Geometry optimization

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Geometry optimization

- Good standard methods are available for minimization
  - Fletcher: "Practical Methods of Optimization" (2nd edn., 1987)
  - Dennis and Schnabel: "Numerical Methods for Unconstrained Optimization and Nonlinear Equations" (1983,1996)
  - Gill, Murray, and Wright: "Practical Optimization" (1982)

- Methods for saddle points are much less developed
  - less intuitive and experimental information available for saddle points
  - many methods have been considered over the years but

> *Localization of a saddle point is easy to make only in laboratories other than our own*
>
> *Havlas and Zahradník*

Overview

1. Introduction
   - Smooth functions
   - Minima and saddle points
   - Strategies for optimization
2. Local region
   - Local region
   - Linear and quadratic models
   - Newton's method
   - The quasi-Newton method
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3. Global strategies for minimization
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4. Global strategies for saddle points
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   - Levenberg–Marquardt trajectories
   - Gradient extremals
   - Image functions

Section 1

Introduction

Outline

Multivariate smooth functions

- Taylor expansion of a smooth function f about the current point x_c:

$$f(x) = f_c + \tilde{s} g_c + \tfrac{1}{2} \tilde{s} H_c s + \cdots, \quad s = x - x_c$$

- Multivariate function f in x with gradient g_c and Hessian H_c at x_c:

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad g_c = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}, \quad H_c = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

- Diagonal Hessian representation:

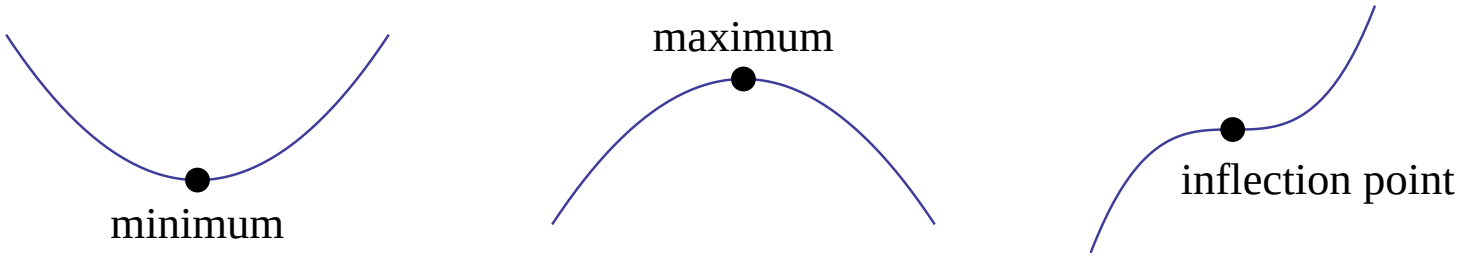
$$f(x) = f_c + \sum_i \phi_i \sigma_i + \tfrac{1}{2} \sum_i \lambda_i \sigma_i^2 + \cdots$$

  - gradient in the diagonal representation ϕ_i
  - Hessian eigenvalues λ_i
  - Hessian index: the number of negative Hessian eigenvalues

Stationary points

- A smooth function $f(x)$ has a stationary point at x_* if the gradient vanishes:

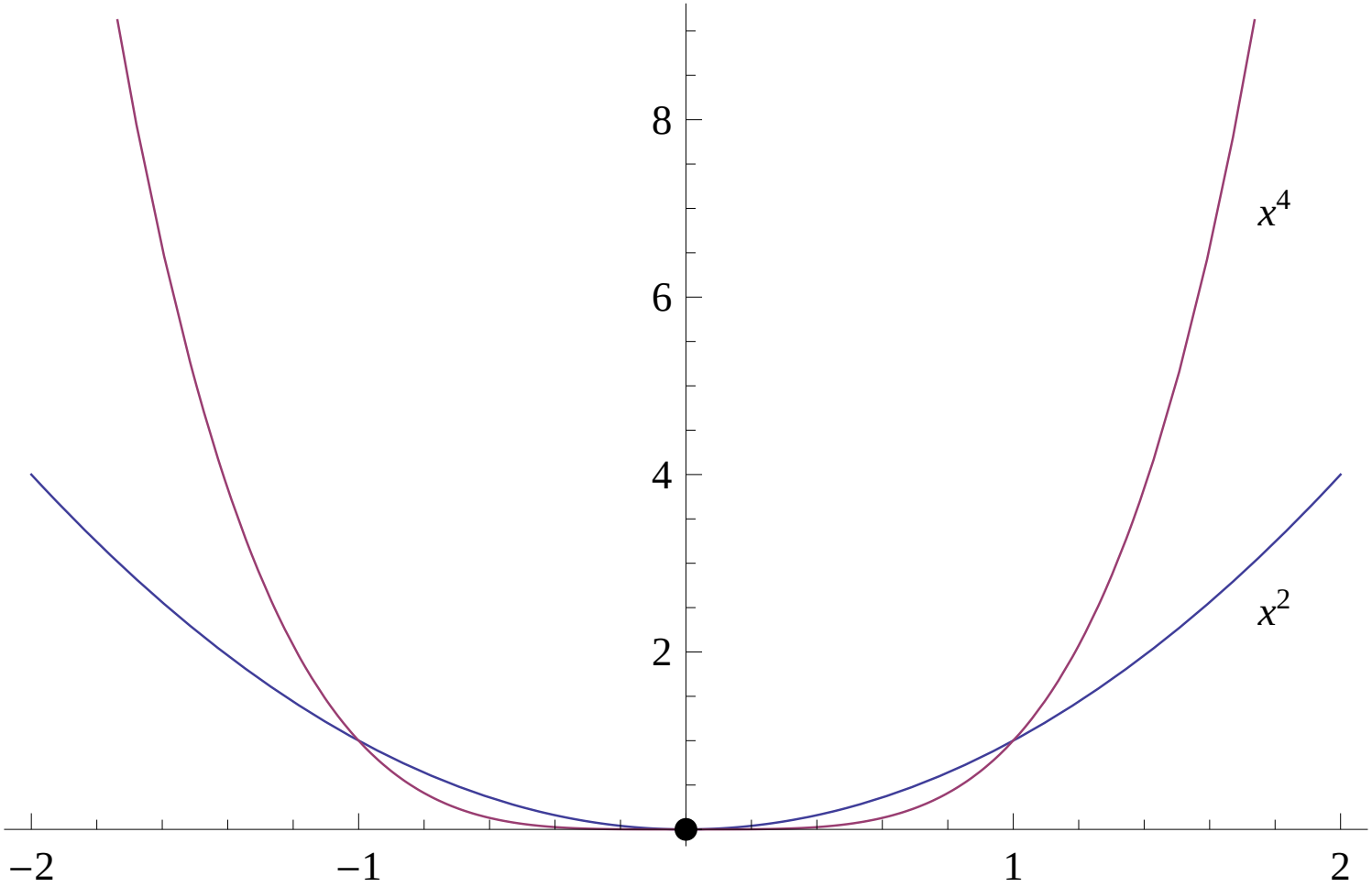
$$g(x_*) = 0 \quad \text{(zero slope)}$$



- The function $f(x)$ has a minimum at x_* (the minimizer) if the Hessian index is zero:

