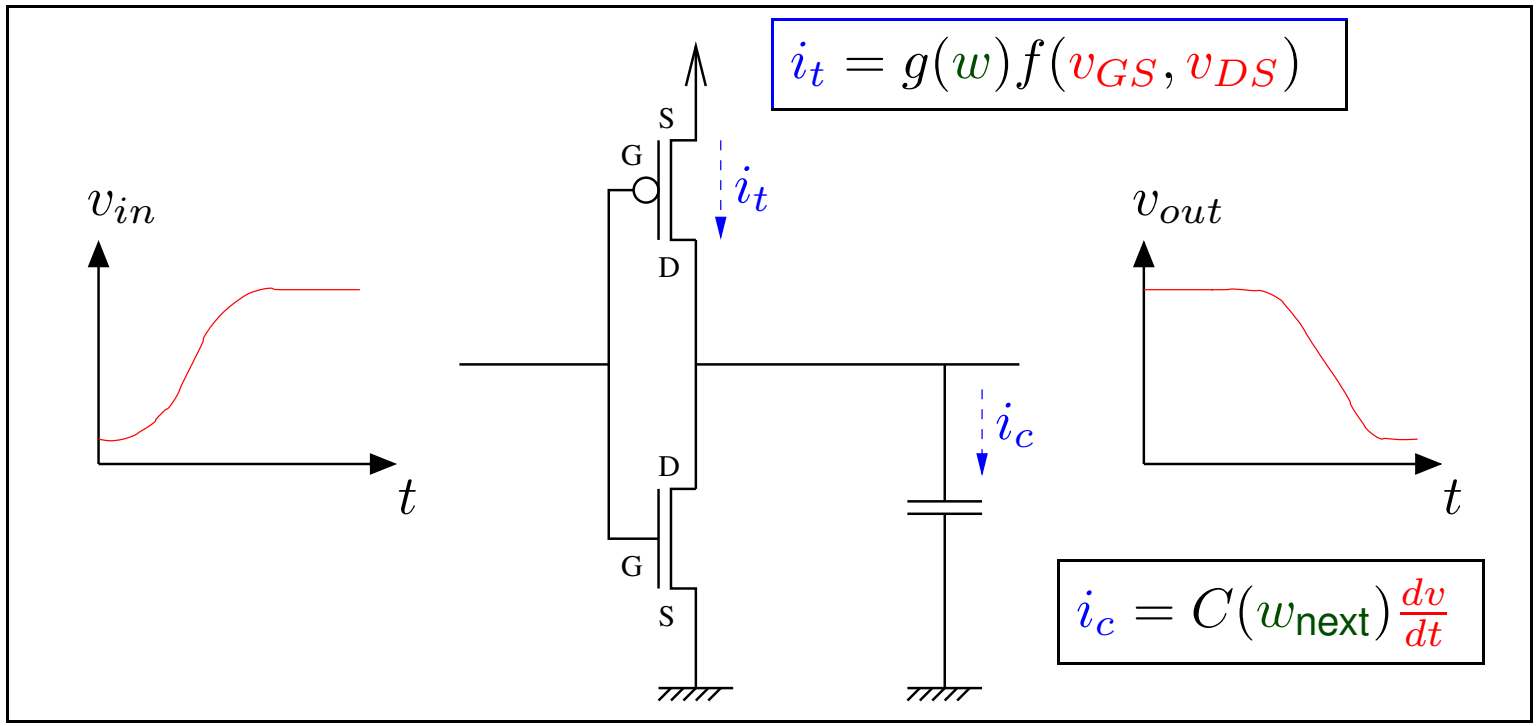


- Two transistors (P-FET and N-FET)
  - Input Lo $\longrightarrow$ Output Hi
  - Input Hi $\longrightarrow$ Output Lo

Dynamic Behavior of a Gate

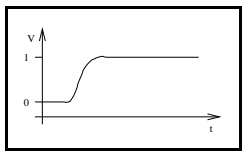


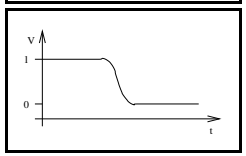
Dynamic Behavior of a Gate

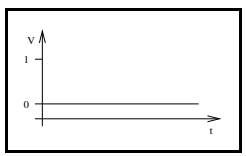


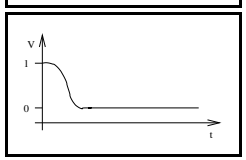
- System of differential and algebraic equations:
  - Conservation laws
  - (Parasitic) capacitors: Include dv/dt terms
  - I-V characteristics for conducting devices

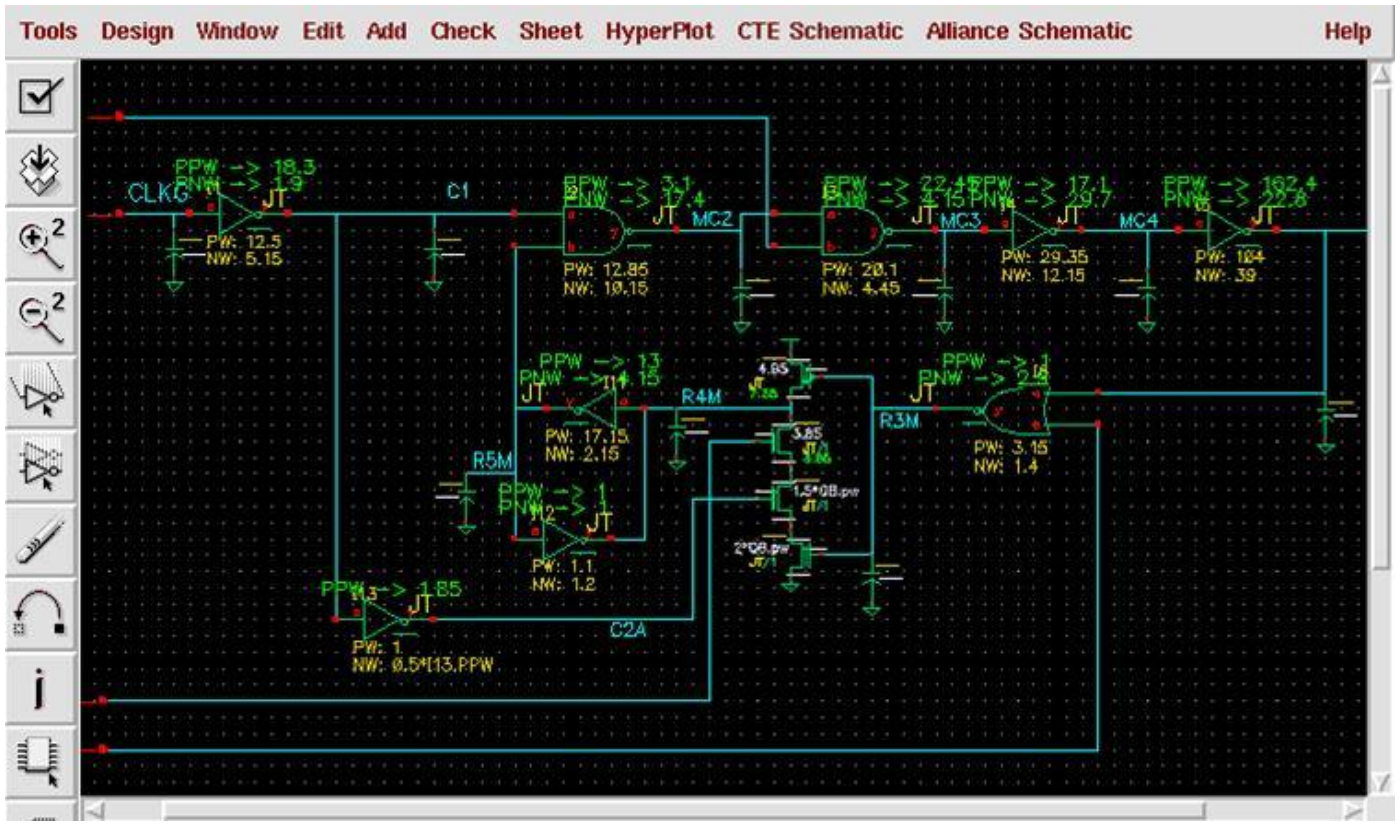
Circuit Tuning: Basic Concepts

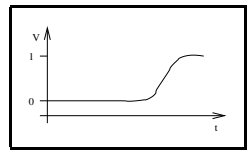






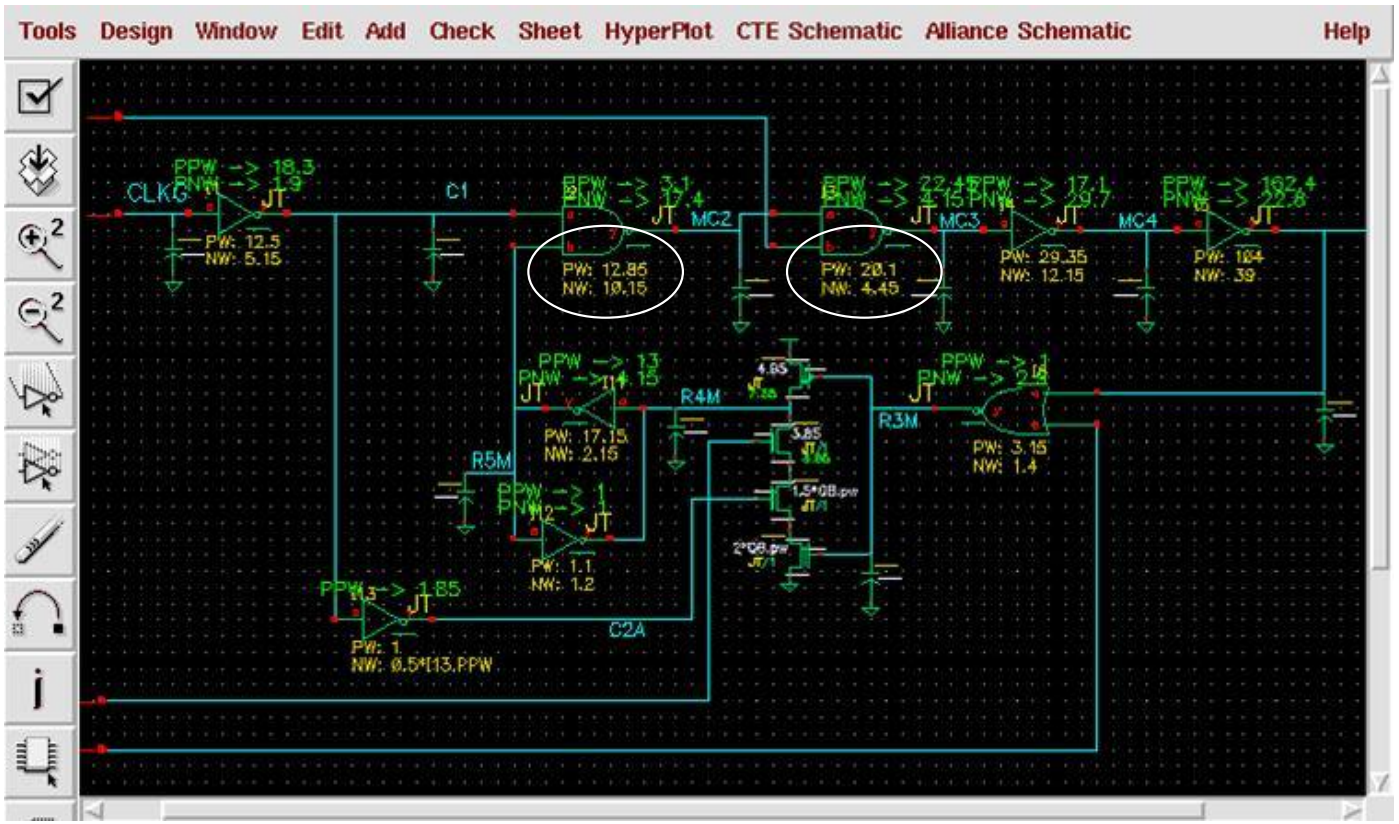






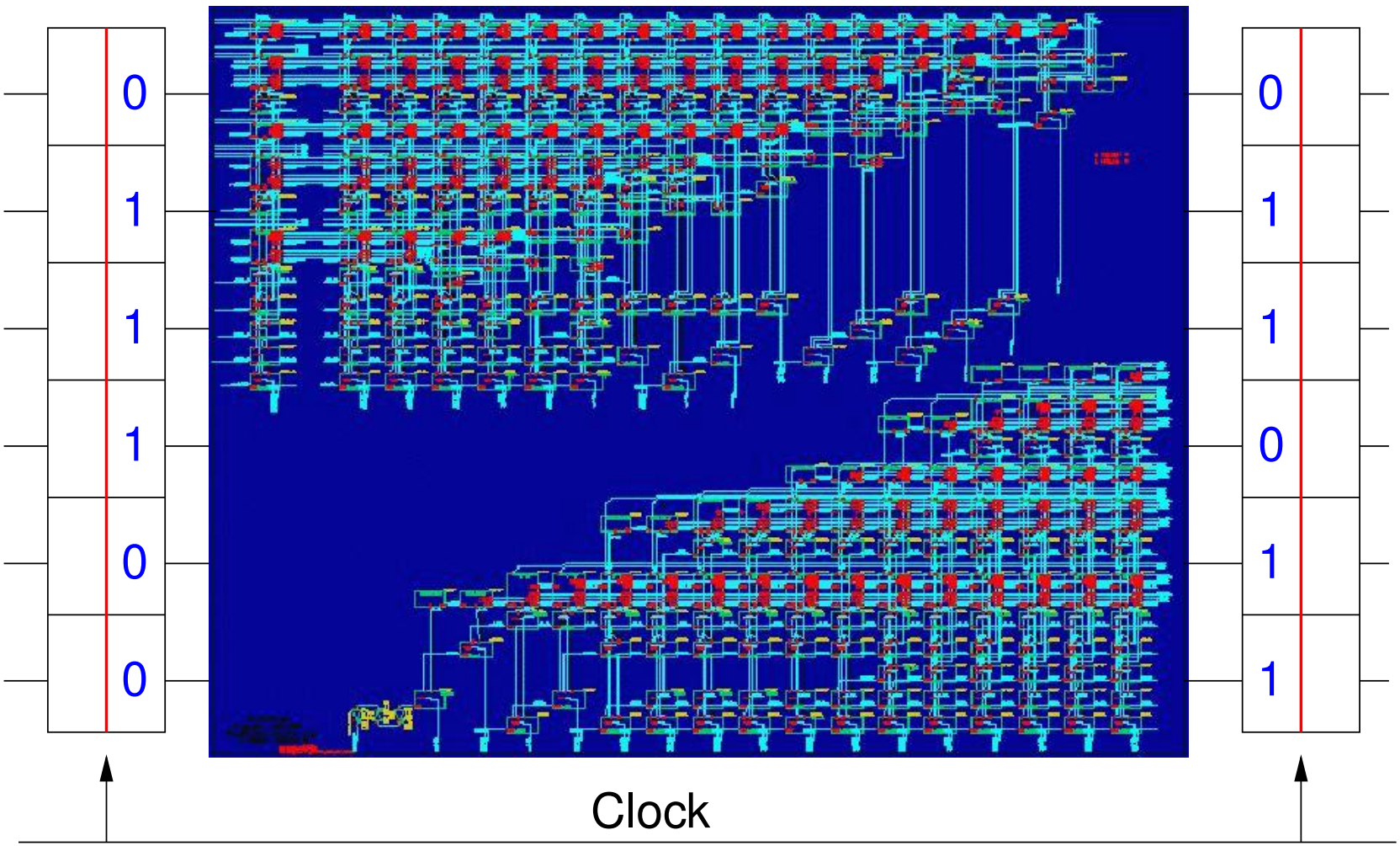
- Signals arrive at the inputs, pass through the circuit, and leave at the outputs (switches at gates on order of 10^{-12} seconds)

Circuit Tuning: Basic Concepts



- Can change the “speed” of a gate by changing the widths of its transistors (PFETs and NFETs)

Proper Timing is essential!



