Data Driven Process Engineering

Mixed Integer Programming

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Bounding Functions

Learning Objectives

- Demonstrate bounding of nonconvex functions for minimization and maximization
- Illustrate convex relaxations on exponential terms
- Illustrate McCormick relaxations for bilinear terms

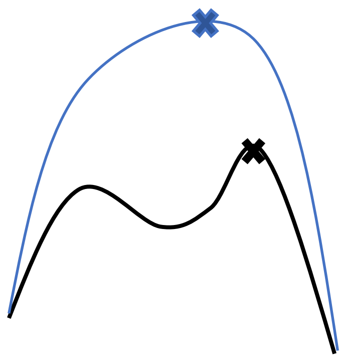
Relaxations and Bounding in Continuous Space – Max Problem

If continuous, nonlinear, non convex ???

Convex relaxation (over-estimator) of original nonconvex function.

Must bound function everywhere "from above"

Global Optimum of convex relaxation (easy to find even with local NLP)



Original max problem (non-convex)

Original global maximum

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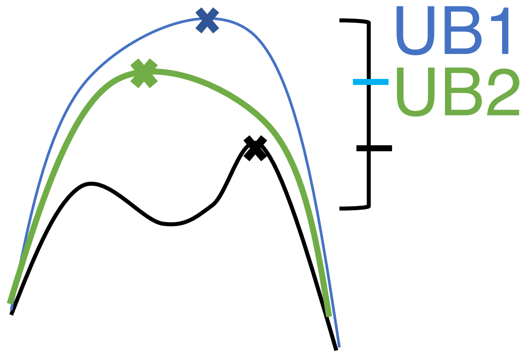
- Upper Bound 2 < Upper Bound 1



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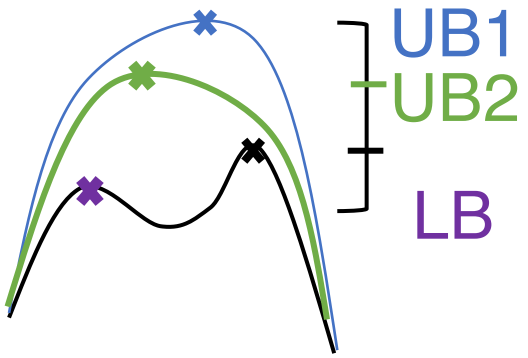

- Lower Bound:
  - Any feasible solution
  - Any local optimum

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Relaxations and Bounding in Continuous Space – Min Problem

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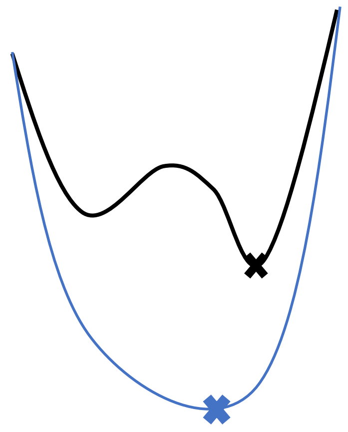

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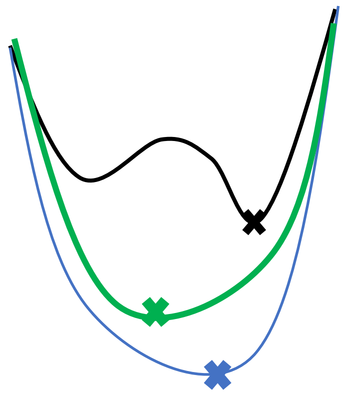

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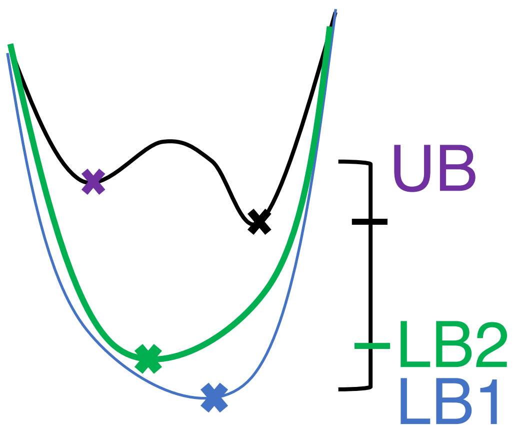

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The Art and Science of Making Relaxations

- Active area of research
- People spend entire careers coming up with relaxations:
  - Of specific terms
  - General relaxations
- We will show two, but many exist!
- Interesting papers:
  - C.E. Gounaris, C.A. Floudas, Tight convex underestimators for C2-continuous problems I and II, Journal of Global Optimization