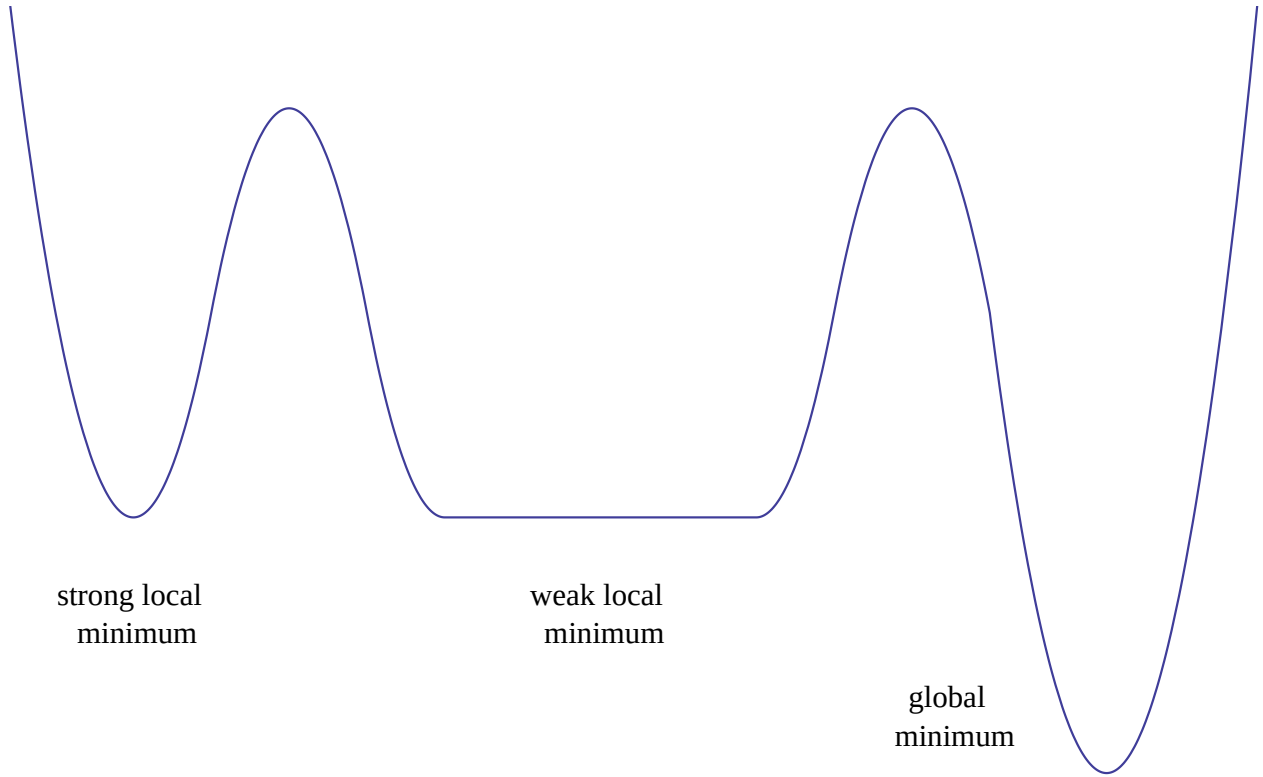
Strong and weak minima

- At a minimum, all Hessian eigenvalues are nonnegative
  - if, in addition, all eigenvalues are positive, we have a strong minimum
  - if one or more eigenvalues are zero, we have a weak minimum



Local and global minima

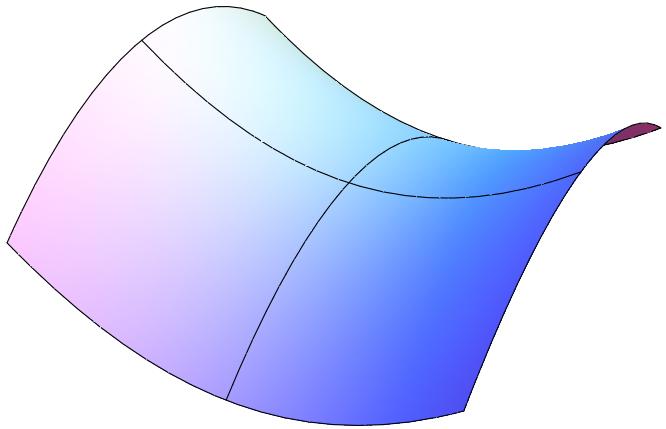
- A minimum x_* is global if $f(x) \geq f(x_*)$ for all x
- A minimum x_* that is not global is said to be local



- Most practical methods do not discriminate between local and global minima

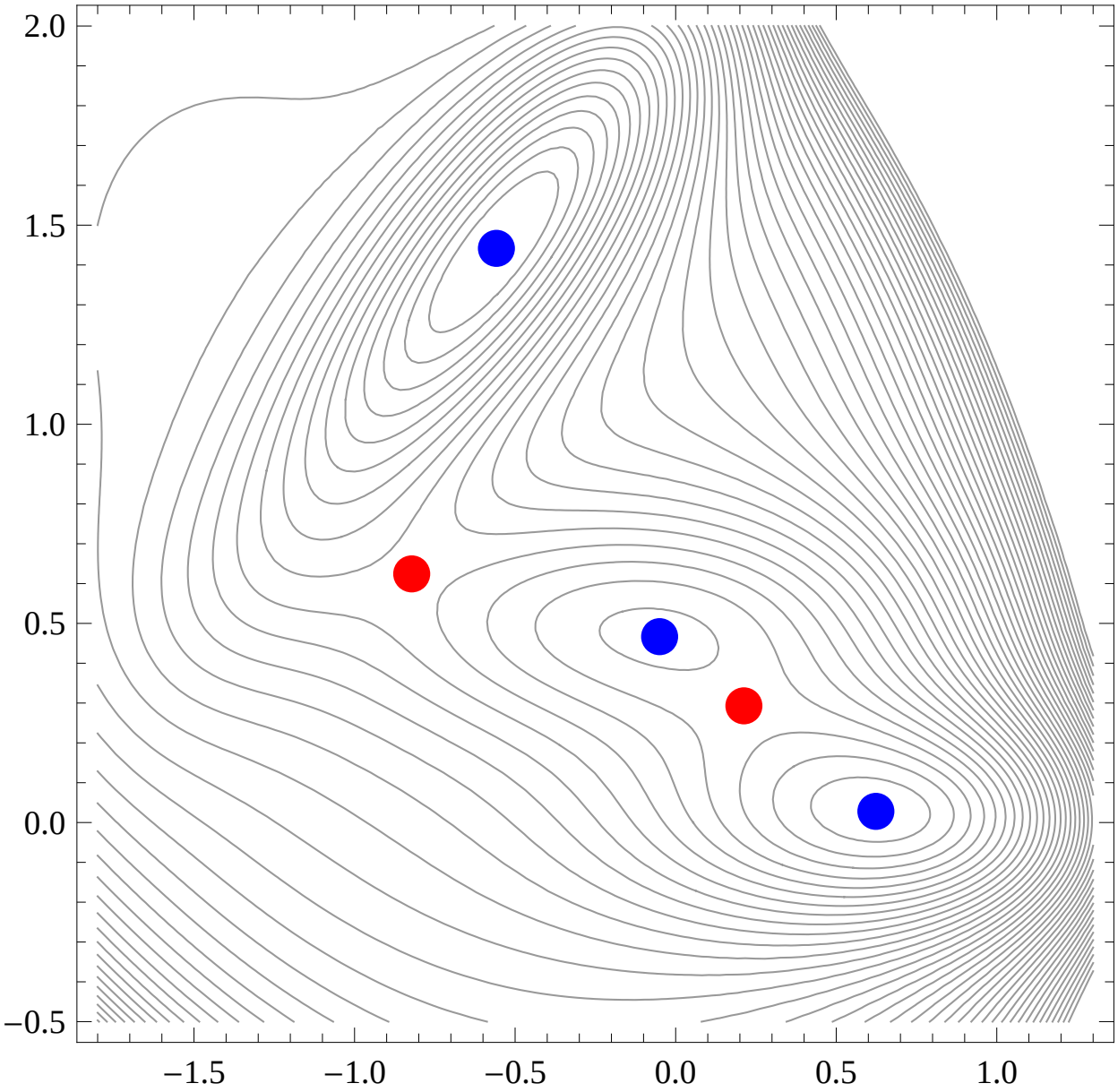
Saddle points

- A saddle point is a stationary point with one or more negative Hessian eigenvalues
  - a kth-order saddle point has Hessian index k



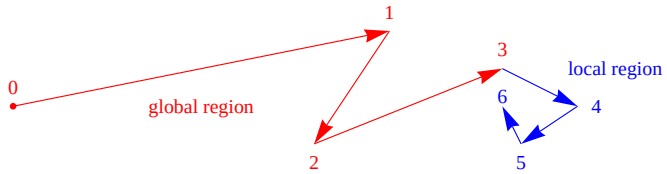
- The gradient and Hessian are both needed to characterize a stationary point
- Potential-energy surfaces:
  - minimum: stable molecular conformation
  - first-order saddle point: transition state
- Electronic-structure energy functions:
  - minimum: ground state
  - saddle point: excited state

Minima and saddle points



Strategies for optimization: global and local regions

- Any optimization is iterative, proceeding in steps or iterations
- At each step, a local model $m(x)$ is constructed of the surface $f(x)$
  - this model must be (locally) accurate, flexible, and easy to determine
- A search proceeds in two regions: the global region and the local region



Local region

- the local model $m(x)$ represents $f(x)$ accurately around the optimizer x_*
- take a step to the optimizer of the model $m(x)$
- this region usually presents few problems