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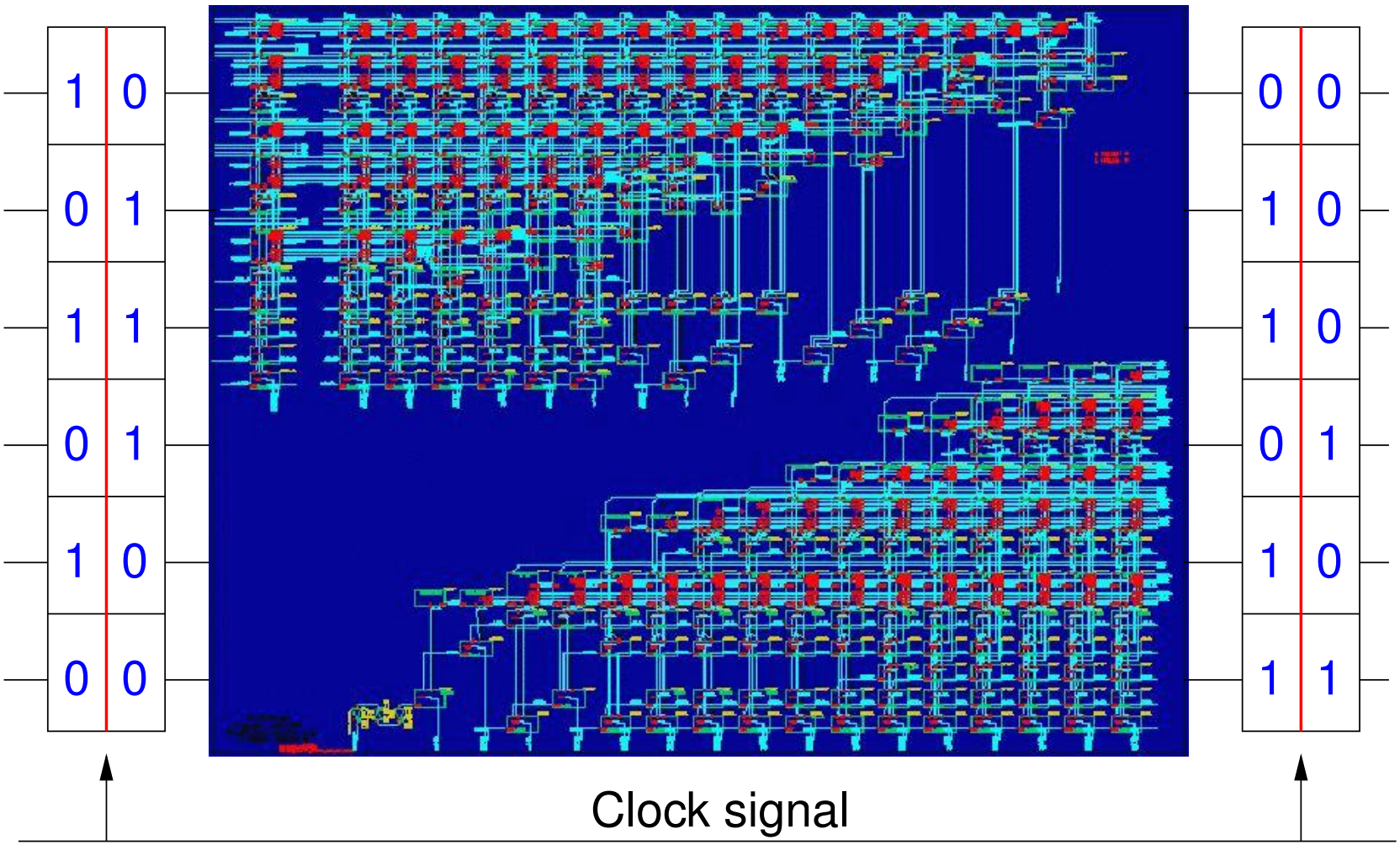

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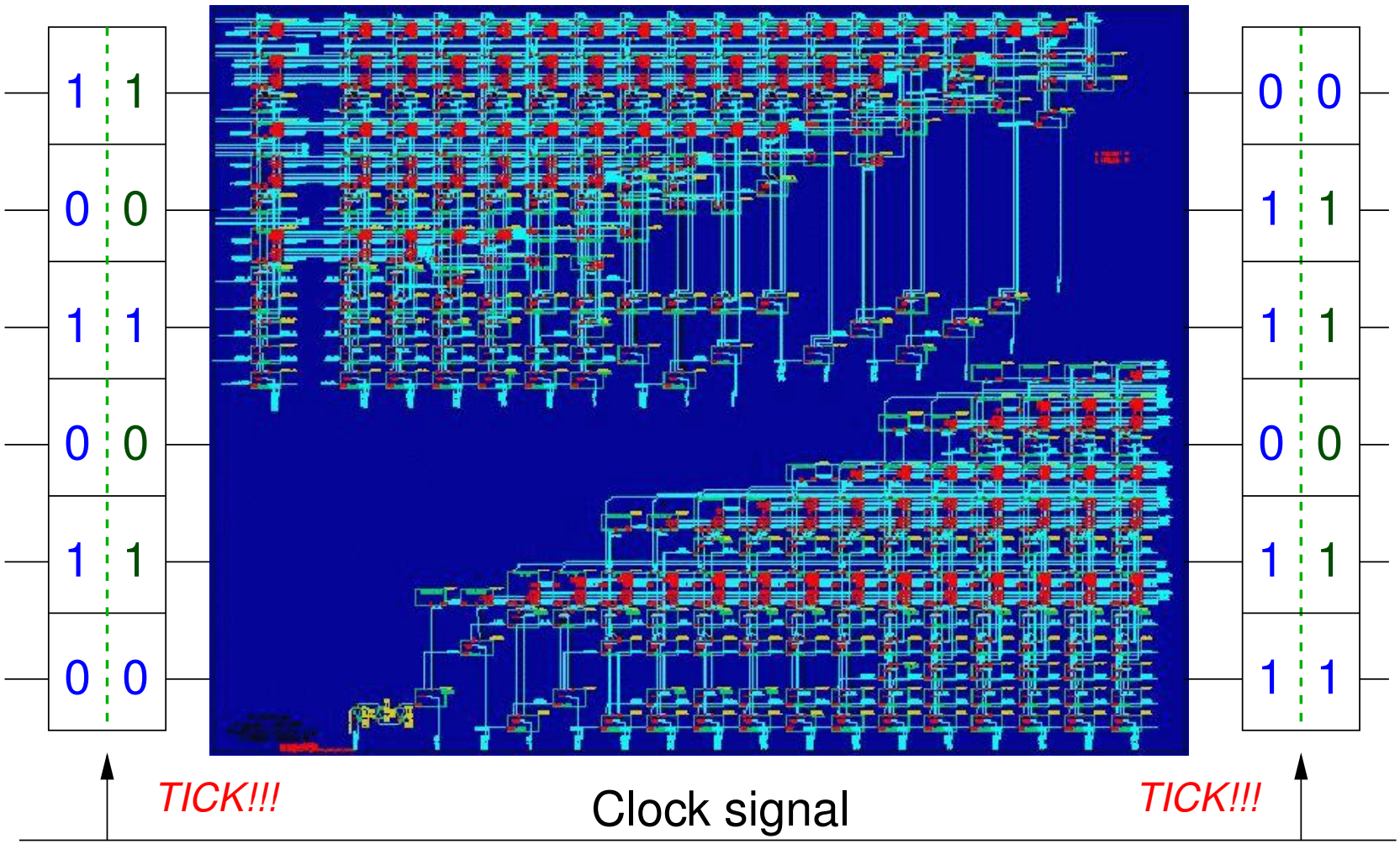

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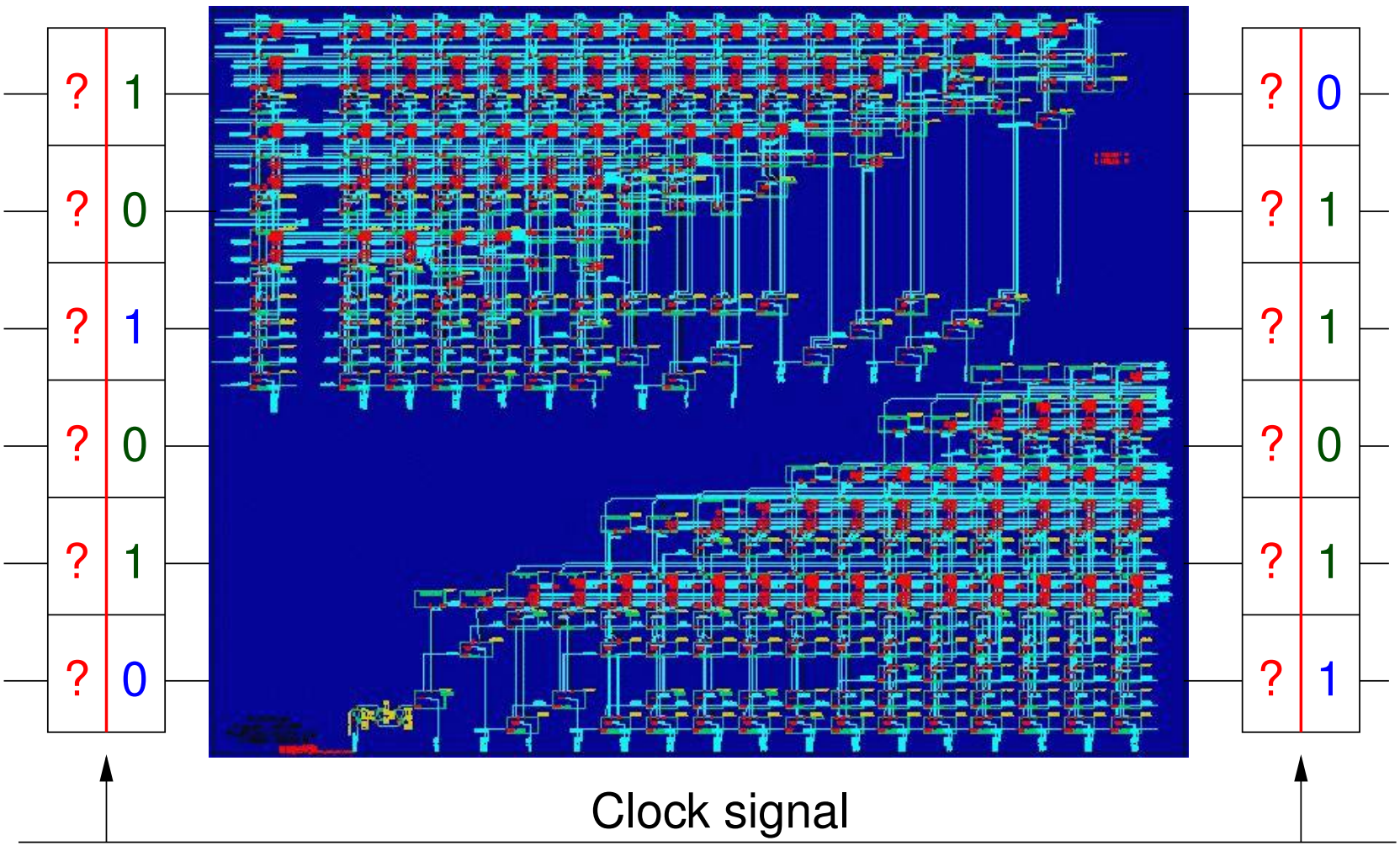

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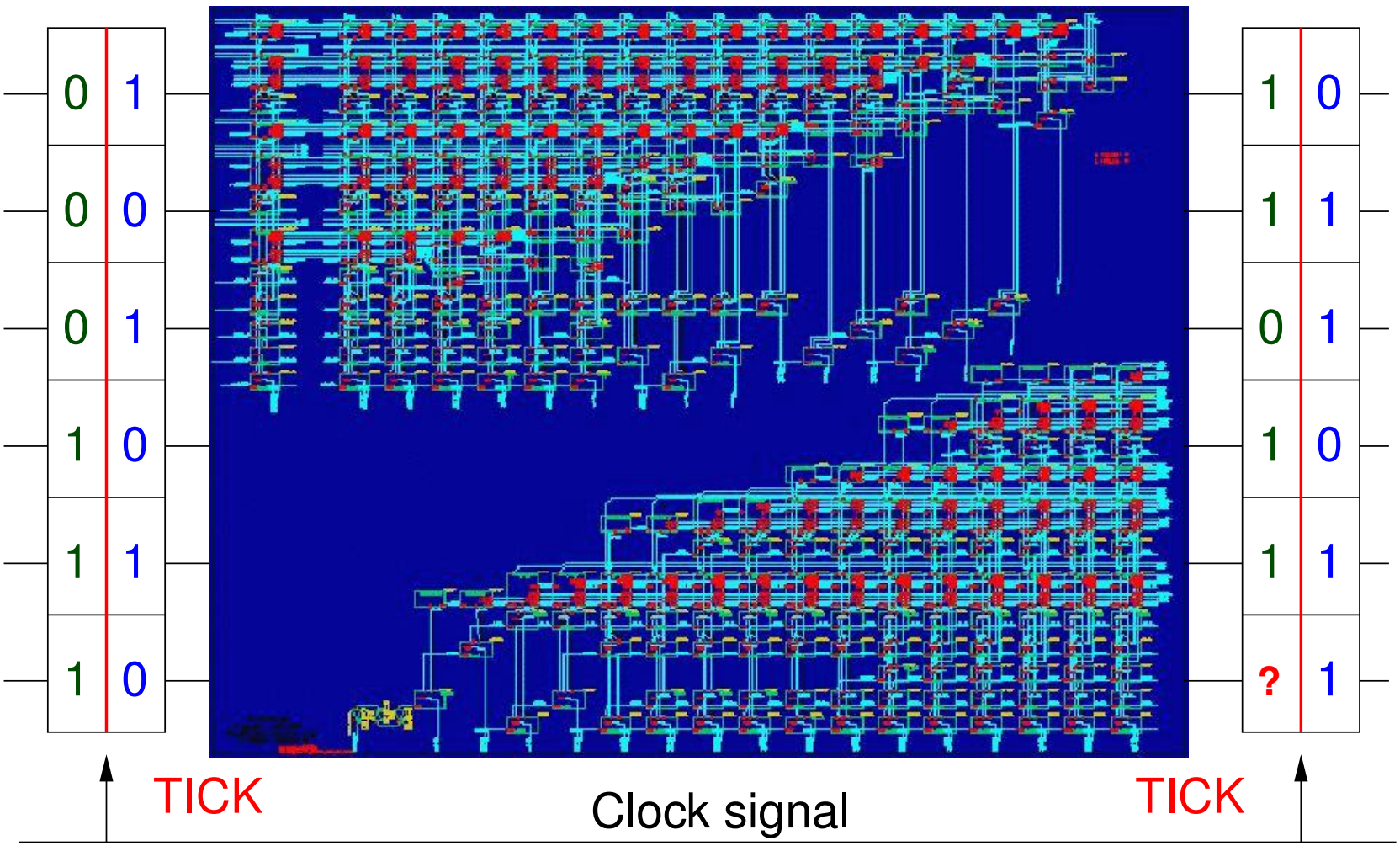


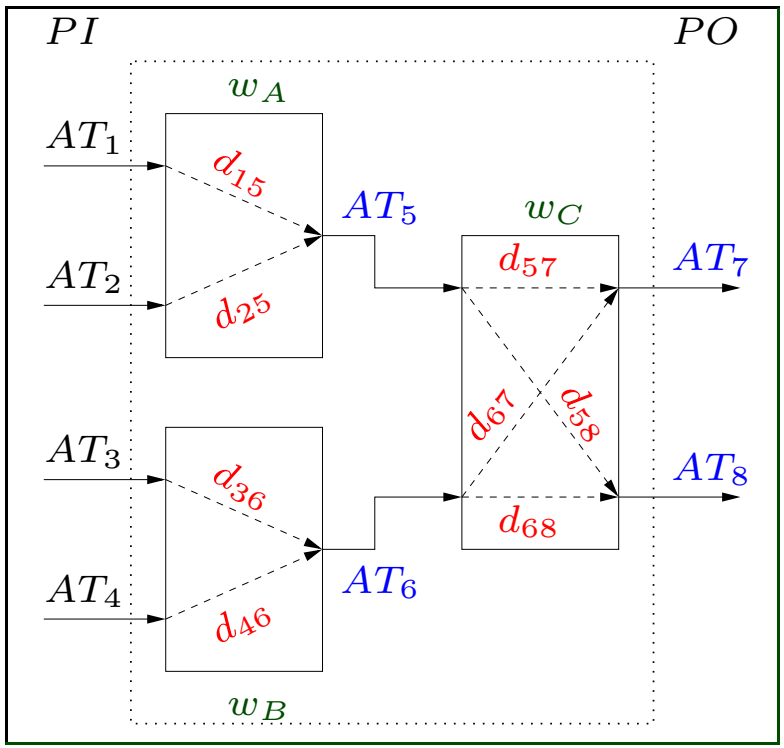
Circuit Tuning

- Stages in Chip Design (iterative)
  - Logic/Functional (boolean)
  - Schematic tuning
  - Physical design (placement/routing)
  - Extracted tuning
- Want to optimize aspects of circuit
  - Delay of signals
  - Area consumption
  - Power consumption

  by changing sizes of transistors
- Often, overall circuit too large
- Simplify circuit (smaller; fix some transistors) $\longrightarrow$ suboptimal solutions
- Currently, tuning circuits with up to 71,022 transistors (19,576 ind.)
- Strong incentive to be able to tune larger circuits in less time

Mathematical Formulation (Static Timing)

Circuit



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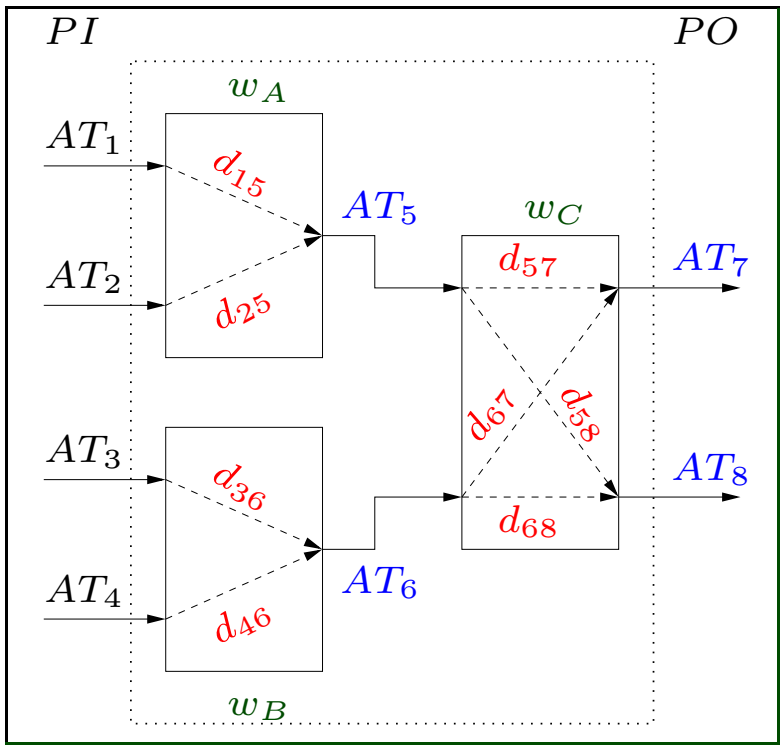

$$
\begin{aligned}
AT_5 &= \max\{AT_1 + d_{15}, AT_2 + d_{25}\} \\
AT_6 &= \max\{AT_3 + d_{36}, AT_4 + d_{46}\} \\
AT_7 &= \max\{AT_5 + d_{57}, AT_6 + d_{67}\} \\
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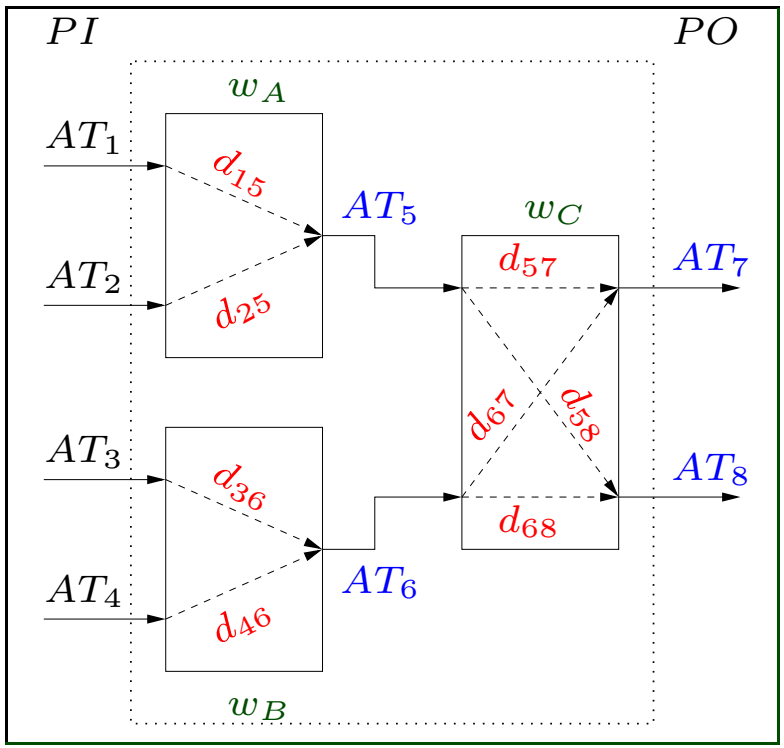