54 J Glob Optim (2008) 42:51–67

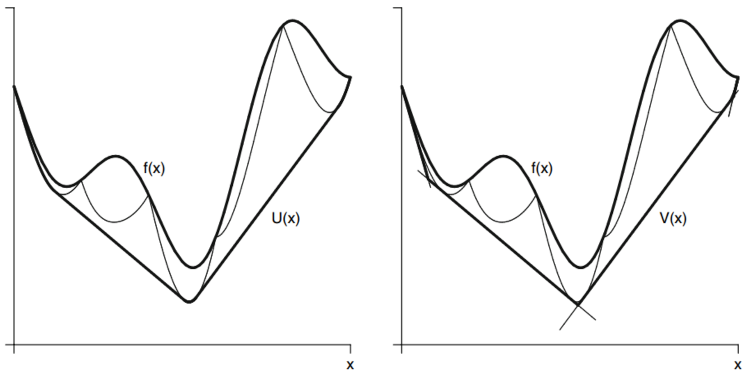


Fig. 1 Function $f(x)$ and underestimators $U(x)$ and $V(x)$

66 J Glob Optim (2008) 42:51–67

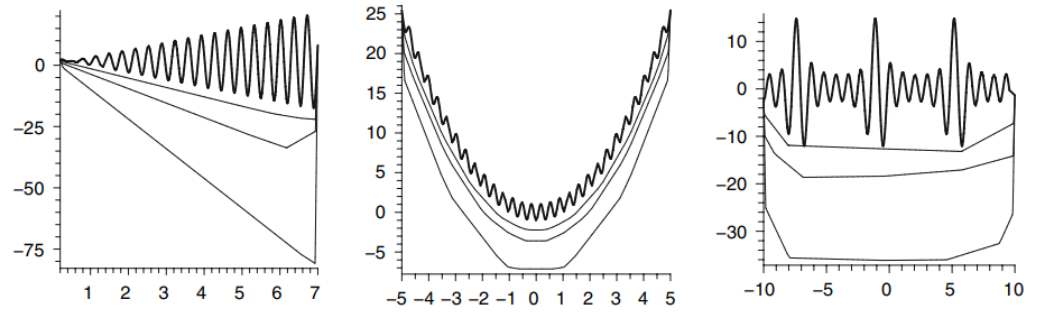
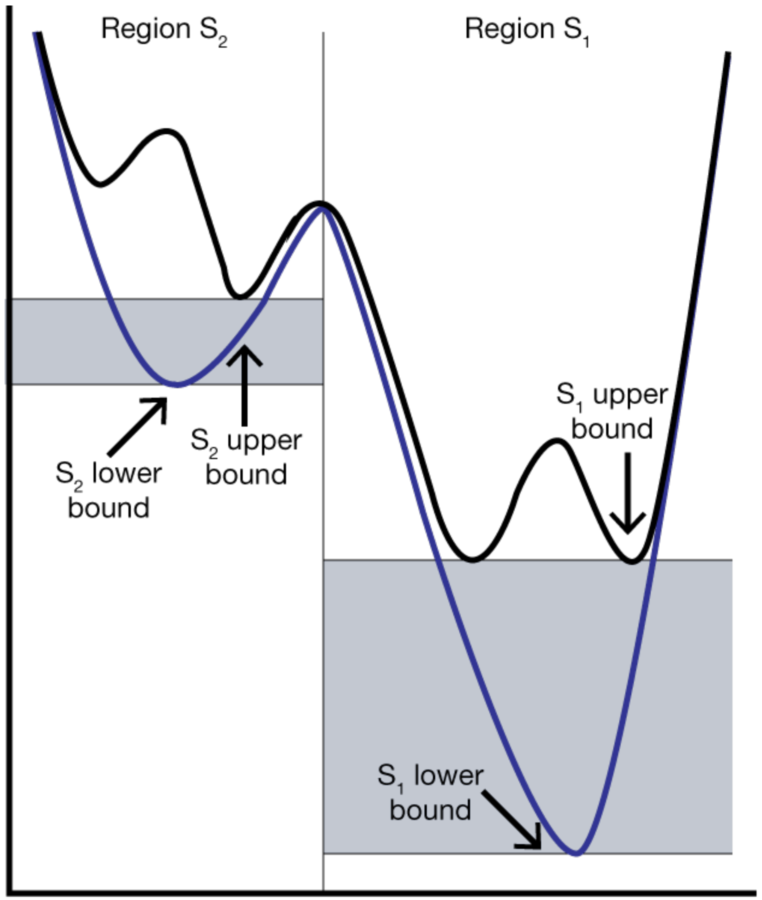


Fig. 5 Functions 4, 19 and 33 with underestimators $V(x)$ for three different partitioning levels ($N = 24$, 36 and 48)

Why Would B&B Work with Continuous Relaxations?