Global region

- the local model $m(x)$ does not represent $f(x)$ accurately around the optimizer x_*
- the model cannot locate x_* but must instead guide us in the right general direction
- relatively simple for minimizations, difficult in saddle-point searches

Section 2

Local region

Outline

Local region

- In the local region, the local model extends to the optimizer x_* of the true function
- We can then proceed in a simple manner:
  1. construct a local model $m_c(x)$ of $f(x)$ around the current point x_c

$$m_c(x_c) = f(x_c)$$
$$m_c(x_*) \approx f(x_*)$$

  2. determine the stationary point x_+ of the local model

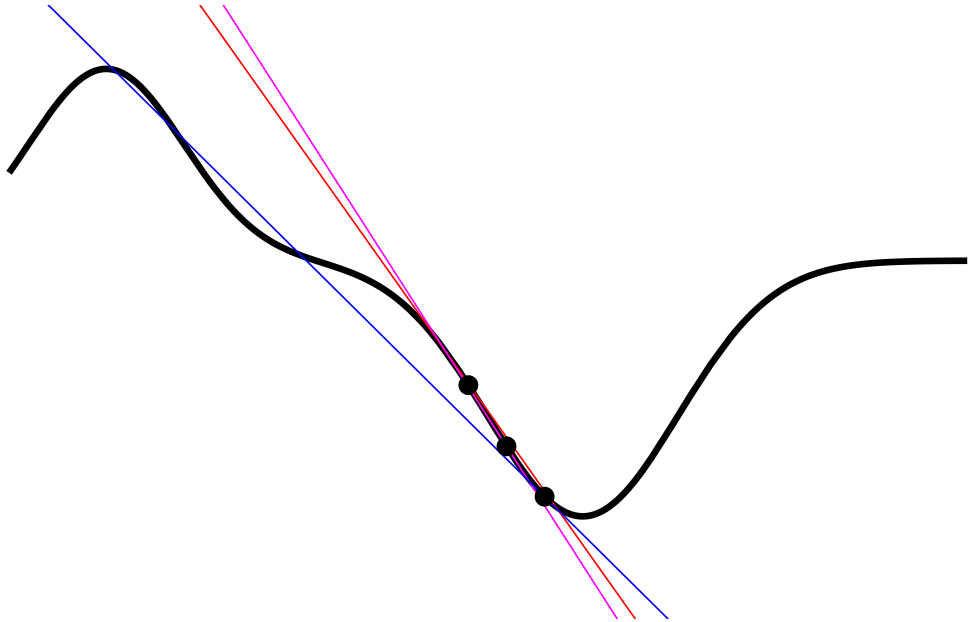
$$\left.\frac{\mathrm{d}m_c(x)}{\mathrm{d}x}\right|_{x=x_+} = 0$$

  3. if $x_+ = x_*$ (to some preset threshold), terminate; otherwise, set $x_c = x_+$ and iterate again
- The convergence of the optimization depends on the quality of the local model
- We shall build the local model by expansion around the current point
  - the linear model
  - the quadratic model

Linear model

- The local linear or affine model arises by truncation after the first-order term:

$$m_A(x) = f(x_c) + \tilde{g}_c s$$



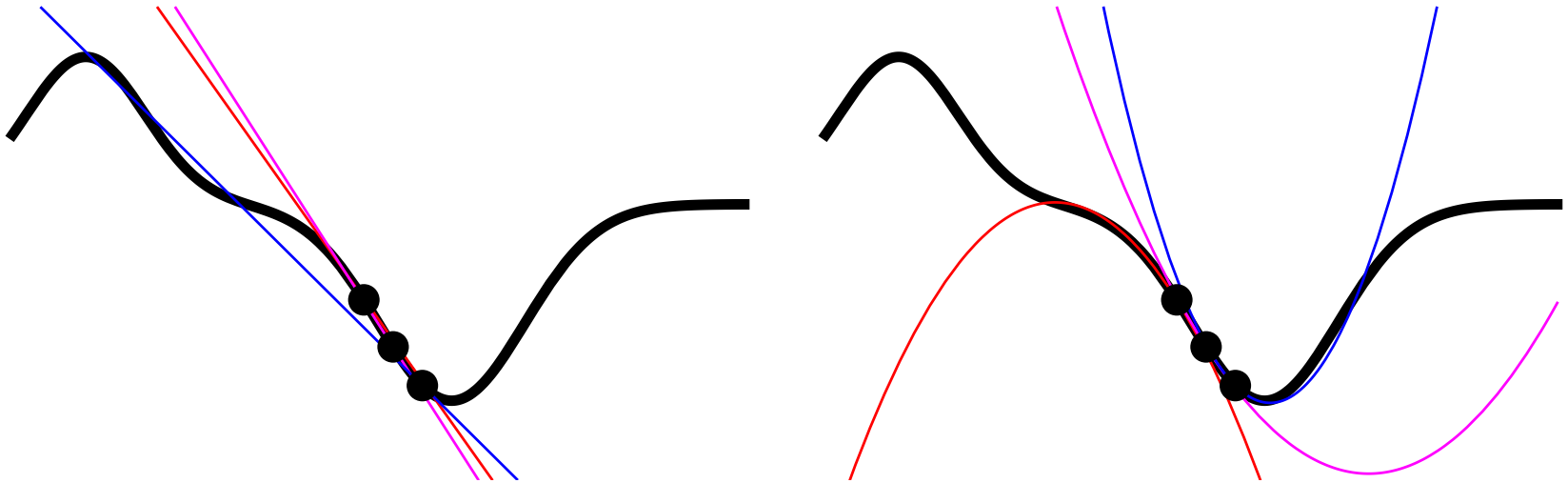
- The linear model is typically constructed from the exact gradient
- The linear model is not very useful since
  - it is unbounded
  - it has no curvature information
  - it has no stationary points
- The linear model forms the basis for the steepest-descent method
  - it is often used in combination with line search (vide infra)

Second-order model

- In the second-order (SO) model, we truncate the expansion after second order:

$$m_{\mathrm{SO}}(x) = f(x_c) + \tilde{g}_c s + \tfrac{1}{2}\tilde{s} H_c s$$

  - requires the exact gradient g_c and Hessian H_c at the current point
- The SO models contains full information about local slope and curvature



- Unlike the first-order (linear) model, the SO model has a stationary point
  - this point may or may not be close to the true stationary point
  - in the local region, the SO stationary point is close to the true stationary point

Newton's method

- The SO model is given by

$$m_{\mathrm{SO}}(x) = f(x_c) + \tilde{g}_c s + \tfrac{1}{2}\tilde{s} H_c s$$

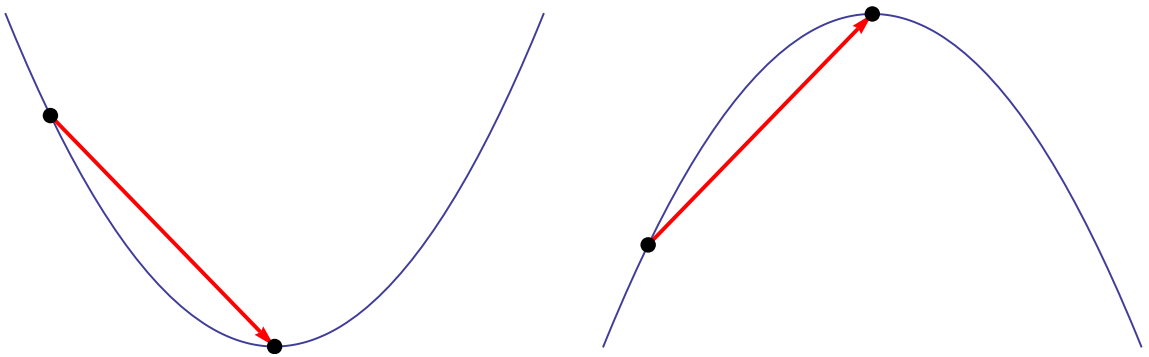
- Differentiating the SO model and setting the result to zero, we obtain

$$\frac{\mathrm{d}m_{\mathrm{SO}}(s)}{\mathrm{d}s} = 0 \quad \Rightarrow \quad g_c + H_c s = 0 \quad \Rightarrow \quad s = -H_c^{-1} g_c$$

- The new point x_+ and the current point x_c are related as

$$x_+ = x_c - H_c^{-1} g_c \quad \leftarrow \text{Newton step}$$

- When iterated, we obtain Newton's method
- Note: the Newton step does not discriminate between minima and maxima