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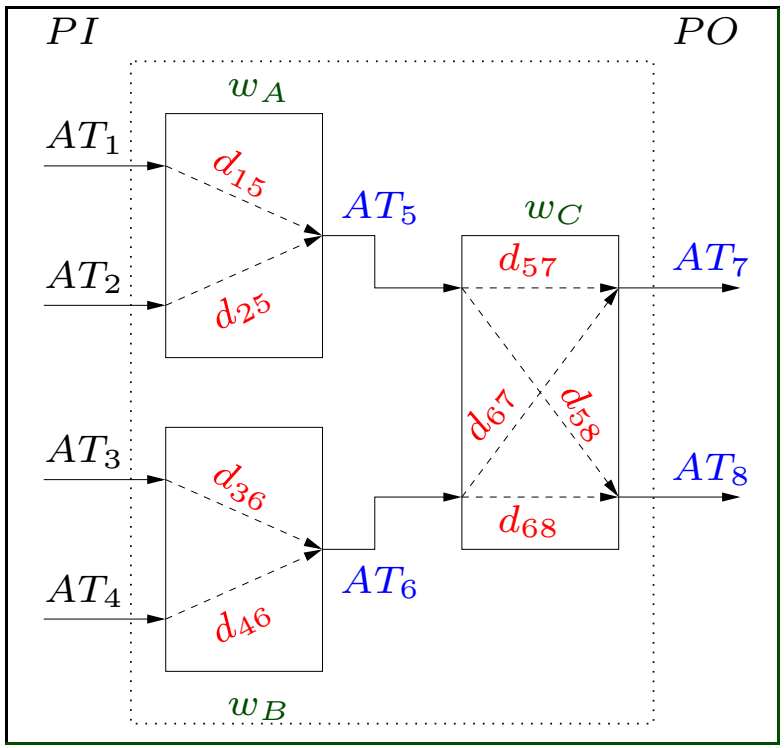

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Delays are functions of transistor widths:

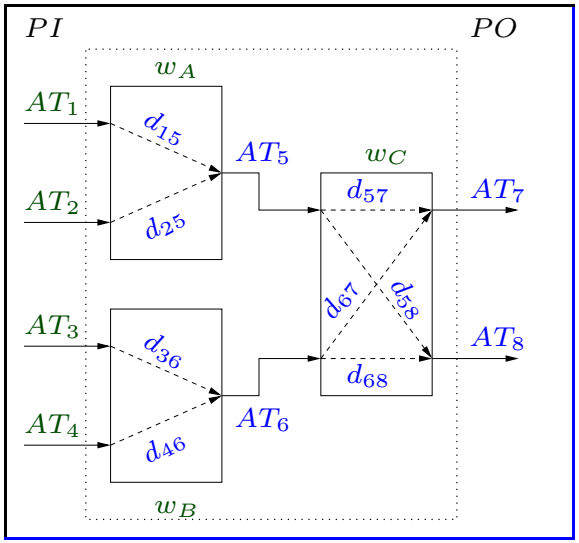
$$d_{ij} = d_{ij}(w_j, w_{\text{next}(j)})$$

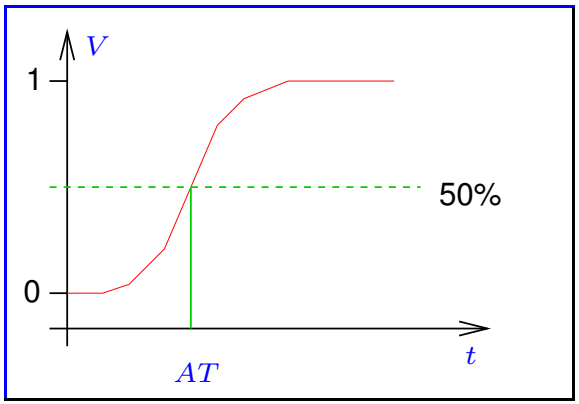
Optimization Problem (Delay Minimization)

$$\min_{AT,w} \quad \max\{AT_i \ : \ i \in PO\}$$

$$s.t. \quad AT_j = \max\{AT_i + d_{ij}(w_j, w_{\text{next}(j)}) \ : \ i \in \text{input}(j)\}$$

$$w_{\min} \leq w \leq w_{\max}$$





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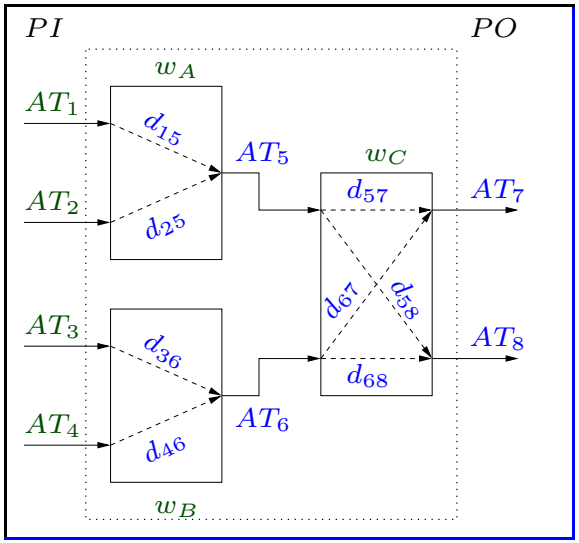

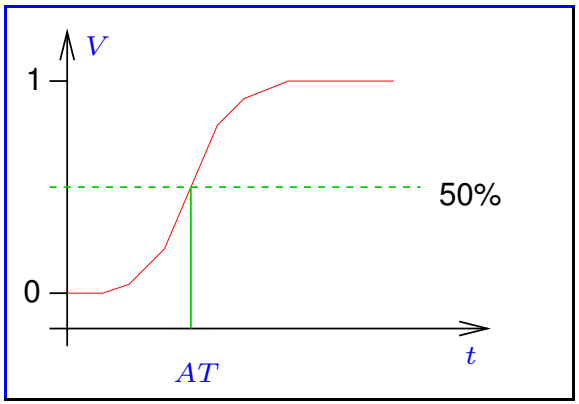

$$\min_{x} \quad \max_{i} f_i(x)$$

$\longrightarrow$

$$\min_{x,z} \quad z$$

$$s.t. \quad z \geq f_i(x) \quad \forall i$$

Optimization Problem (Delay Minimization)

$$\min_{AT,w\ ,z} \quad z$$

$$s.t. \quad z \geq AT_i \qquad i \in PO$$

$$AT_j \geq AT_i + d_{ij}(w_j, w_{\mathsf{next}(j)}\ ) \qquad i \in \mathsf{input}(j)$$

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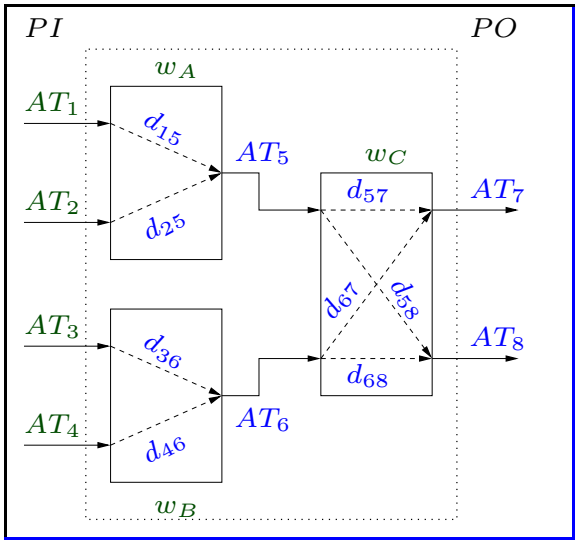

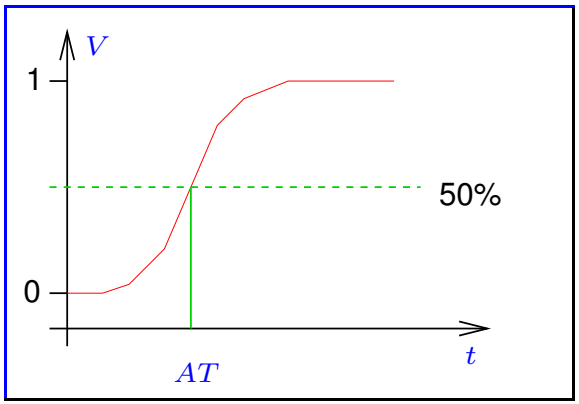

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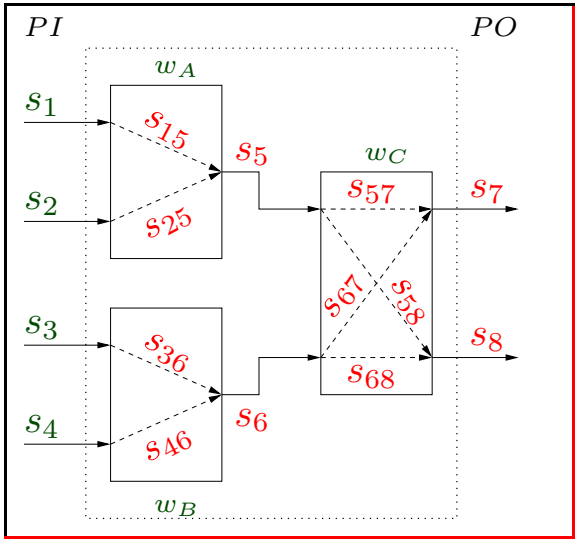

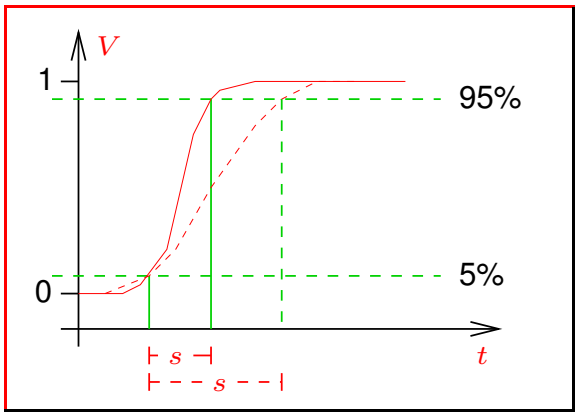

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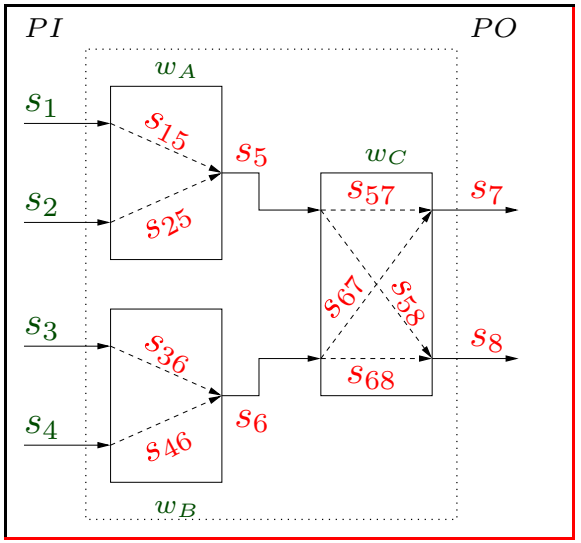
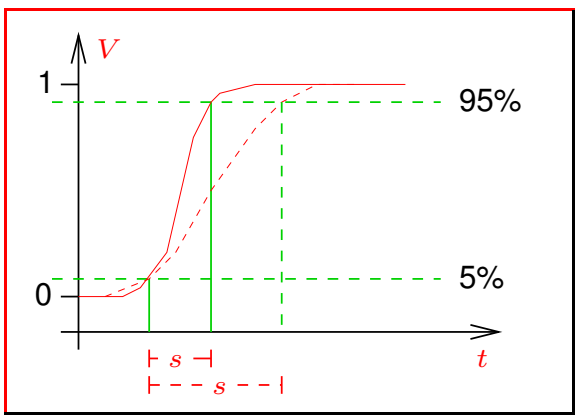
$$\sum A_i w_i \leq A_{\max}$$

$$C_i(w) \leq C_i^{\max} \qquad i \in PI$$

$$\beta_i^{\min} \leq \frac{w_i^{\text{PFET}}}{w_i^{\text{NFET}}} \leq \beta_i^{\max} \qquad i \in G$$

$$w_{\min} \leq w \leq w_{\max}, \qquad s_{\min} \leq s \leq s_{\max}$$





Properties of Optimization Problem

- The nonlinear functions $d_{ij}(w_i, w_{\text{next}(i)}, s_i)$ and $s_{ij}(w_i, w_{\text{next}(i)}, s_i)$ are obtained by SPECS (event driven circuit simulator) (Visweswariah)
  - Very fast compared to standard circuit simulators
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- After optimization, transistor widths are snapped to grid
  - Don't need highly accurate solution
- Many degenerate variables (AT and s in non-critical paths)
- Many variables and many degrees of freedom (n up to $736,000$)
- Computation time can be up to several days

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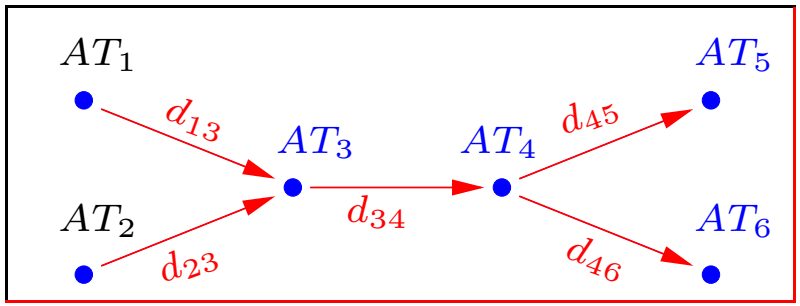
Pruning

1.



$$
\begin{aligned}
AT_3 &\geq AT_1 + d_{13} \\
AT_3 &\geq AT_2 + d_{23} \\
AT_4 &\geq AT_3 + d_{34} \\
AT_5 &\geq AT_4 + d_{45} \\
AT_6 &\geq AT_4 + d_{46}
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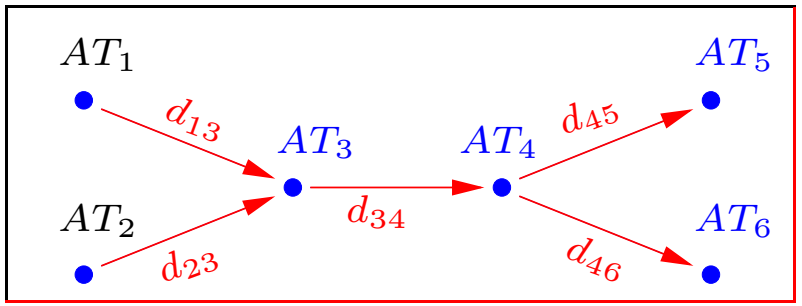

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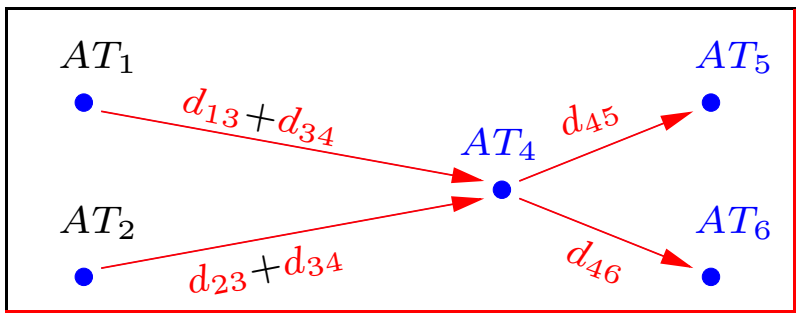

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AT_4 &\geq AT_1 + d_{13} + d_{34} \\
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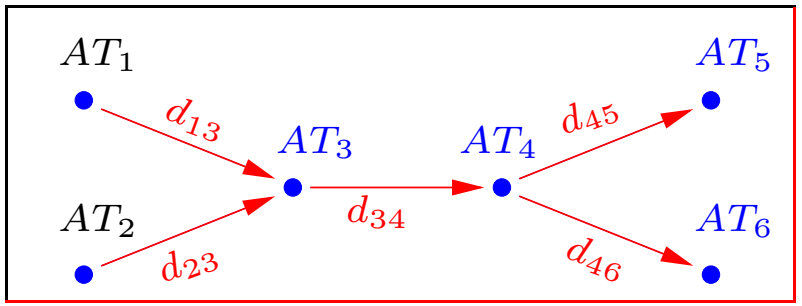