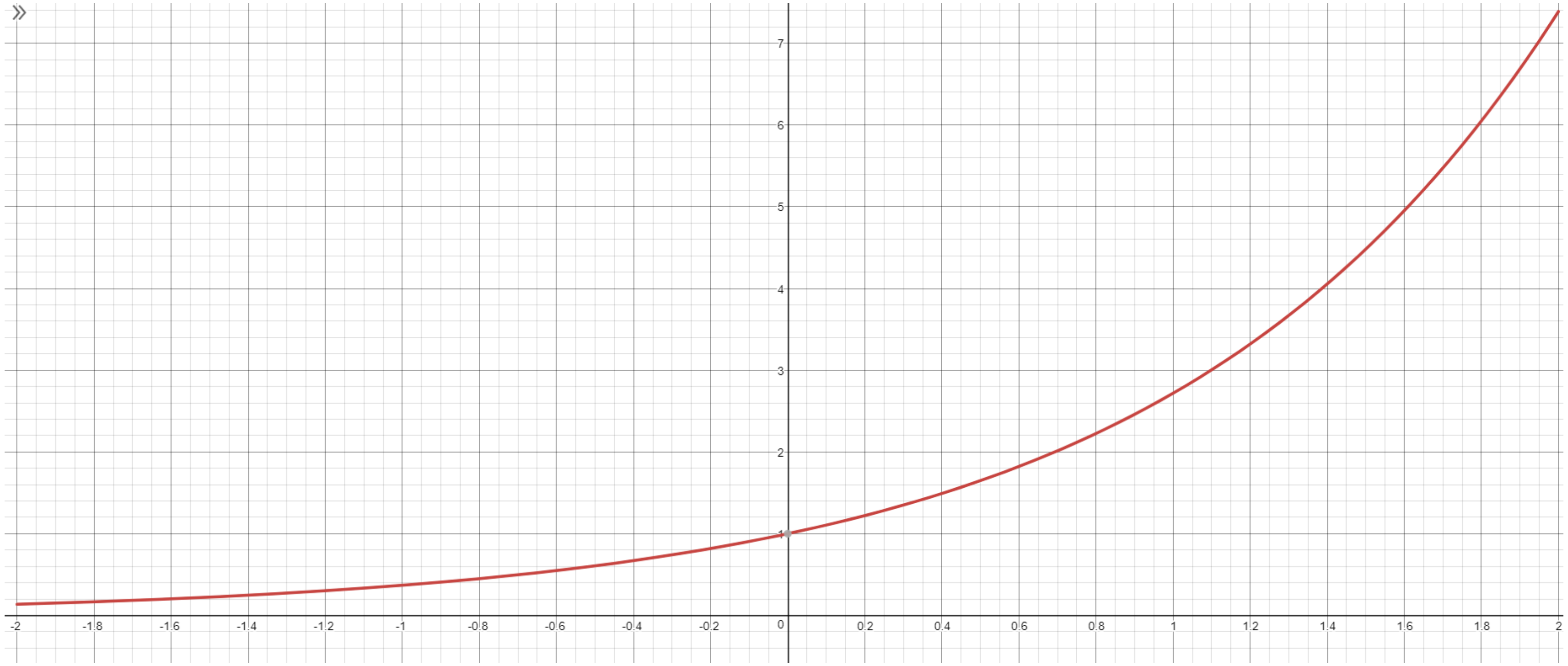
- As we subdivide the space, relaxations may become tighter
- As the space becomes tiny, relaxation should approach actual function
- Key idea is to have good enough relaxations to help us “prune-space”
- If relaxations are too wide, then we will never prune any space and end up having to solve many subproblems/nodes → inefficient



S_2 LB > S_1 UB

Relaxation for Exponential Terms

- A lot of the surrogate functions you fit has exponential terms
- Can you think of an “upper-bound” relaxation and a “lower-bound” relaxation for the following problem?
- $f(x) = \exp(x)$ where $-2 \leq x \leq 2$



Relaxation of Bilinear xy Terms

- xy terms are NONCONVEX
- How can we develop over/under-estimators for them?
- Very popular McCormick Relaxations
- What's the idea?
- First create new variable w:

$xy = w$

Then use bounds on x and y:

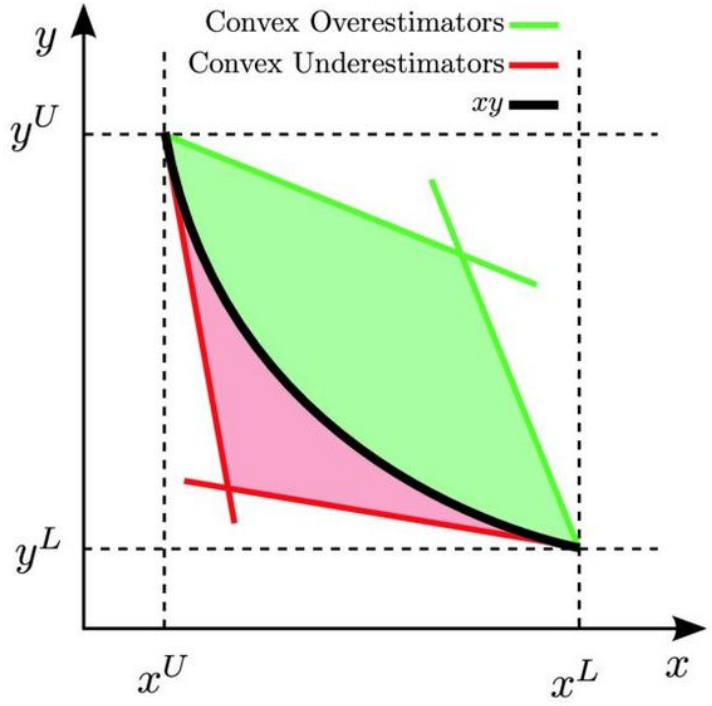
$x^L \le x \le x^U$

$y^L \le y \le y^U$

$a = (x - x^L), b = (y - y^L)$

$\Rightarrow ab = (x - x^L)(y - y^L) = xy - x^L y - x y^L + x^L y^L$

$\Rightarrow ab \ge 0 \Rightarrow w \ge x^L y + x y^L - x^L y^L \dots.$



https://optimization.mccormick.northwestern.edu/images/6/6a/Mccormick.jpg

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FINAL BOUNDS (under-estimator):

$w \geq x^L y + x y^L - x^L y^L$

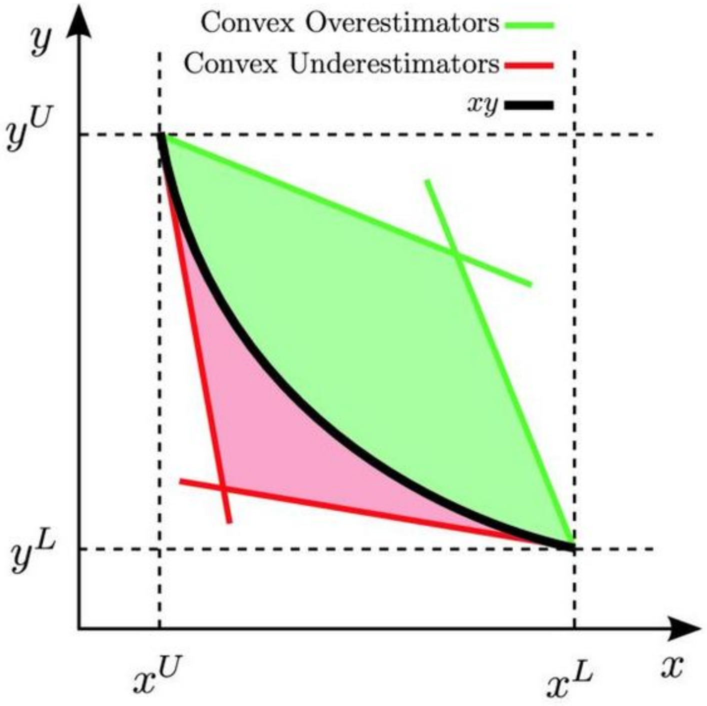
$w \geq x^U y + x y^U - x^U y^U$

Then: $a = (x - x^L), b = (y^U - y)\ldots$

FINAL BOUNDS (over-estimator):

$w \leq x^U y + x y^L - x^U y^L$

$w \leq x y^U + x^L y - x^L y^U$



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Summary

- Relaxations must be valid over and under estimators
- The tighter the relaxation, the better (closer) bound it leads to
- Relaxations exist or may be derived for many types of functions
- Relaxations for specific functions is an active area of research in optimization