Convergence of Newton's method

- The relation between the new and old points is given by

$$x_+ = x_c - H_c^{-1} g_c \quad \leftarrow \text{Newton step}$$

- Subtracting the true optimizer x_*, we obtain a relation between new and old errors

$$e_+ = e_c - H_c^{-1} g_c, \quad e_+ = x_+ - x_*, \quad e_c = x_c - x_*$$

- We next expand the gradient and inverted Hessian around the true optimizer x_*:

$$g_c = g_* + H_* e_c + \mathcal{O}(e_c^2) = H_* e_c + \mathcal{O}(e_c^2) \quad (\text{since } g_* = 0)$$
$$H_c^{-1} = H_*^{-1} + \mathcal{O}(e_c)$$

- Inserted in the error expression above, these expansions give

$$e_+ = e_c - H_c^{-1} g_c = e_c - \left(H_*^{-1} + \mathcal{O}(e_c)\right)\left(H_* e_c + \mathcal{O}(e_c^2)\right) = \mathcal{O}(e_c^2)$$

- We conclude that Newton's method converges quadratically

$$e_+ = \mathcal{O}(e_c^2)$$

  - close to the optimizer, the number of correct digits doubles at each iteration

The quasi-Newton method

- If the exact Hessian is unavailable or expensive, use an approximate Hessian
  - this gives the more general quadratic model

$$m_Q(x) = f(x_c) + \tilde{g}_c s + \tfrac{1}{2}\tilde{s} B_c s, \quad B_c \approx H_c$$

  - the associated quasi-Newton step is given by

$$x_+ = x_c - B_c^{-1} g_c$$

- In the quasi-Newton method, B is iteratively improved upon
  - at each iteration, the exact Hessian satisfies the relation

$$(g_+ - g_c) = H_+ (x_+ - x_c) + \mathcal{O}((x_+ - x_c)^2)$$

  - by analogy, we require the new approximate Hessian to satisfy the relation

$$(g_+ - g_c) = B_+ (x_+ - x_c) \quad \leftarrow \text{the quasi-Newton condition}$$

  - the new Hessian is updated in a simple manner from B_c, $g_+ - g_c$ and $x_+ - x_c$

$$B_+ = f(B_c, g_+ - g_c, x_+ - x_c)$$

  - several update schemes are available

Hessian updates

- Apart from the quasi-Newton condition, other conditions are often imposed
- Hereditary symmetry:

$$B_c \text{ symmetric} \Rightarrow B_+ \text{ symmetric}$$

- Powell–symmetric–Broyden (PSB) update:

$$B_+ = B_c + \frac{(\tilde{s}_c s_c) T_c \tilde{s}_c + (\tilde{s}_c s_c) s_c \tilde{T}_c - (\tilde{T}_c s_c) s_c \tilde{s}_c}{(\tilde{s}_c s_c)^2}$$

$$T_c = (g_+ - g_c) - B_c s_c$$

  - simple matrix and vector manipulations
- Hereditary positive definiteness:

$$B_c \text{ positive definite} \Rightarrow B_+ \text{ positive definite}$$

- Broyden–Fletcher–Goldfarb–Shanno (BFGS) update:

$$B_+ = B_c + \frac{y_c \tilde{y}_c}{\tilde{y}_c s_c} - \frac{B_c s_c \tilde{s}_c B_c}{\tilde{s}_c B_c s_c}$$

$$y_c = g_+ - g_c$$

- Many other schemes exist

Convergence in local region

- Consider a sequence x_k that converges to x_*

$$\lim_{k\to\infty} x_k = x_* \qquad \leftarrow \text{convergent sequence}$$

$$e_k = x_k - x_* \qquad \leftarrow \text{error vector}$$

- Linear, superlinear and quadratic rates of convergence:

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|} = a \qquad \leftarrow \text{linear convergence} \qquad \text{(steepest descent, gradient)}$$

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|} = 0 \qquad \leftarrow \text{superlinear convergence} \qquad \text{(quasi-Newton, updated Hessian)}$$

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^2} = a \qquad \leftarrow \text{quadratic convergence} \qquad \text{(Newton, exact Hessian)}$$

- The local region presents few problems for methods based on the quadratic model
  - convergence to weak or near-weak minima will still be slow
  - such minima require a quartic model for fast convergence
- As our model improves, fewer but more expensive steps are needed for convergence

Stopping criteria

- An optimization is terminated when one or several convergence criteria are satisfied
- Typically, the following criteria are used
  - the gradient norm:
$$\|g_c\| \leq \varepsilon_g$$
  - the norm of the predicted second-order change in the function:
$$\tfrac{1}{2}|\tilde{g}_c H_c^{-1} g_c| \leq \varepsilon_f$$
  - the norm of the (quasi-)Newton step:
$$\|H_c^{-1} g_c\| \leq \varepsilon_s$$
- In addition, we should always check the structure of the Hessian (the Hessian index)
- Finally, inspect the solution and use common sense!

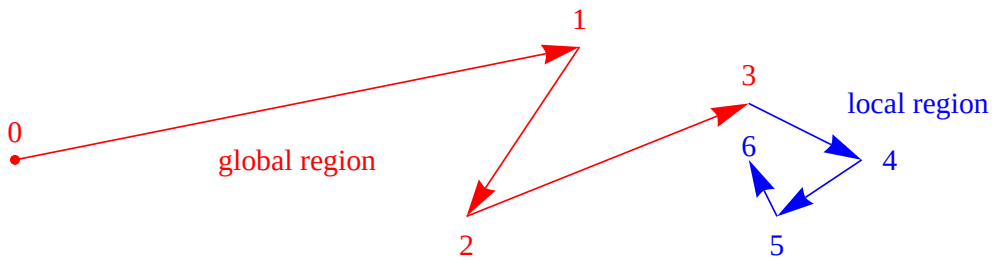
Section 3

Global strategies for minimization

Outline

Global region

- Optimization in the local region is fairly simple
- We shall now consider the more difficult global region . . .



Local region

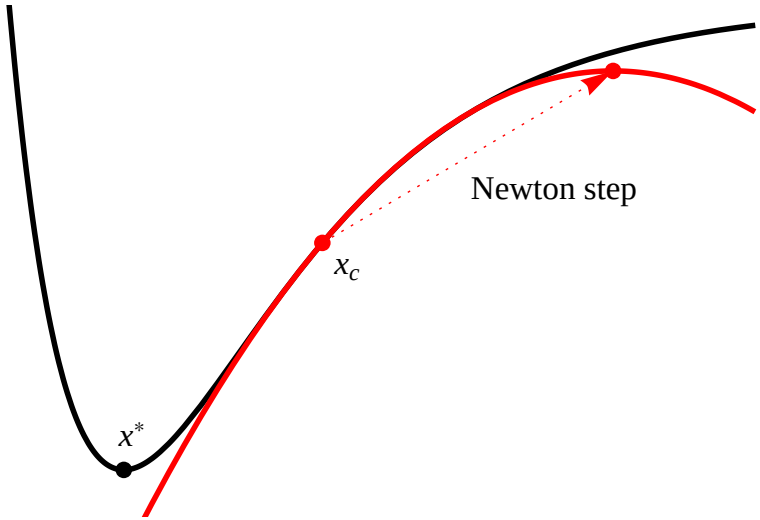
- the local model $m(x)$ represents $f(x)$ accurately around the optimizer x_*
- take a step to the optimizer of the model $m(x)$
- the same method works for minima and saddle points

Global region

- the local model $m(x)$ does not represent $f(x)$ accurately around the optimizer x_*
- the model must guide us in the right general direction
- this is relatively simple in minimizations but difficult in saddle-point searches

Strategies for minimization

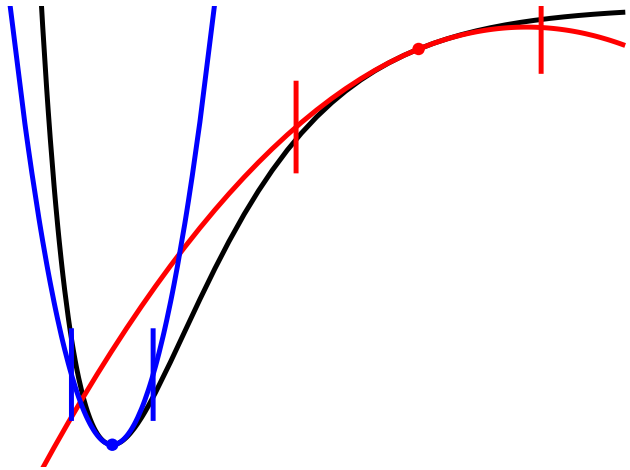
- Global strategies are needed when the local model represents $f(x)$ poorly around x_*