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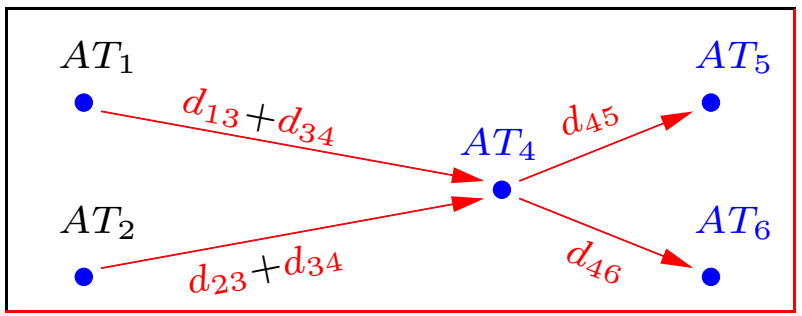

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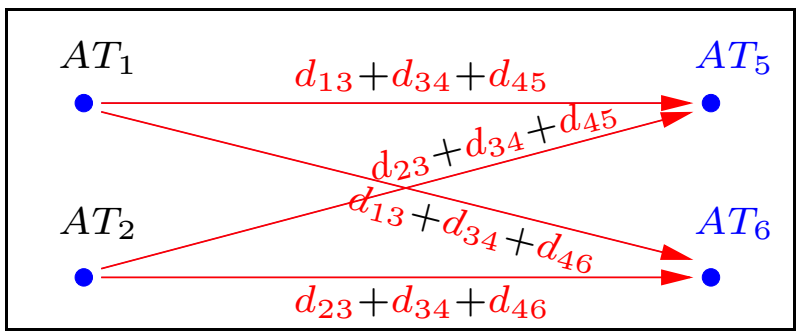

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- IBM-internal software tool for designers of custom digital circuits
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  - *Equivalent* formulation
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  - Usual reduction on large problems:
    33%↓ vars, 22%↓ cons, 1.7-4.1x↓ CPU time (Lancelot)

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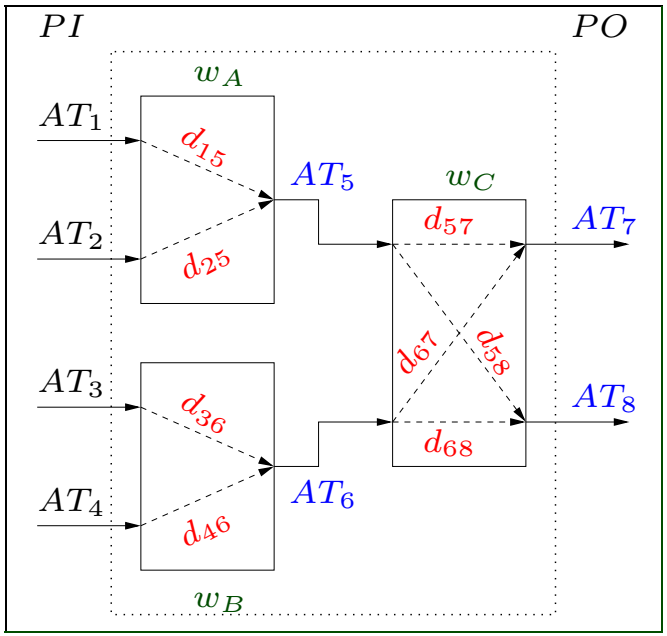
- Integration of IPOPT optimization code

Integration of IPOPT in EinsTuner



$$\min_{AT,w} \quad AT_{\text{latest}}$$

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$$AT_j \geq AT_i + d_{ij}(w_i)$$

$$\sum_i \text{Area}_i w_i \leq \text{Area}_{\text{max}}$$

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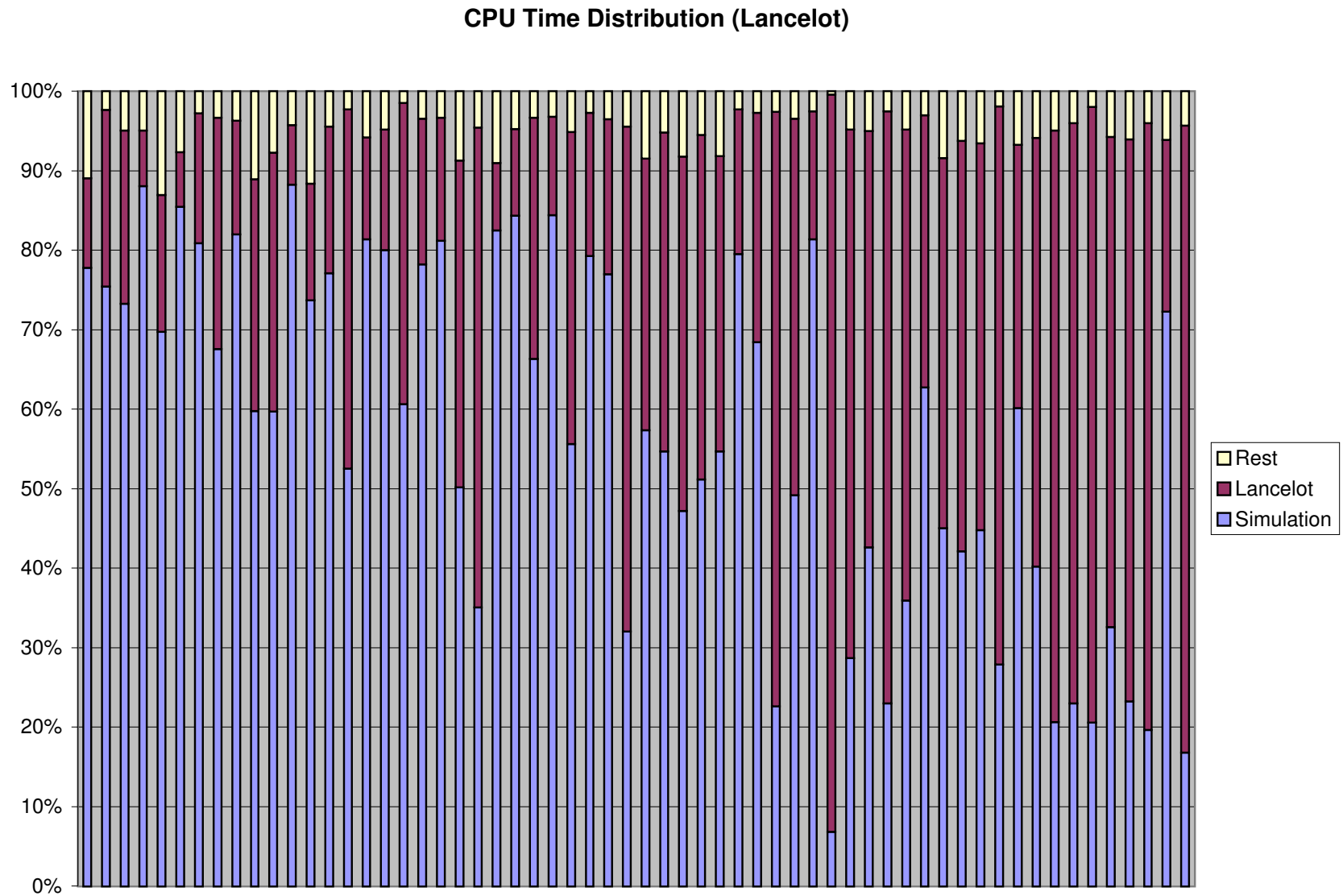
- Approximate 2nd derivatives with limited-memory BFGS
- Factorize linear system with WSMP (Gupta), a sparse direct parallel solver
- Overall faster and more robust than previous optimization engine
- Used extensively in production
- Since recently using adaptive barrier parameter strategy

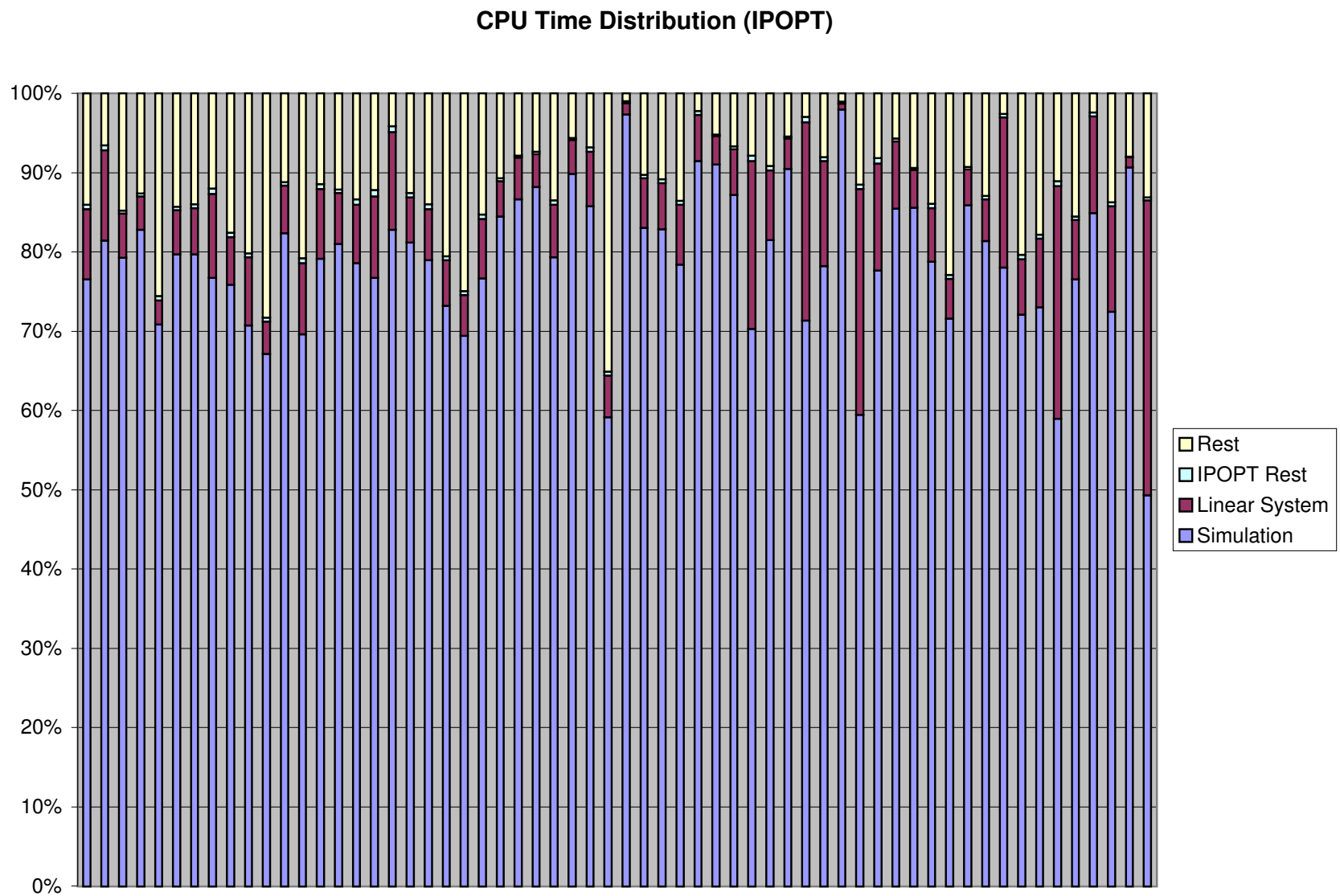
Next slide:

- 51 benchmark problems (n=1,261,. . . ,161,701)

Breakdown of CPU time — Lancelot



Breakdown of CPU time — Ipopt



Mixed-Integer Nonlinear Optimization

The CMU–IBM Bonmin Collaboration

- Goals:
  - Develop MINLP algorithms
  - Implement as open course software (as BONMIN in COIN-OR)
  - Release publicly available MINLP test set

- The Gang:

CMU

- Pietro Belotti
- Larry T. Biegler
- Gérard Cornuéjols
- Ignacio E. Grossmann
- Carl D. Laird
- François Margot
- Nick Sawaya

IBM

- Pierre Bonami
- Andrew R. Conn
- John J. Forrest
- Oktay Günlük
- Laci Ladanyi
- Jon Lee
- Andrea Lodi (U Bologna)
- Andreas Wächter

Outline

- Algorithms implemented in BONMIN
  - Branch-and-bound
  - Outer approximation
  - A hybrid approach
- Numerical comparison

- Improving branching rules for branch-and-bound
  - Variants of strong branching
- Numerical comparison

- Related and future work

Mixed Integer Nonlinear Programming

$$(P) \quad \boxed{\begin{array}{ll} \min & f(x,y) \\ s.t. & c(x,y) \leq 0 \\ & x \in \{0,1\}^n, \quad y \in \mathbb{R}^p \end{array}}$$

- If f and c linear $\Longrightarrow$ MILP
- If f and c nonlinear $\Longrightarrow$ MINLP
- If f and c convex $\Longrightarrow$ convex MINLP (focus here)

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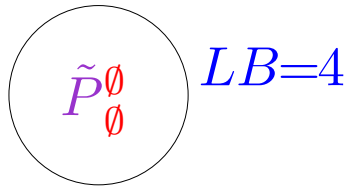
- If f and c linear $\implies$ MILP
- If f and c nonlinear $\implies$ MINLP
- If f and c convex $\implies$ convex MINLP (focus here)

$$(\tilde{P}^{\mathcal{U}}_{\mathcal{D}}) \quad \begin{array}{ll} \min\limits_{x\in[0,1]^n, y\in\mathbb{R}^p} & f(x,y) \\ s.t. & c(x,y) \leq 0 \\ & x_{\mathcal{D}} = 0, \quad x_{\mathcal{U}} = 1 \end{array}$$

$\mathcal{D},\mathcal{U} \subseteq \{1,\ldots,n\}$ with $\mathcal{D} \cap \mathcal{U} = \emptyset$ (partially relaxed/fixed continuous subproblem)

$$\mathcal{D} \subseteq \bar{\mathcal{D}}, \mathcal{U} \subseteq \bar{\mathcal{U}} \implies OPT(\tilde{P}^{\mathcal{U}}_{\mathcal{D}}) \leq OPT(\tilde{P}^{\bar{\mathcal{U}}}_{\bar{\mathcal{D}}})$$

Branch & Bound Procedure



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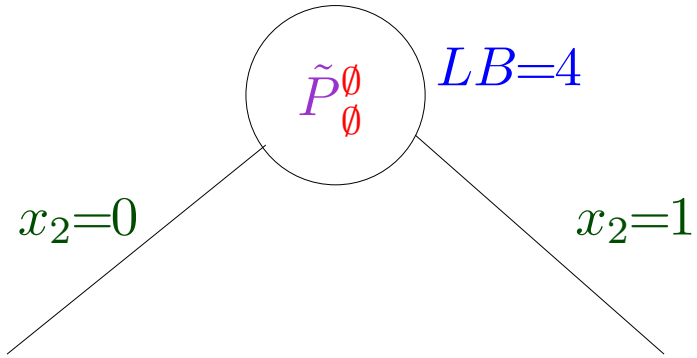

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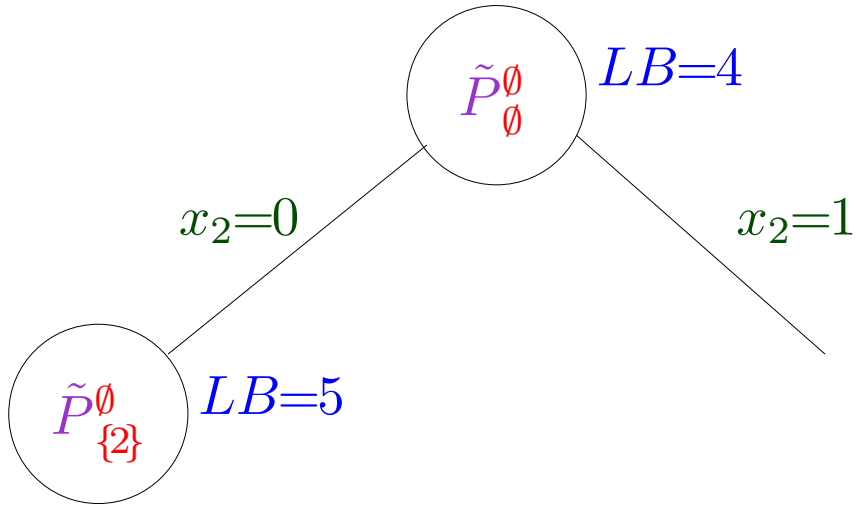

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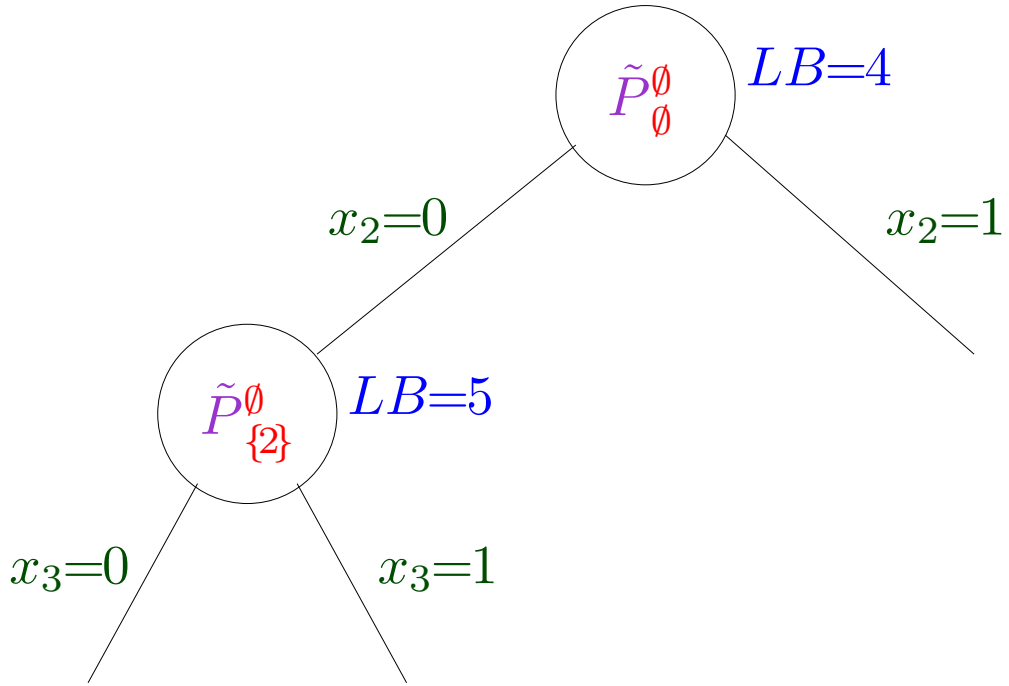