- The Newton step above leads us away from the minimizer, increasing $f(x)$
- The following is a useful global strategy for the minimization method:
  - the function $f(x)$ must be (sufficiently) reduced at each step
- In addition, the method we seek should be globally convergent:
  - it should converge to some (possibly local) minimum from any starting point
  - however, we cannot ensure that the minimum is global
- There are two standard global strategies:
  - the trust-region method
  - the line-search method

The trust region and the RSO model

- In the trust-region method, we recognize that the second-order model is good only in some region around x_c: the trust region (TR)



- The trust region cannot be specified in detail, we assume that it is a hypersphere

$$\sqrt{\tilde{s}s} \leq h \quad \leftarrow \text{trust radius } h$$

  - the trust radius is updated by a feedback mechanism
- This gives us the restricted second-order (RSO) model

$$m_{SO}(x) = f(x_c) + \tilde{g}_c s + \tfrac{1}{2}\tilde{s} H_c s, \quad \tilde{s}s \leq h^2$$

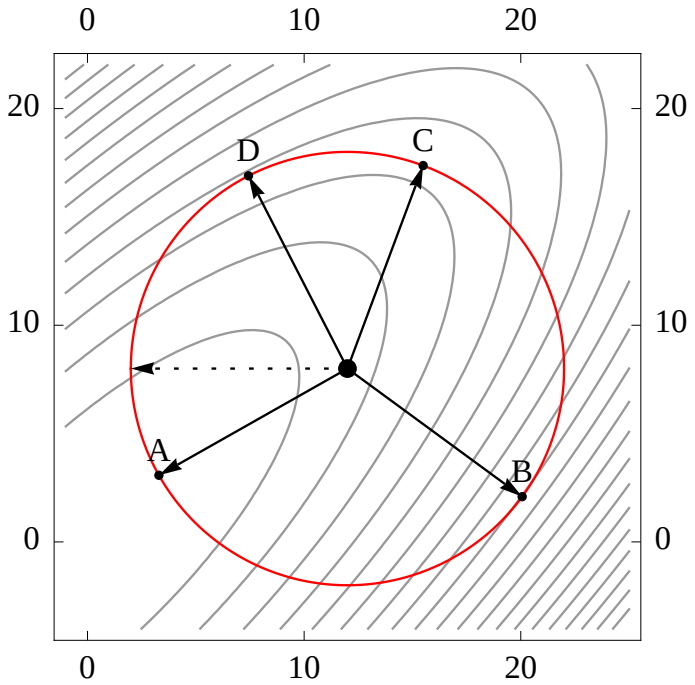
- At each iteration, we minimize $m_{SO}(x)$ subject to the constraint that $\tilde{s}s \leq h^2$

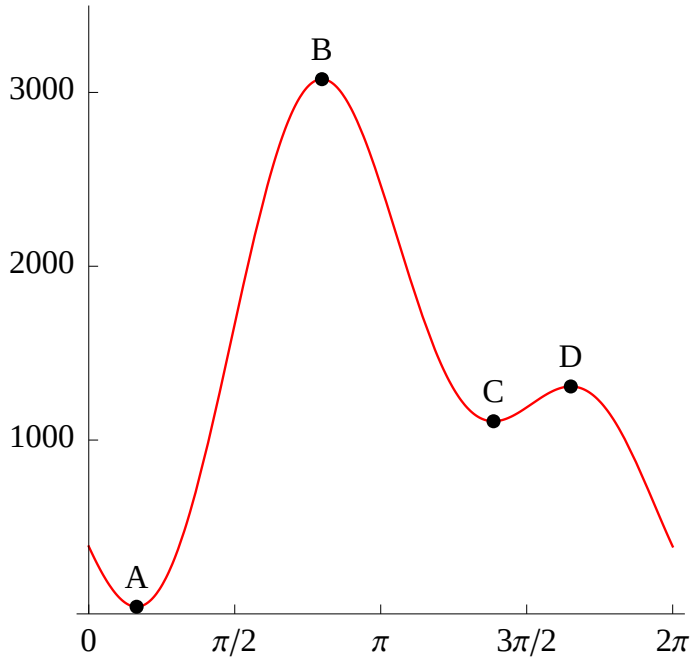
Stationary points in the trust region

- The trust region may or may not have a stationary point in the interior
- However, there are always two or more stationary points on the boundary
- Consider $f(x, y)$ below expanded about $(12, 8)$ in $s_x = x - 12$ and $s_y = y - 8$:

$$f(x,y) = 8(x-y)^2 + (x+y)^2 = 528 + \begin{bmatrix} s_x, s_y \end{bmatrix} \begin{bmatrix} 104 \\ -24 \end{bmatrix} + \frac{1}{2} + \begin{bmatrix} s_x, s_y \end{bmatrix} \begin{bmatrix} 18, -14 \\ -14, 18 \end{bmatrix} \begin{bmatrix} s_x \\ s_y \end{bmatrix}$$

  - with trust radius $h = 10$, there are four stationary points on the boundary





- In the global region, we minimize f globally on the boundary and go to point A

The level-shifted Newton step

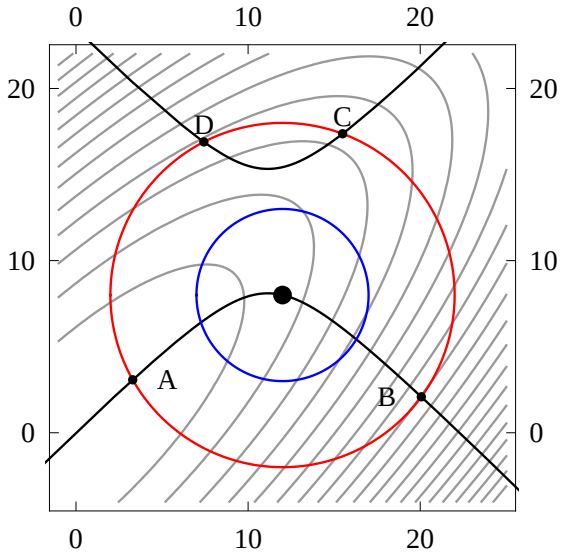
- To determine stationary points on the boundary, we use Lagrange's method

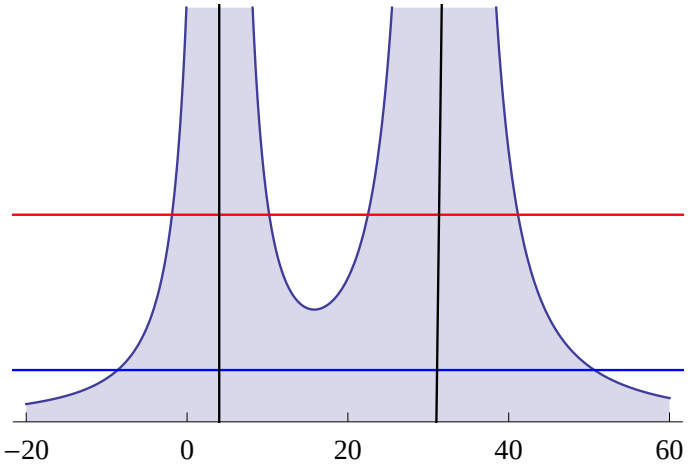
$$L(s,\mu) = m_{SO}(s) - \tfrac{1}{2}\mu(\tilde{s}s - h^2) \quad \leftarrow \text{Lagrangian}$$

- The stationary points are now obtained by setting the gradient to zero

$$\mathrm{d}L/\mathrm{d}s = g_c + H_c s - \mu s = 0 \quad \Rightarrow \quad s(\mu) = -(H_c - \mu I)^{-1} g_c$$

- We obtain a level-shifted Newton step $s(\mu)$ that depends on μ
  - we select μ such that the step is to the boundary





- Note: we have always at least two stationary points on the boundary

The trust-region algorithm

1. Construct a restricted second-order model of the surface at x_c:

$$m_{\mathrm{RSO}}(s) = f(x_c) + \tilde{g}_c s + \tfrac{1}{2}\tilde{s} H_c s, \quad \|s\| \leq h_c$$