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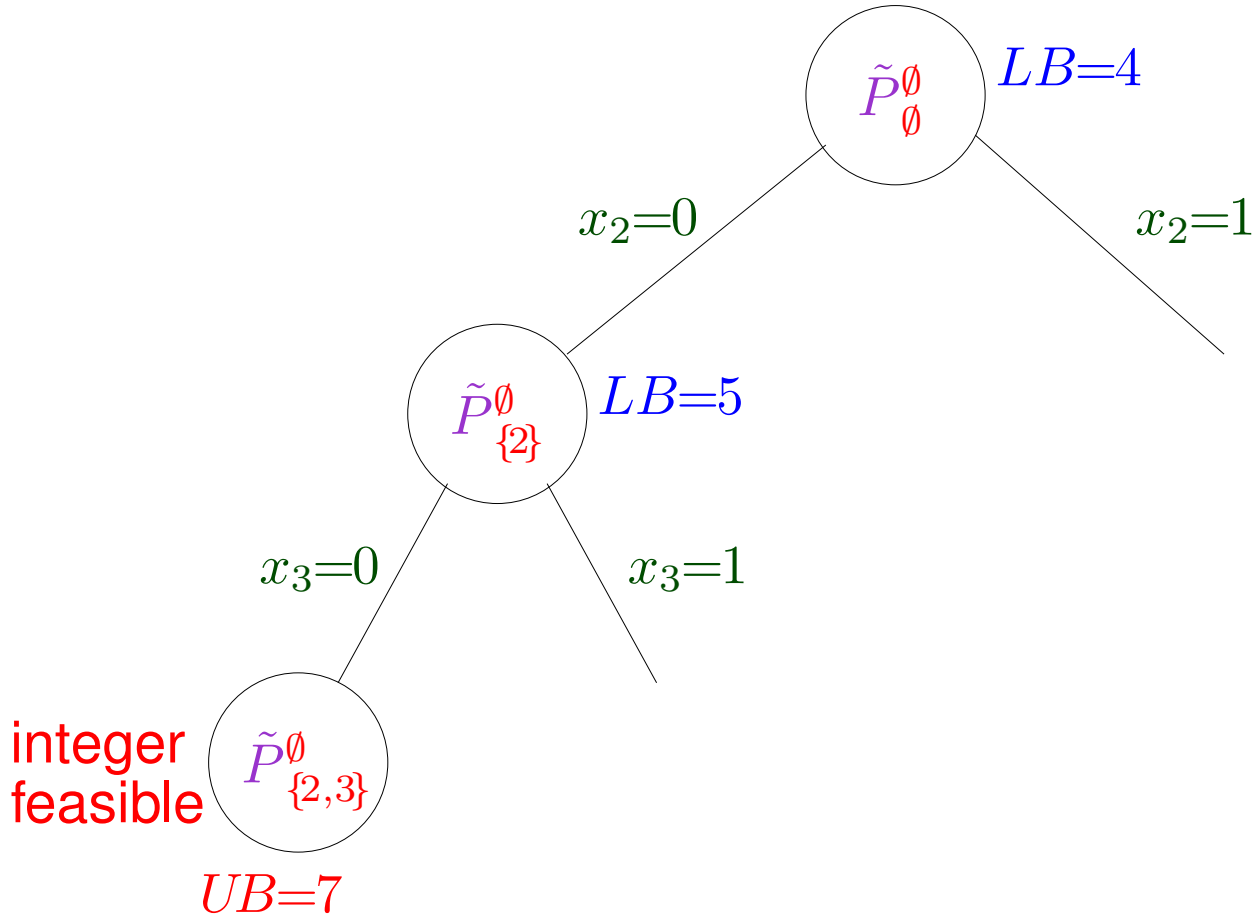

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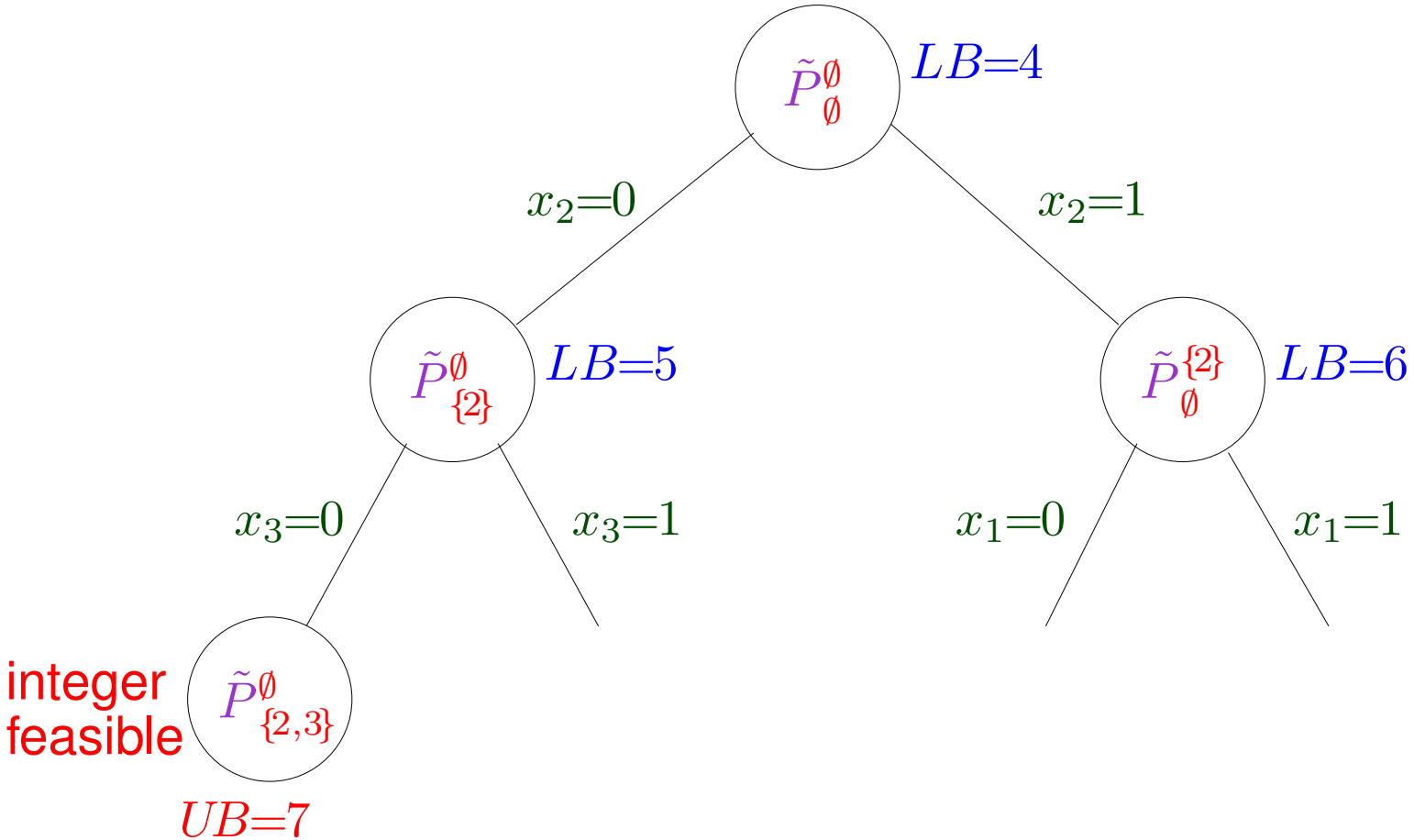

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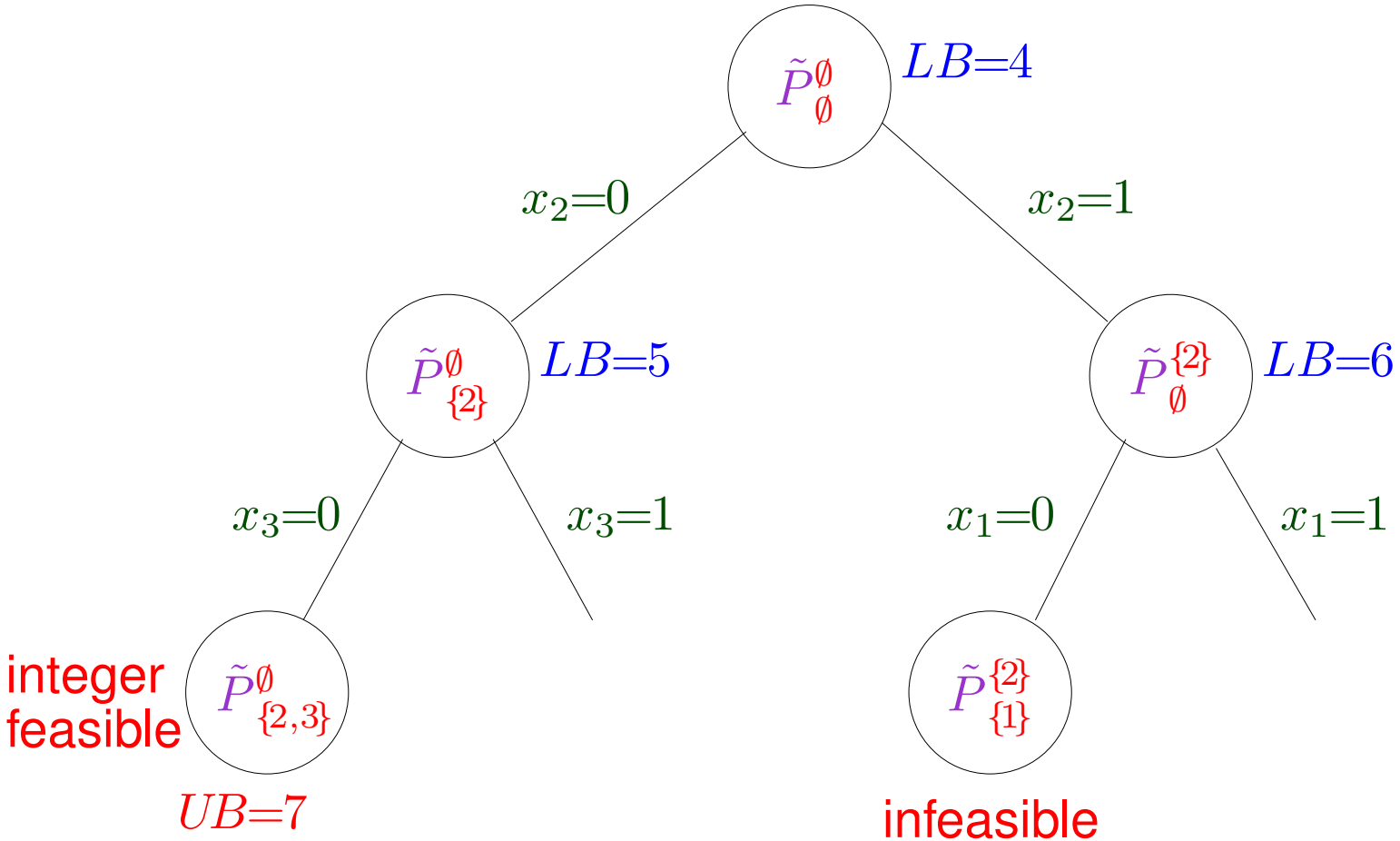

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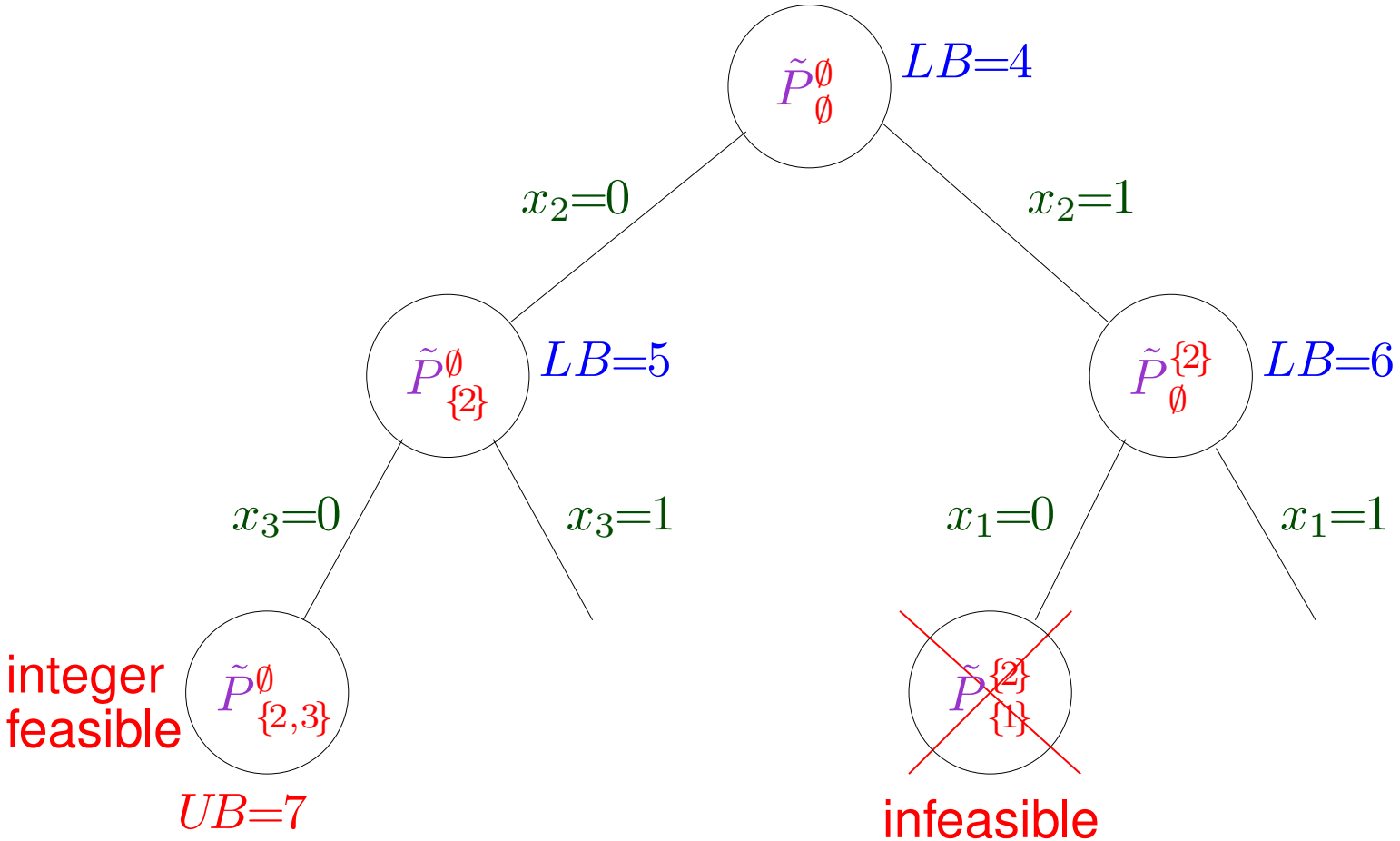

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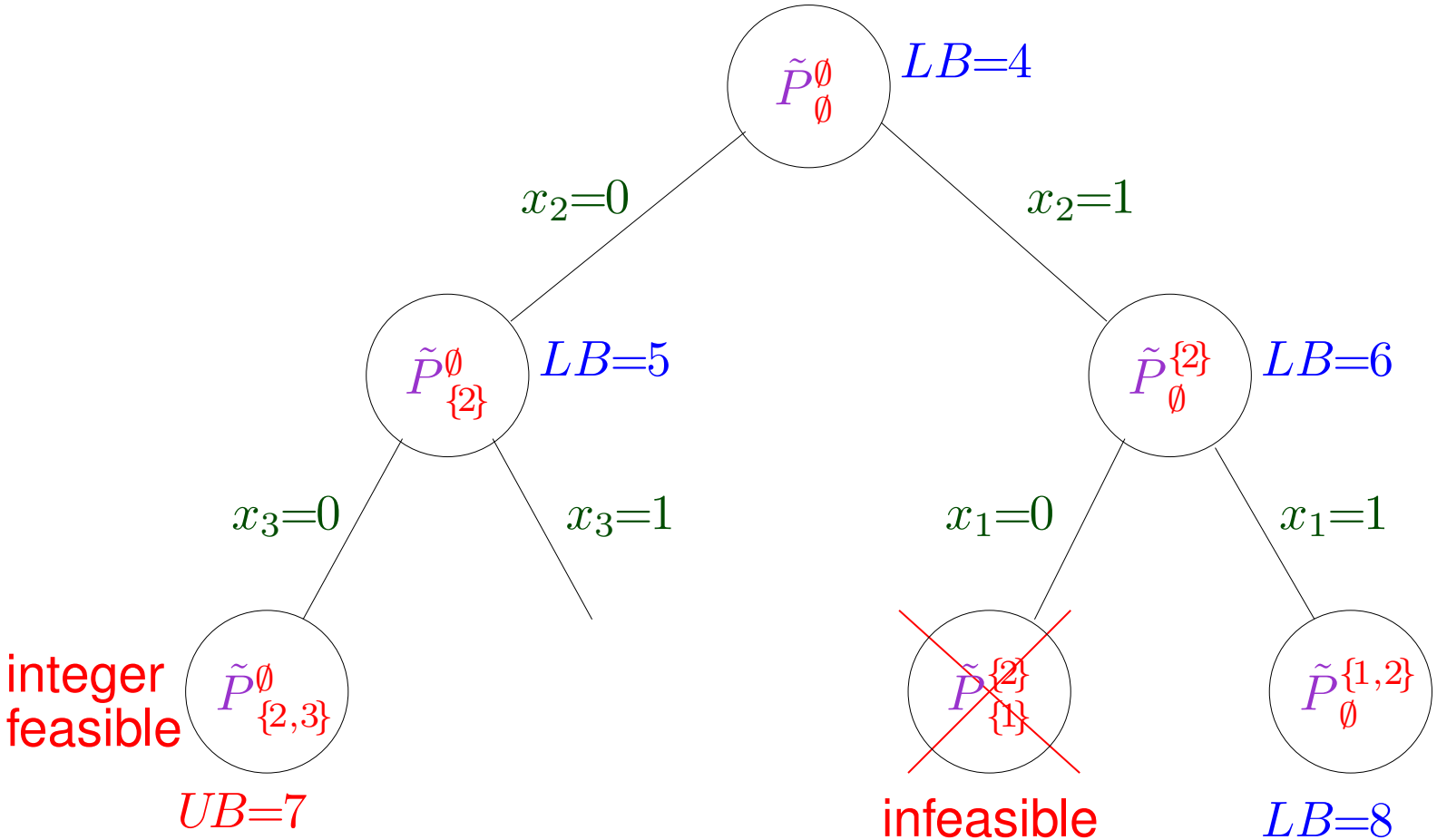

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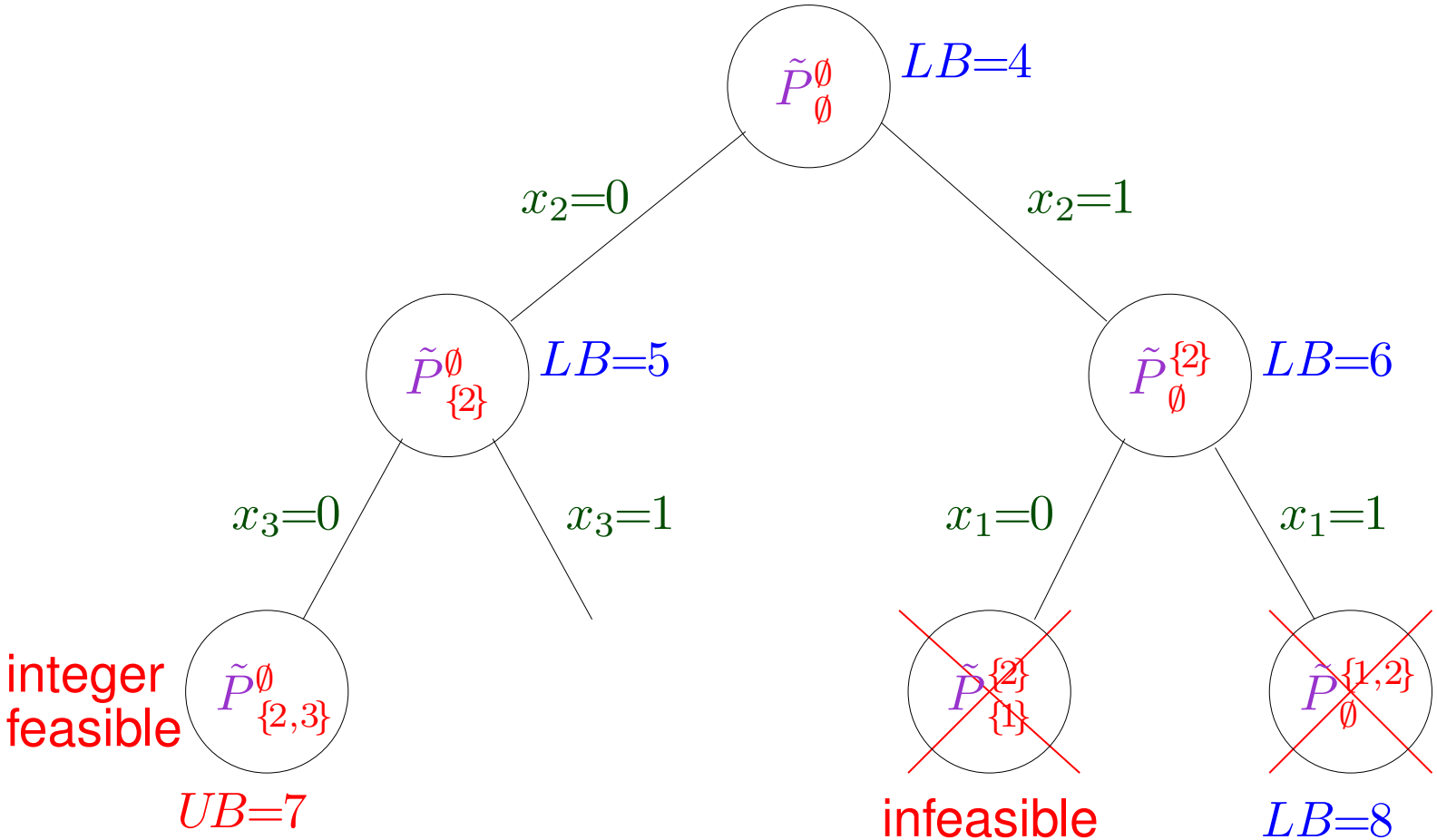

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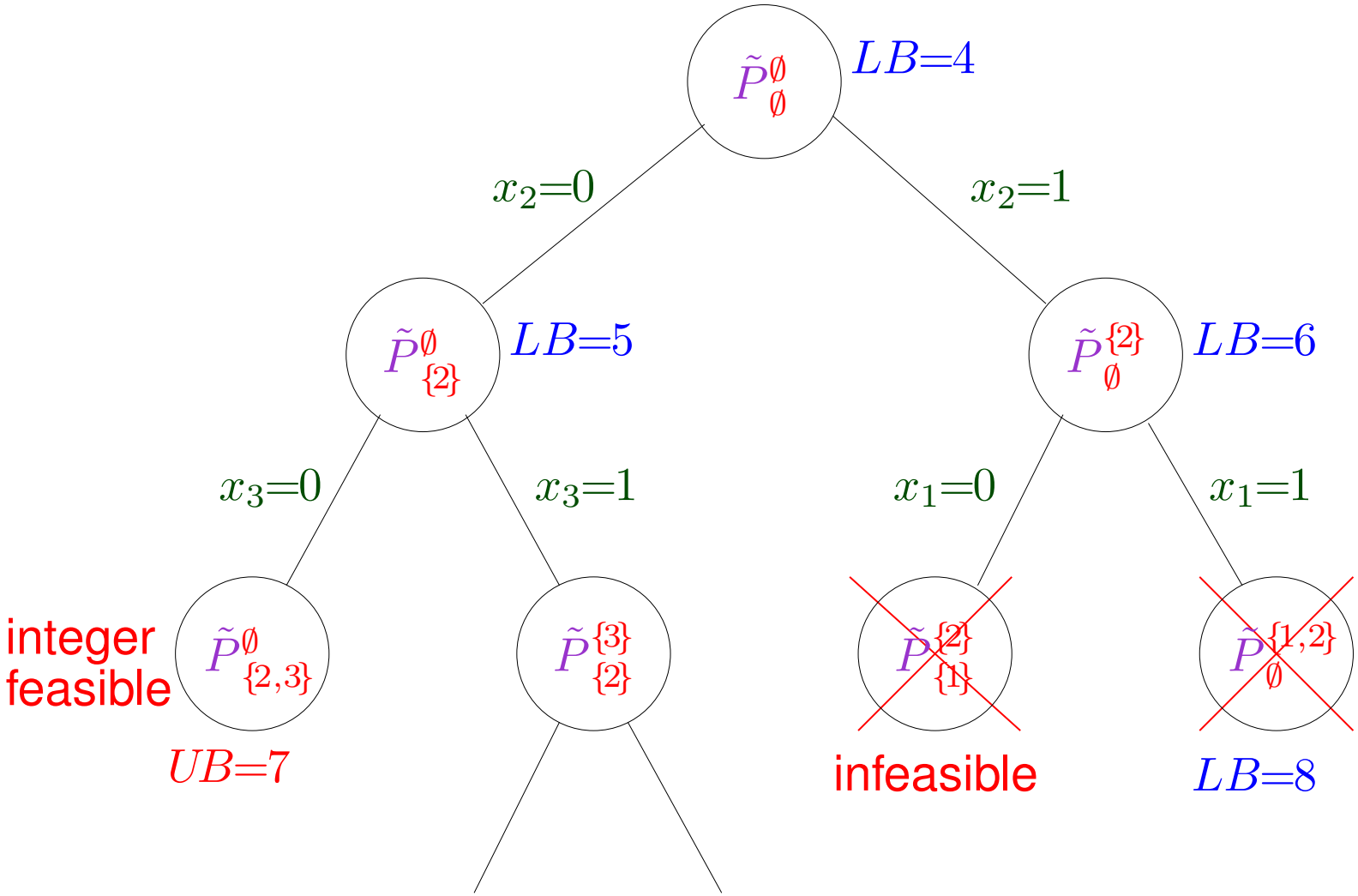

Branch & Bound

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  - Use optimal solution from parent node
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    (re-use factorization; matrices don't change)
- Different branching rules
  - Most integer-infeasible variable
  - Pseudo-costs (based on average past effect on objective function)
  - Strong branching (later)
  - ...
- Different node selection strategies
  - Depth first (quickly gives upper bounds)
  - Best bound (minimum number of nodes, wide tree)
  - ...

Difficulties in MINLP

- Algorithms in MILP well-developed
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- Complications:
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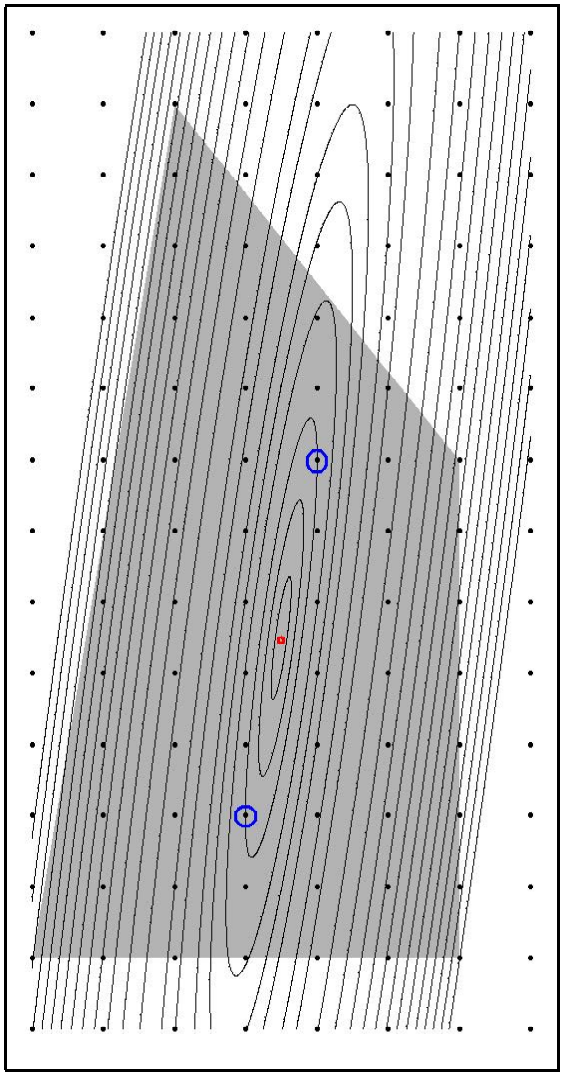
  - Even in convex case:
    optimal solution can lie in the interior;
    finding convex hull of integer feasible points not sufficient
  - MINLP solution not obtained by rounding NLP solution
  - NLP solver cannot be hot-started



Outer Approximation

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\begin{array}{lll}
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s.t. & f(x,y) \leq z & \\
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\end{array}
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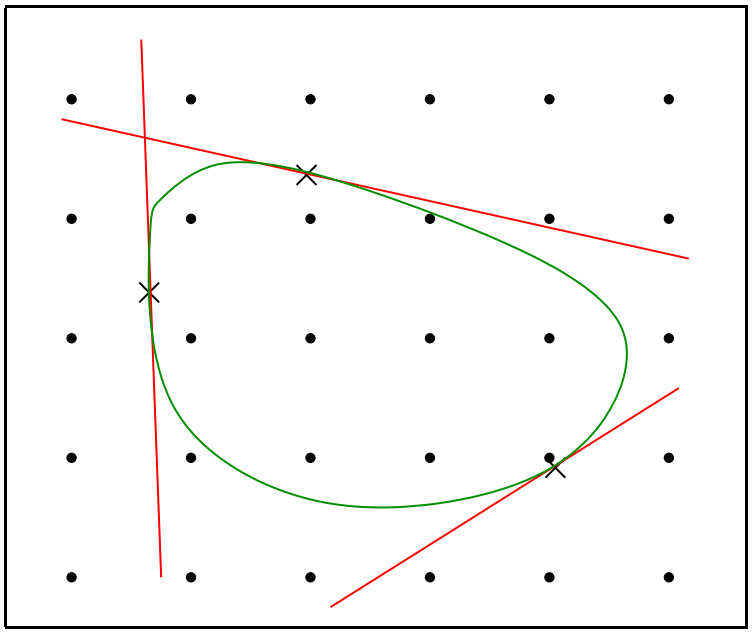
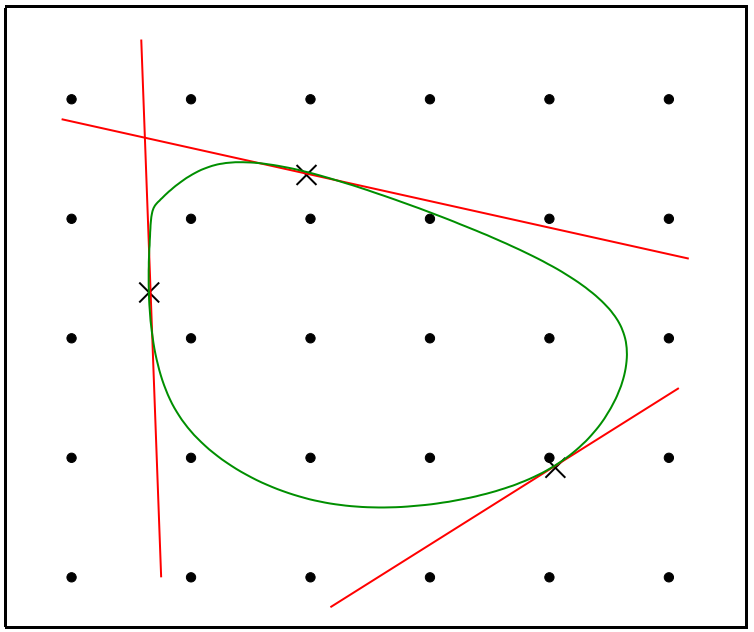
Idea: approximate by MILP (hyperplanes)



Outer Approximation

$$\begin{aligned} \min \quad & z && \text{(linear objective)} \\ s.t. \quad & f(x,y) \le z \\ & c(x,y) \le 0 \\ & x \in \{0,1\}^n, y \in \mathbb{R}^p, z \in \mathbb{R} \end{aligned}$$



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$$\begin{aligned} \min \quad & z \\ s.t. \quad & \nabla f(x^k,y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} + f(x^k,y^k) \le z \\ & \nabla c(x^k,y^k)^T \begin{pmatrix} x - x^k \\ y - y^k \end{pmatrix} + c(x^k,y^k) \le 0 \\ & \qquad\qquad \text{for all } (x^k,y^k) \in \mathcal{T} \\ & x \in \{0,1\}^n, y \in \mathbb{R}^p, z \in \mathbb{R} \end{aligned}$$

$\mathcal{T}$ contains linearization points (augmented during algorithm)

Outer Approximation Algorithm

relaxed MINLP

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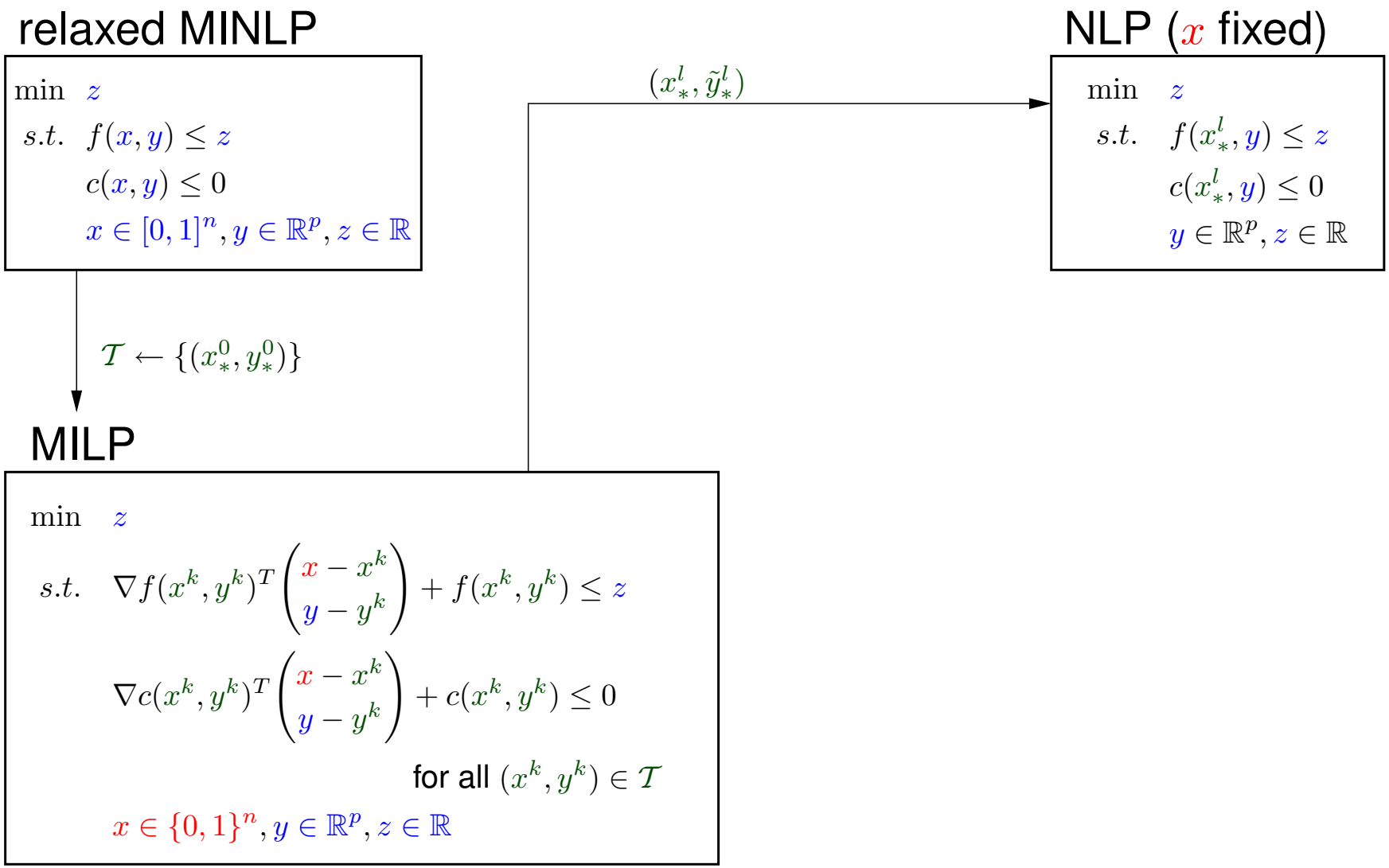