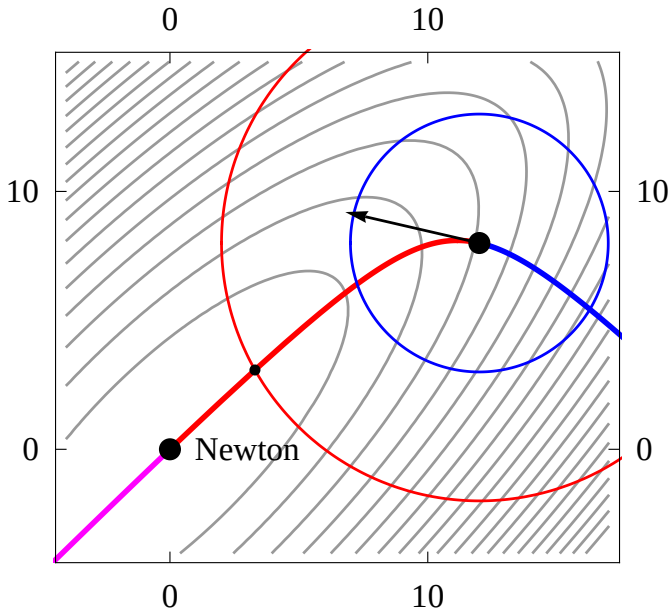
2. Take the Newton step if $\|s(0)\| < h_c$ and if H_c has correct structure

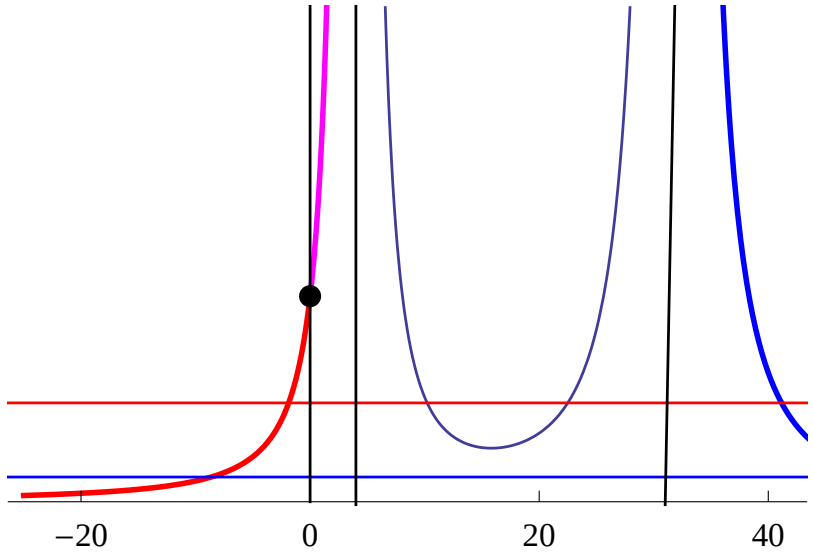
$$s(0) = -H_c^{-1} g_c$$

3. Otherwise, take the level-shifted Newton step to the minimum on the boundary

$$s(\mu) = -(H_c - \mu I)^{-1} g_c, \quad \mu < \min(0, \lambda_1), \quad \|s(\mu)\| = h_c$$

- The Levenberg–Marquardt trajectory: the step $s(\mu)$ as a function of μ:

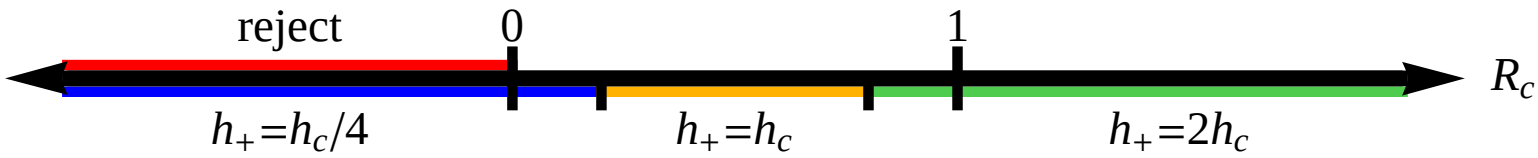




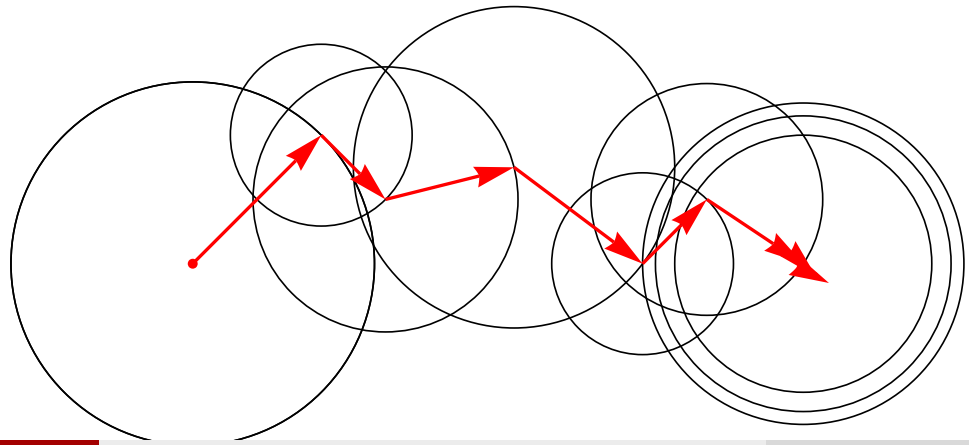
Trust-radius update

- The trust radius h_c is updated by a feedback mechanism:

$$R_c = \frac{\text{actual change}}{\text{predicted change}} = \frac{f_+ - f_c}{\tilde{g}_c s + \frac{1}{2}\tilde{s} H_c s} = 1 + \mathcal{O}(s^3)$$



- Important safety measure:
  - always reject the step if the function increases
  - calculate new step with reduced radius
- Typically implemented with the exact Hessian: an updated Hessian may not be accurate enough for an unbiased search in all directions



The line-search method

- If the Newton step must be rejected, it may still provide a direction for a line search
- In the line-search method, such searches form the basis for the global optimization

Line search

a one-dimensional search along a descent direction until an acceptable reduction in the function is obtained

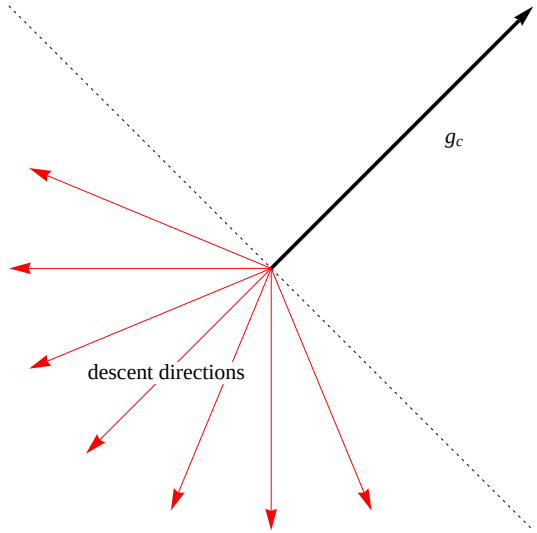
- A descent direction is a vector z such that $\tilde{g}_c z < 0$
  - examples of descent directions:
    - steepest-descent step:

      $$z = -g_c \quad \text{since} \quad -\tilde{g}_c g_c < 0$$

    - Newton step with a pos. def. Hessian:

      $$z = -B_c^{-1} g_c \quad \text{since} \quad -\tilde{g}_c B_c^{-1} g_c < 0$$

  - the BFGS step guarantees p. d. Hessian
  - the Newton step is usually better than the steepest-descent step



Line searches

- Exact line search:
  - expensive, unnecessary
- Inexact or partial line search:
  - try Newton step first
  - if necessary, backtrack until an acceptable step is found
- Line searches are often used with updated Hessians: quasi-Newton methods
  - relatively stable
  - efficient
- Backtracking does not make full use of available information
  - the Hessian is used to generate the direction of the step but not its length
  - the coupling between direction and length is ignored

trust-region method	line-search method
first step size, next direction	first direction, next step size
handles indefinite Hessians naturally	handles indefinite Hessians poorly
less suited for updated Hessians	well suited for updated Hessians
"guaranteed" convergence	no guarantee of convergence
conservative	risky

Coordinate systems for geometry optimizations

- A judicious choice of coordinates may improve convergence by reducing
  - quadratic couplings
  - higher-order (anharmonic) terms

Cartesian coordinates

- simple to set up and to automate
- provides universal and uniform quality
- yields strong couplings and large anharmonicities
- contains rotations and translations