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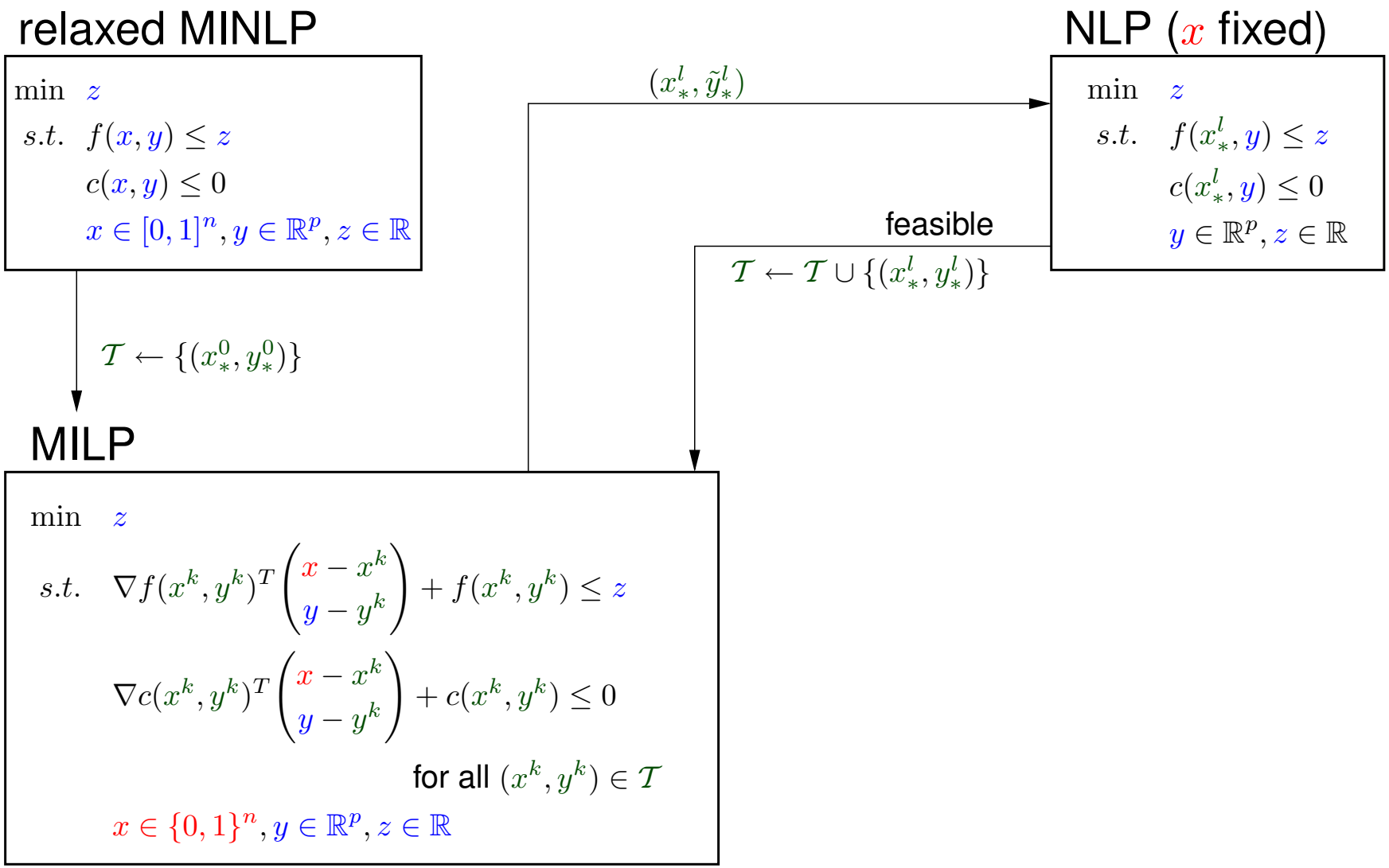

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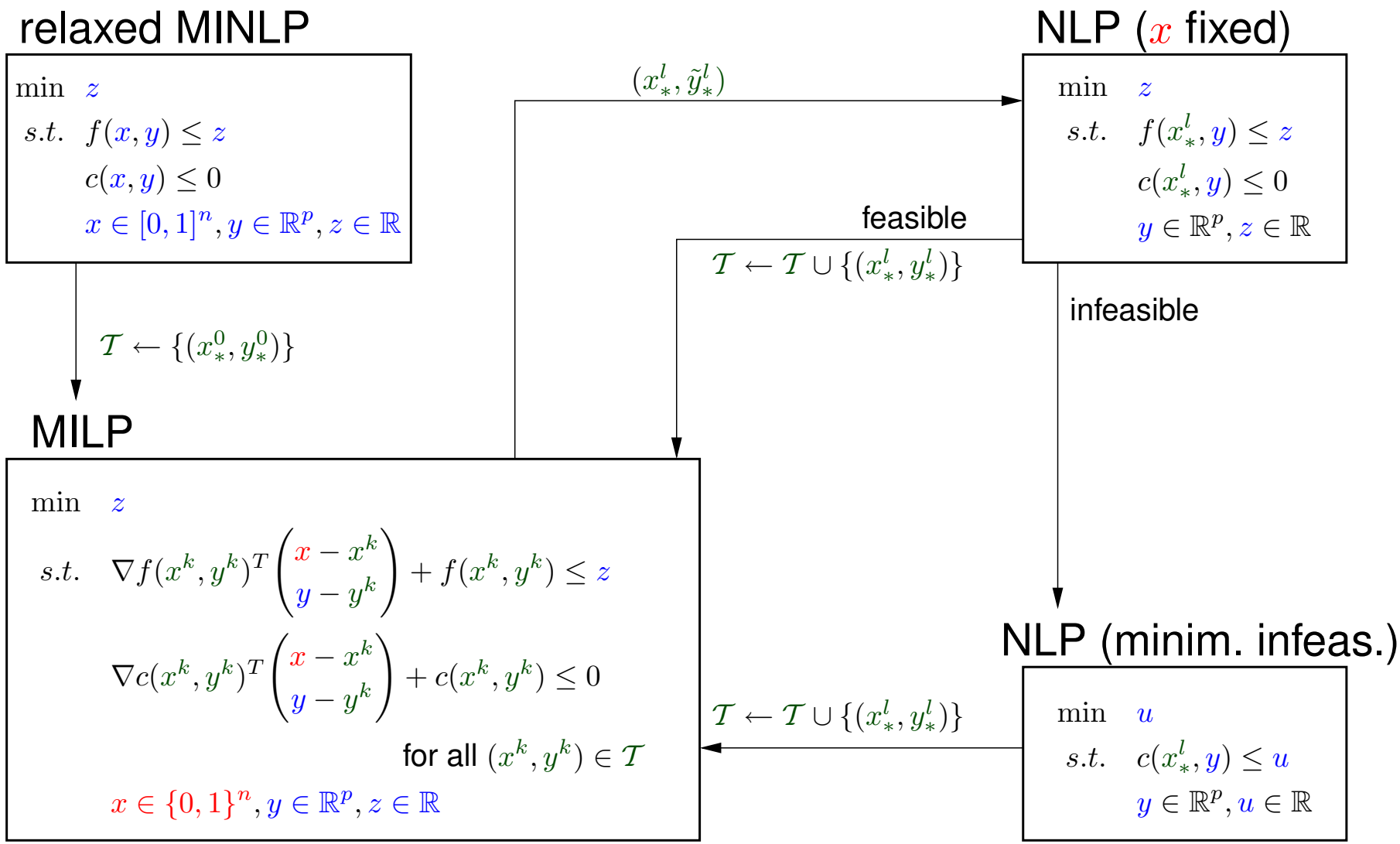

Outer Approximation Discussion

- Alternatingly solve MILPs and NLPs
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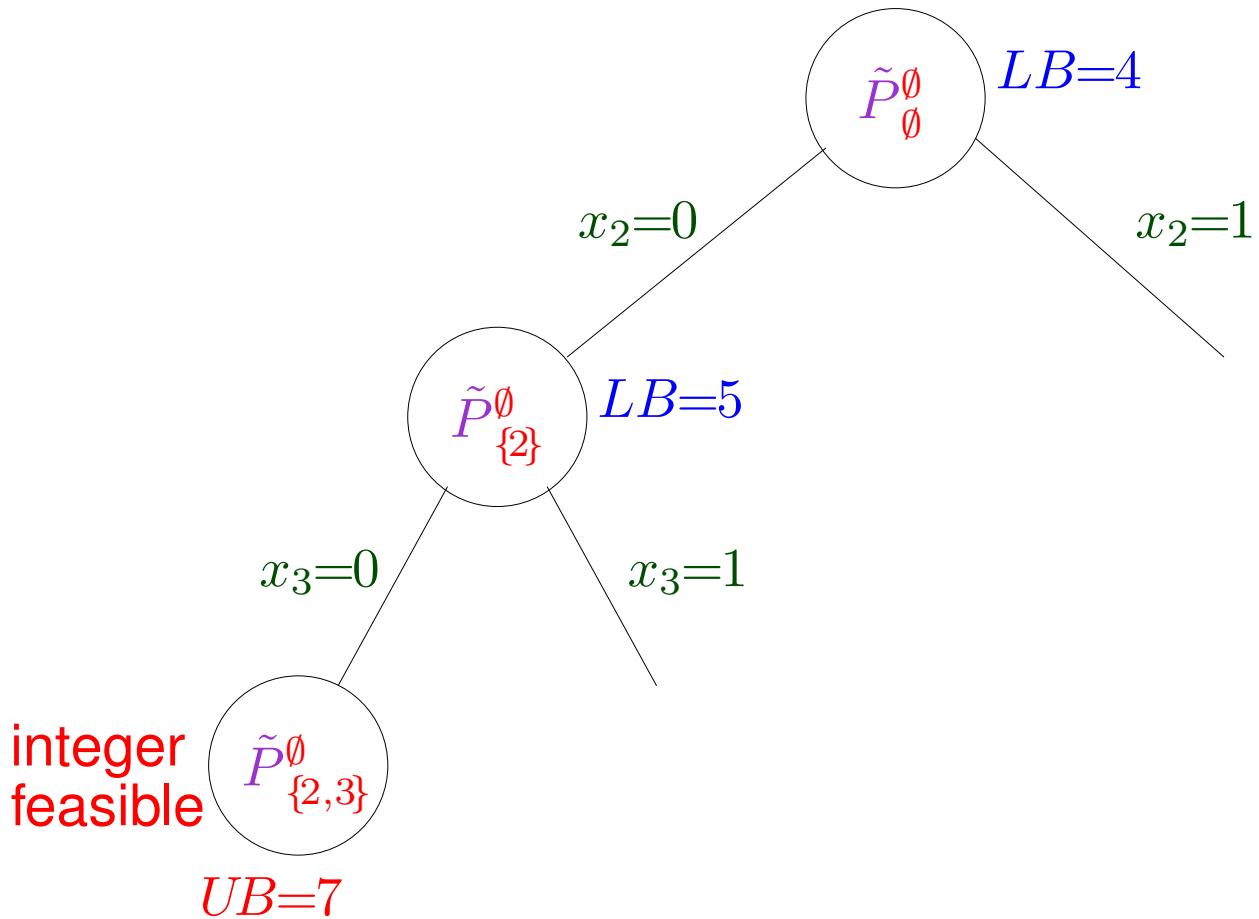
Branch & Bound Procedure



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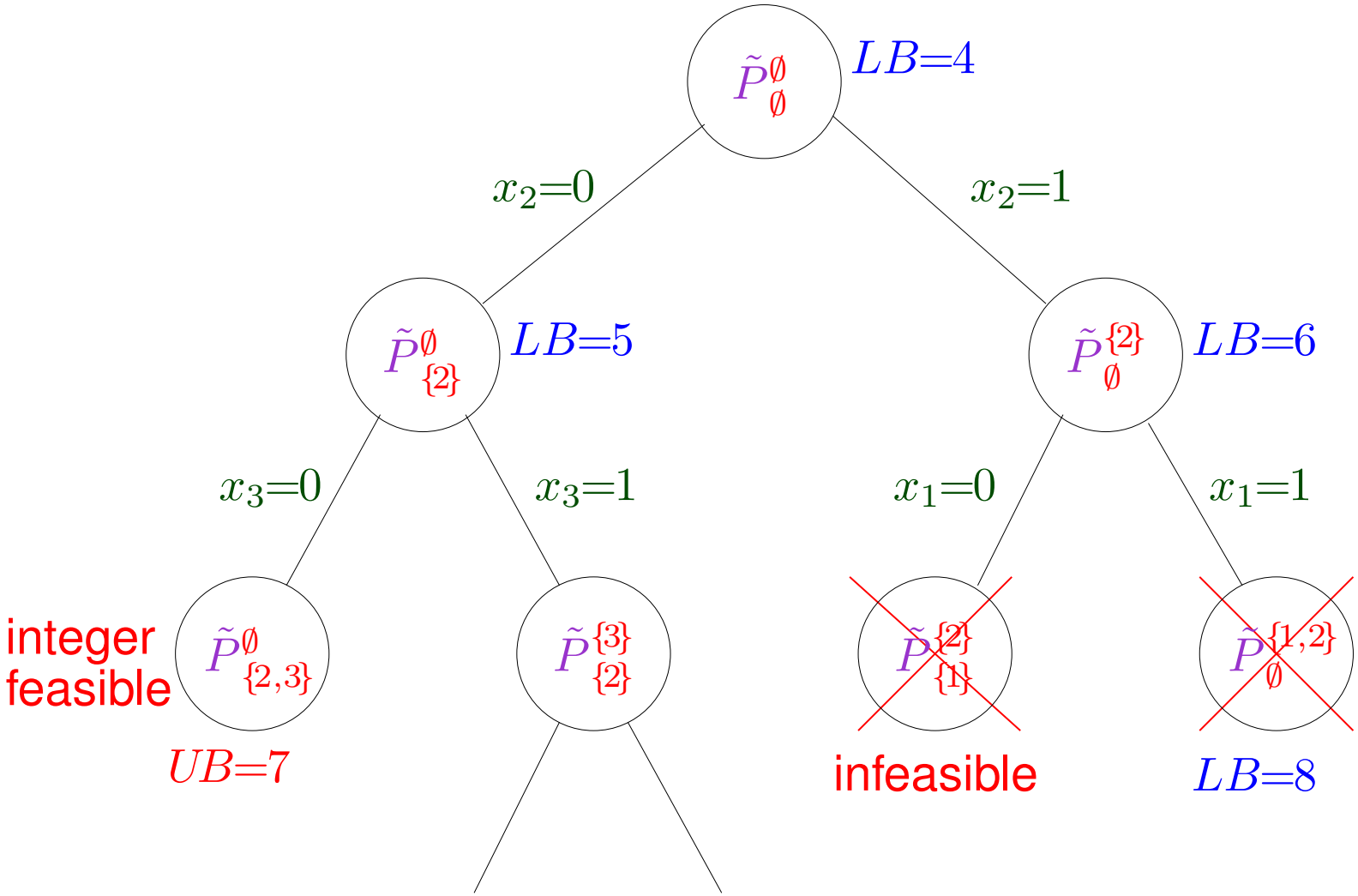
- A "hybrid" approach:
  - Solve NLPs also at nodes where only some x_i are integer
  - For example, solve partially relaxed MINLP every 10th MILP node
    - Includes information about nonlinear geometry more quickly
    - Requires solution of more NLPs
  - Includes outer approximation and branch & bound as two extremes

Branch & Bound Procedure



Bonmin

- Basic Open-source Nonlinear Mixed-INteger programming
- Implementation of MINLP algorithms
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  - `Clp`: Coin LP solver
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  - Essential for fast development: availability of open source
- Can also use Cplex as (MI)LP solver, FilterSQP as NLP solver

I-BB

- Branch and bound for MINLP
- For numerical experiments (other options implemented):
  - Branching rule: Most integer-infeasible variable
  - Search strategy: Best bound
  - Use root node solution as warm start point in nodes
    - using parent node solution didn't seem to pay off (with `Ipopt`)
    - storing parent node solutions requires a lot of memory
- If NLP solver fails
  - Try different starting point
  - Continue branching

I-OA, I-QG, and I-Hyb

- I-OA
  - Standard outer approximation algorithm
  - MILP solver: I-OA: `Cbc` ; I-OA_Cpx: `Cplex`
- I-QG
  - Quesada-Grossmann algorithm
- I-Hyb
  - Hybrid algorithm
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- Branching rule: pseudo costs with strong branching initialization
- Use cuts from `Cgl` to strengthen MILP formulation
  - Gomory, Cover, Mixed-integer rounding cuts
- Use root node solution as warm start point in NLP nodes

MINLP Test Set

- A library of currently 152 convex MINLPs
  - Existing problem from literature (layout and trimloss problems) (T. Westerlund et al.)
  - Disjunctive problems from chemical engineering formulated both with big-M and convex-hull formulation (N. Sawaya)
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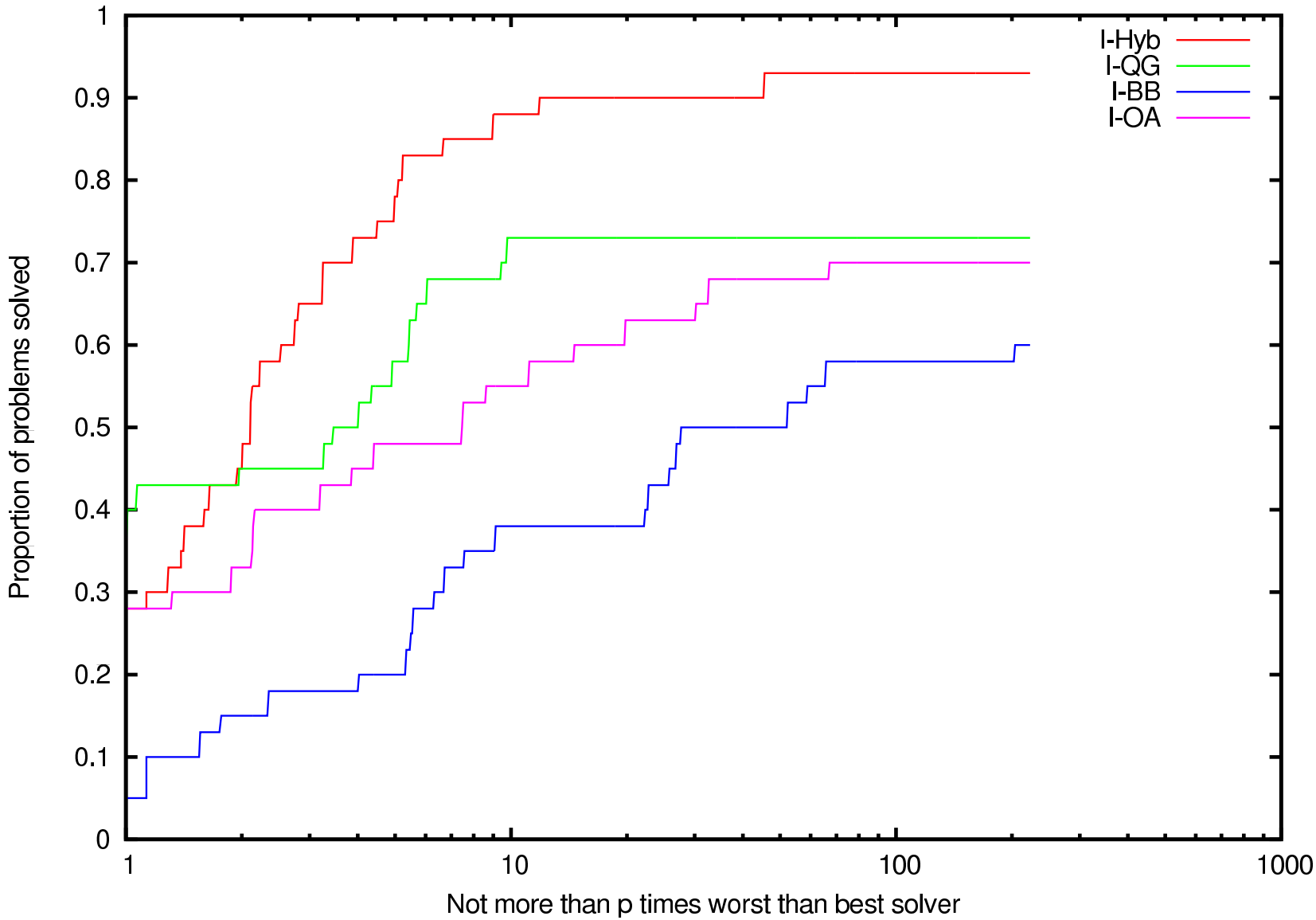
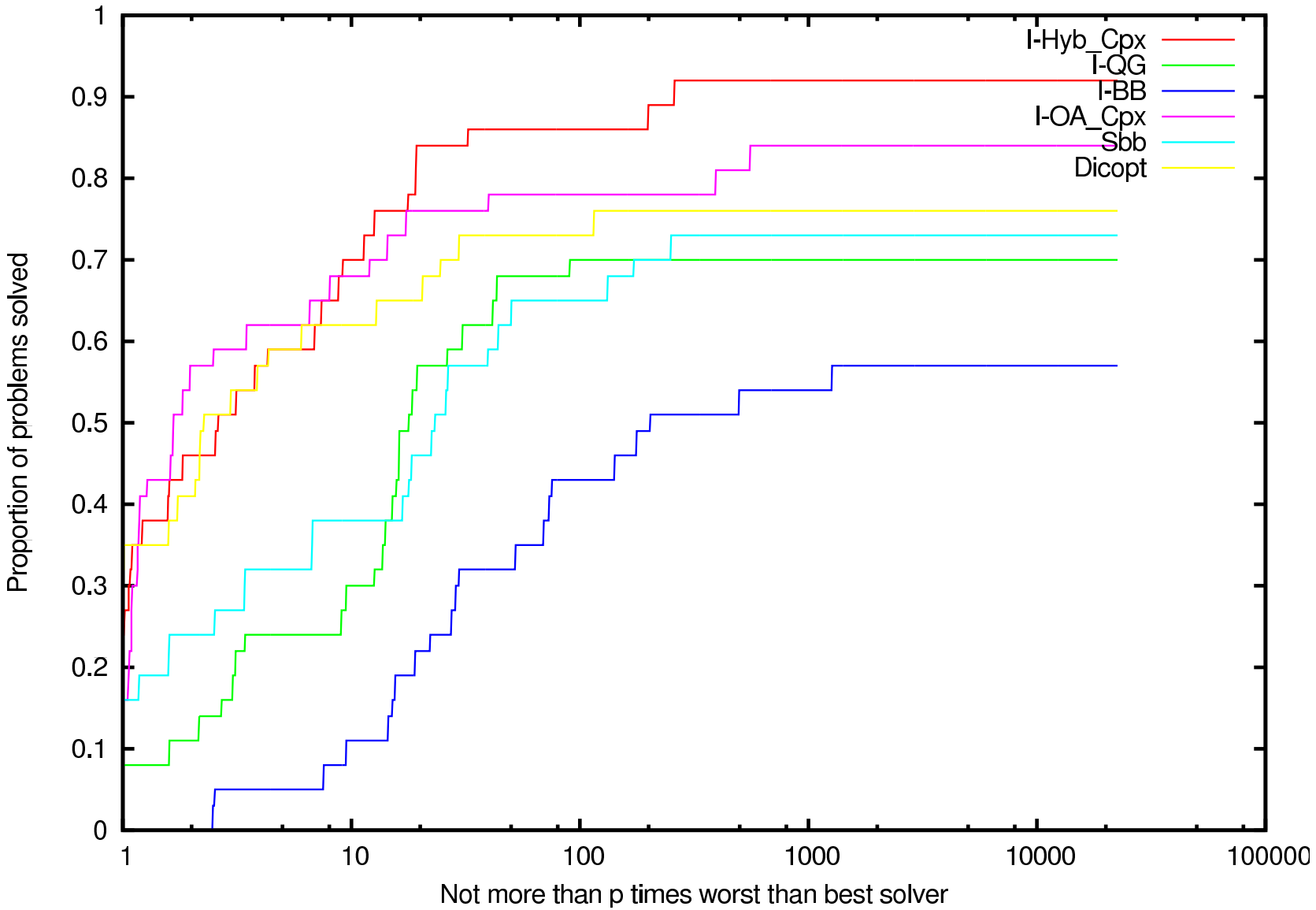
- Numerical results for 38 problems (with `Ipopt`)
  - # cont. var: 33–2720 # disc. var: 18–576 # constr: 65–4980
  - 3 hrs. CPU time limit
- Comparison of I-BB, I-OA, I-Hyb with commercial solvers
  - `SBB` (Arki Consulting & Development): Nonlinear branch and bound
    NLPs solved with `Conopt`
  - `Dicopt` (GAMS Corporation): Outer approximation
    MILPs solved with `Cplex`, NLPs solved with `Conopt`

Comparing Bonmin *Algorithms*



Comparing All Solvers



Numerical Results

- I-Hyb is most robust algorithm within time limit
- Only I-Hyb can solve `trimloss4` in 3 hrs.
- I-Hyb almost always faster than I-BB and I-OA
- I-Hyb has usually smaller enumeration tree than I-BB
- Time in `Ipopt` below 5% for I-OA, can be dominant part for I-Hyb
- Average time for NLP node: `SBB` 0.27 secs, I-BB 0.21 secs
  - Using interior point solver does not necessarily seem to be disadvantageous
- Wall clock time for `SBB` is much larger than CPU time (lots of I/O)

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Motivation:

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- Outer-approximation based algorithms difficult to modify for *nonconvex* problems
  - Linearization may cut off feasible points
  - I-BB still exact for pseudo-convex problems
- Simple I-BB heuristics for nonconvex MINLP:
  - Solve nodes for different, randomly generated starting points
  - Negative cut-off value (continue even if lower bound is larger than current best integer feasible solution)
  - Continue branching even if node is infeasible

Explore different branching rules

Most-Fractional:

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Strong Branching:

- Get list of k possible candidates $x_i \in (0,1)$
  (e.g., k most integer-infeasible)
- For each variable x_i in list:
  - Solve corresponding relaxed MINLPs $\tilde{P}_{\mathcal{D}_i}^{\mathcal{U}_i}$ (approximately)
    for $x_i = 0$ and $x_i = 1$
  - Obtain (estimate of) change in objective function
- Choose most promising candidate
  - Most change in objective function (weighted)
  - (Most integer feasible non-fixed variables)
  - If NLP for one candidate proven to be infeasible, pick this candidate.

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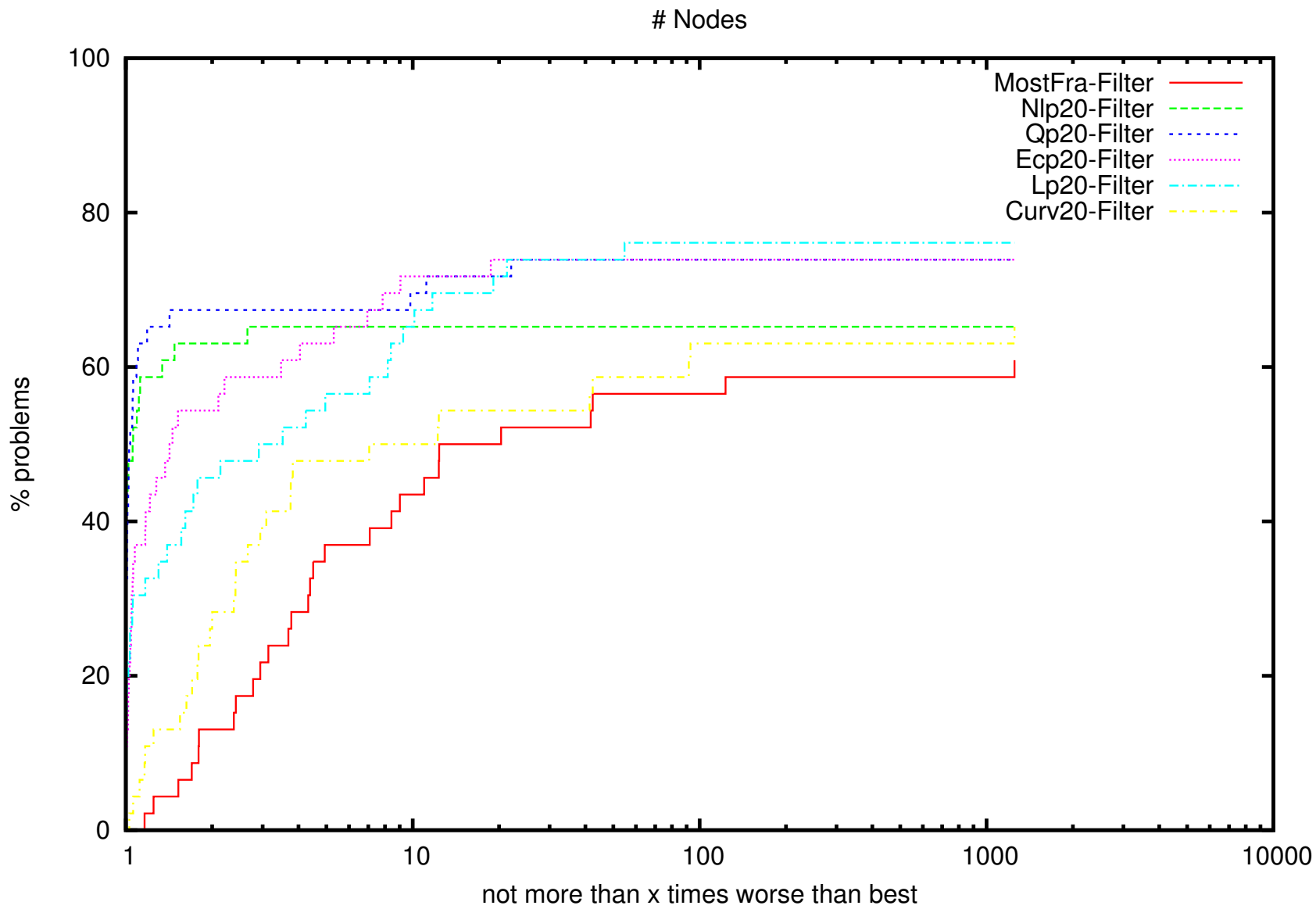
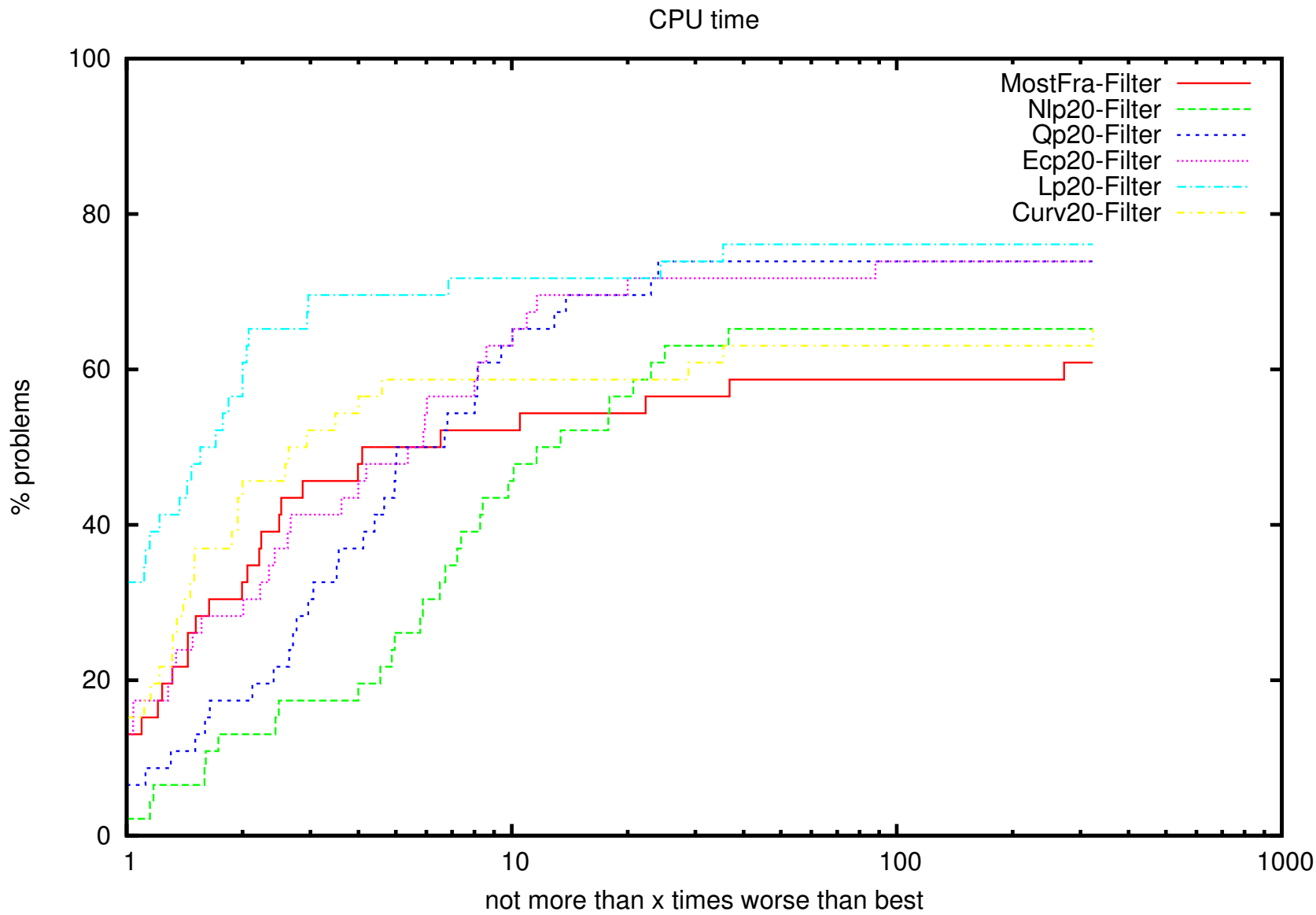
- Comparing options for 50 difficult problems (using `FilterSQP`)

Comparison Branching Options (Nodes)



Comparison Branching Options (CPU*)



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- Research for nonconvex MINLP
  - P. Belotti working on implementation of automatic convexification
  - Will be used in BONMIN for global optimization

What Did We Learn?

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- Handling inequality constraints
  - (active set) SQP methods; have trouble for large problems
  - interior point methods overcome combinatorial complexity
  - primal-dual methods combine advantages of Newton's method and globalization schemes

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- No reason to get bored yet. . .

Literature

- Books on nonlinear optimization
  - J. Nocedal and S. J. Wright: *Numerical Optimization (2nd edition)*
  - R. Fletcher: *Practical Method of Optimization*
  - S. G. Nash and A. Sofer: *Linear and Nonlinear Programming*
- Websites with optimization codes:
  - COIN-OR: `http://www.coin-or.org`
  - NEOS Guide: `http://www-fp.mcs.anl.gov/otc/Guide`
- IPOPT paper:
  - A. Wächter and L. T. Biegler: *On the Implementation of an Interior-Point Filter Line-Search Algorithm for Large-Scale Nonlinear Programming*
- BONMIN paper:
  - P. Bonami *et al.*: *An Algorithmic Framework For Convex Mixed Integer Nonlinear Programs*