Internal coordinates

- primitive internal coordinates: bond lengths, bond angles, dihedral angles
- physically well motivated: small couplings and anharmonicities
- nonredundant system difficult to set up
- solution: use redundant internal coordinates
- redundancies controlled by projections

The initial Hessian

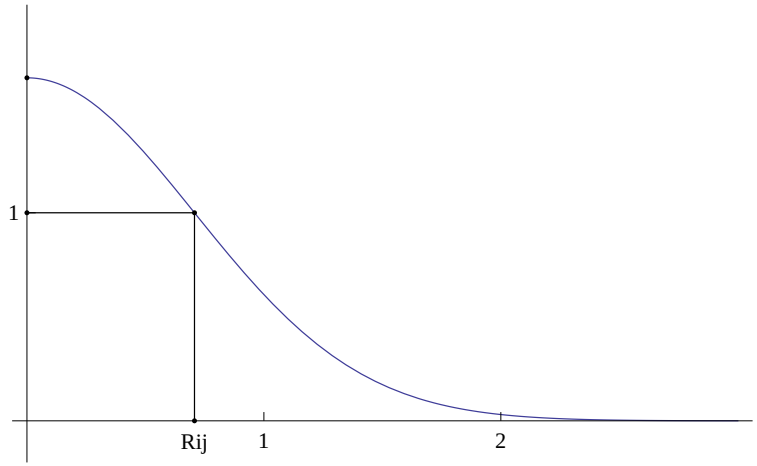
- The efficiency of update methods depends on the quality of the initial Hessian
- The exact initial Hessian gives fewest iterations but is expensive
- A more efficient scheme may be to use a less accurate but cheaper initial Hessian
- A good approximate Hessian is easiest to set up in primitive internal coordinates
  - diagonal harmonic model Hessian

$$B_{pp} = \begin{cases} 0.45\,\rho_{ij} & \text{bond length} \\ 0.15\,\rho_{ij}\rho_{jk} & \text{bond angle} \\ 0.005\,\rho_{ij}\rho_{jk}\rho_{kl} & \text{dihedral angle} \end{cases}$$

  - here ρ_{ij} is a decaying model function for each atom pair ij

$$\rho_{ij}(r_{ij}) = \exp\left[\alpha_{ij}(R_{ij}^2 - r_{ij}^2)\right]$$

α_{ij} and R_{ij} tabulated for all atom pairs



Numerical comparisons

- Total number of iterations/timings for 30 representative molecules (Baker set)
- 1st-order quasi-Newton (BFGS) with different initial Hessians
- 2nd-order Newton method
- Optimizations in Cartesian and redundant internal coordinates

		quasi-Newton					Newton
		Cart. diagonal		int. diagonal		exact	
		1.0	0.4	1.0	hmh		
Cart. coor.	iter.	768	619	318	309	210	123
	time	2261	1873	931	911	907	1163
inter. coor.	iter.	503	363	269	208	158	113
	time	1475	1064	781	664	757	1491

- The best method:
  the BFGS quasi-Newton method in redundant internal coordinates with initial harmonic model Hessian (hmh)

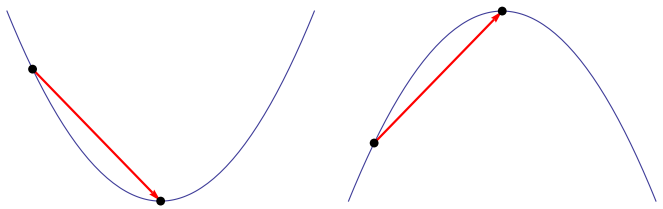
Section 4

Global strategies for saddle points

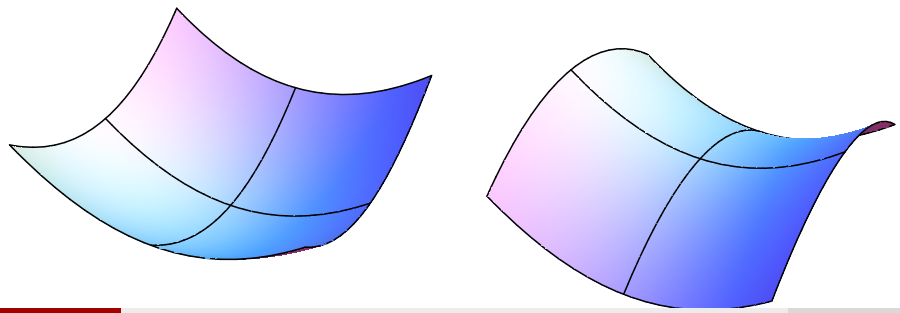
Outline

Saddle points

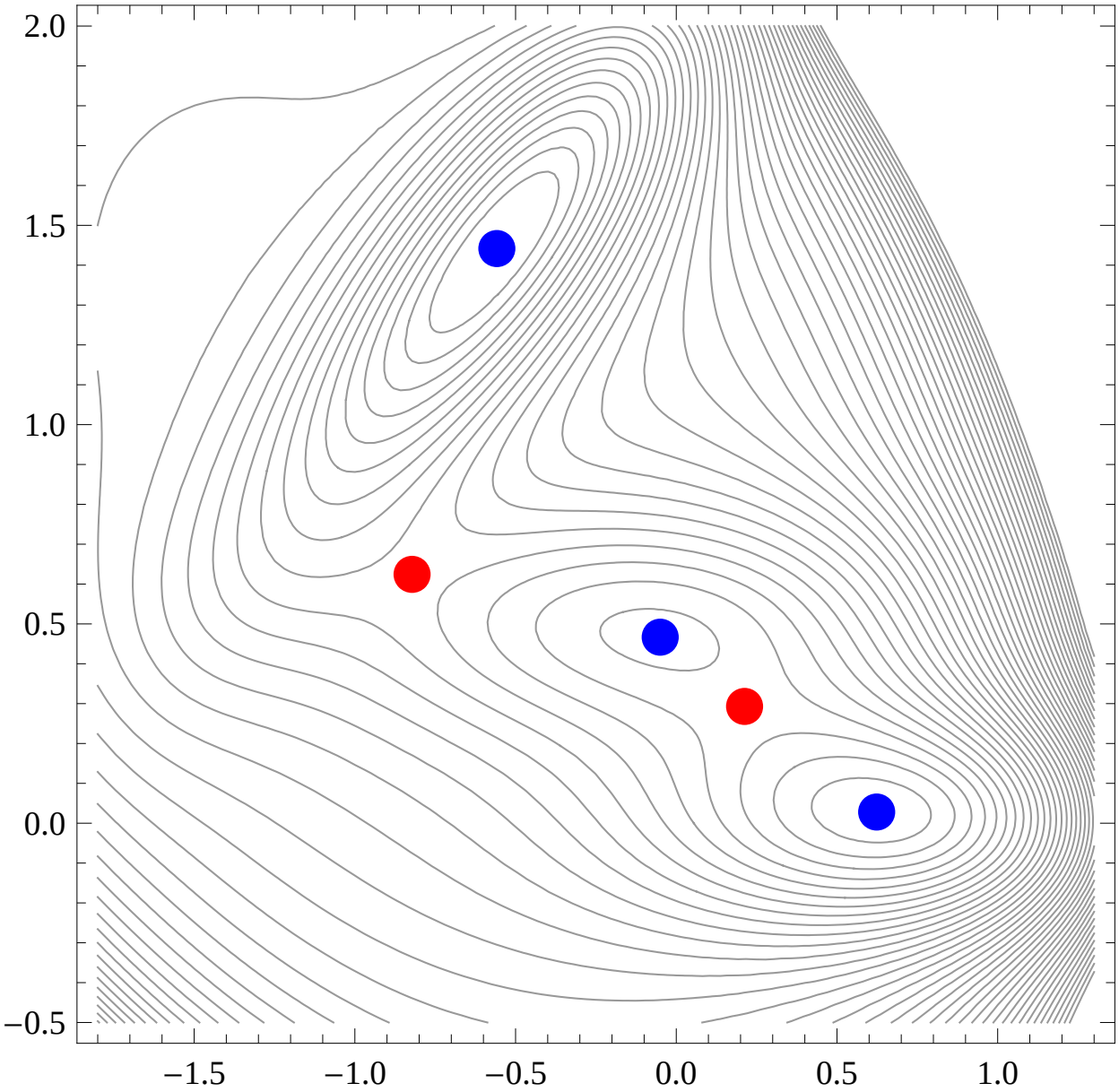
- Saddle-point optimizations are more difficult than minimizations
  - less experimental and intuitive information available
  - less developed and stable
- There are a large number of methods in use
- The local region presents few problems provided a second-order model is used
  - the Newton step is always to the stationary point of the second-order model, be it a minimum, a maximum or a saddle point



- All difficulties with saddle-point optimizations are in the global region
  - it is hard to measure progress in saddle-point optimizations



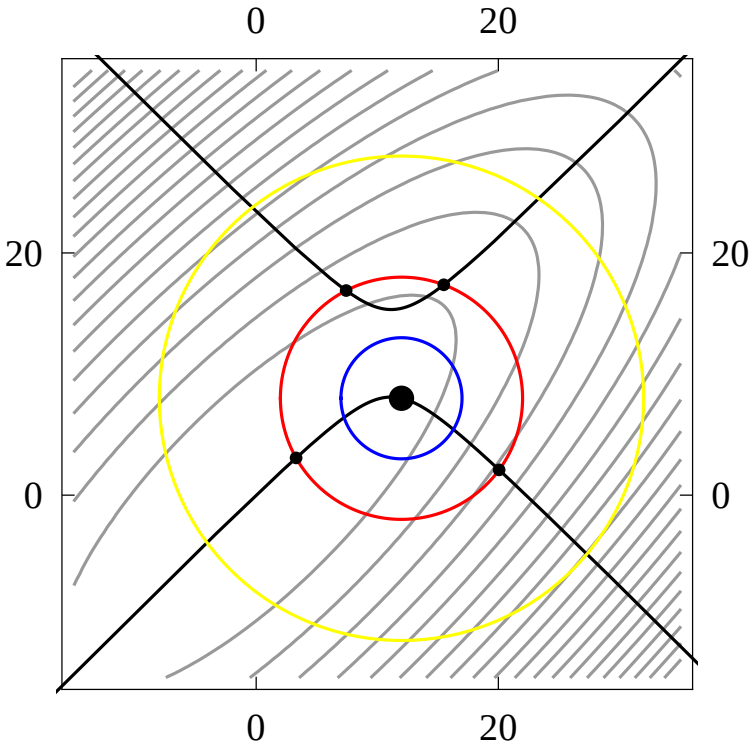
Minima and saddle points

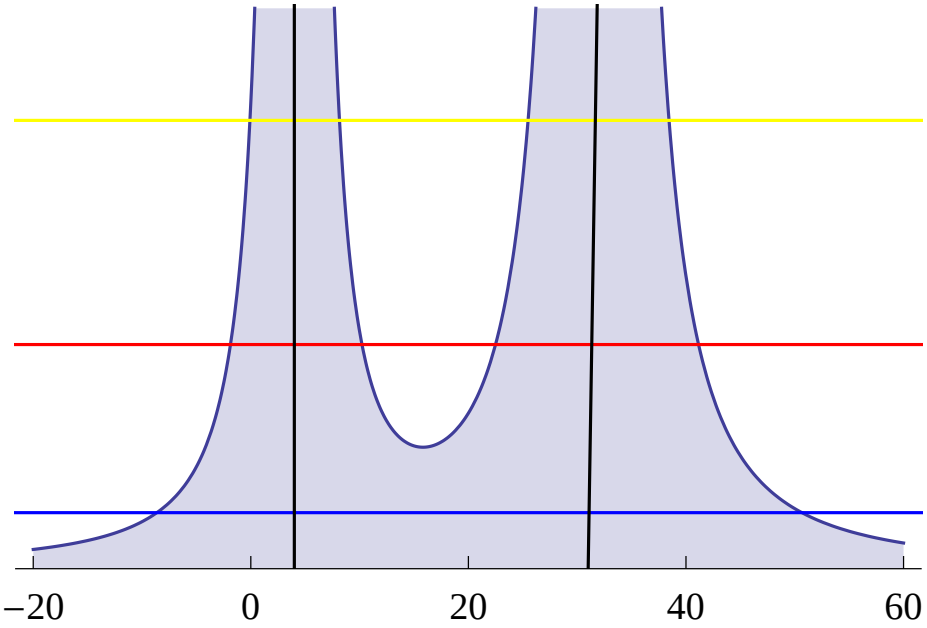


Levenberg–Marquardt trajectories

- A simple approach is to explore other solutions to the restricted 2nd-order problem

$$s(\mu) = -(H_c - \mu I)^{-1} g_c$$





- Select walks to reduce or increase the function along the various modes
  - note: the trajectories depend on the expansion point
  - this approach has been used with some success

Gradient extremals

- Levenberg–Marquardt trajectories are dependent on the expansion point
- Are there well-defined lines connecting stationary points of a smooth function?
- Steepest-descent paths:
  - follow gradient down from the saddle point
  - not locally defined (not recognizable)
  - intrinsic reaction coordinate
- Gradient extremals:
  - connect stationary points
  - locally defined (recognizable) by the condition

$$H(x)g(x) = \lambda(x)g(x)$$

- The gradient is an eigenvector of the Hessian at gradient extremals

From stationary points to gradient extremals

- Consider the gradient in the diagonal representation of the Hessian
  - at a stationary point, all elements are zero
  - at a gradient extremal, all elements except one are zero

$$\phi(x_{\mathrm{sp}}) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \rightarrow \quad \phi(x_{\mathrm{ge}}) = \begin{bmatrix} 0 \\ \vdots \\ \phi(t) \\ \vdots \\ 0 \end{bmatrix}$$

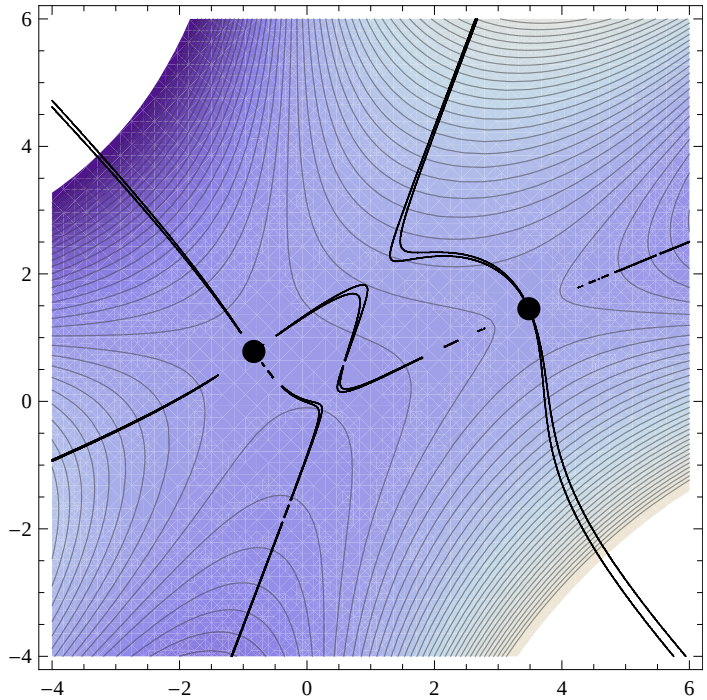
- Gradient extremals are therefore points where we have relaxed just one of the conditions for a stationary point
  - $3N-6$ conditions specify a point
  - $3N-7$ conditions specify a line
- Only one nonzero gradient component in the eigenvector basis implies the condition

$$H(x)g(x) = \lambda(x)g(x)$$

- It should be possible to follow gradient extremals between stationary points

Gradient extremals as optimum ascent paths

- A gradient extremal corresponds to an optimum ascent path



- Optimize the gradient norm on a contour line $f(x) = k$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\tilde{g}g - 2\mu(f(x) - k)\right] = 0 \quad \Rightarrow \quad H(x)g(x) = \mu(x)g(x)$$

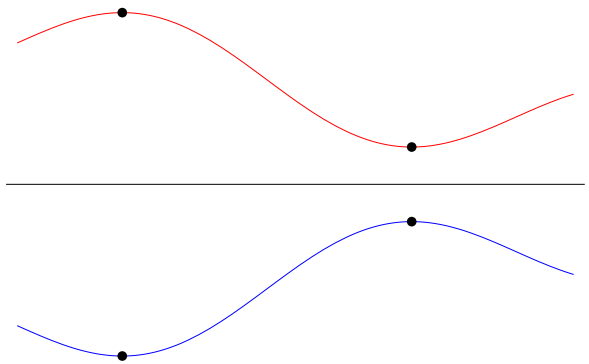
- Some properties of gradient extremals:
  - locally defined, intersect at stationary points
  - not necessarily tangent to gradient, curves a lot and difficult to follow

Image functions

- Imagine a function $\bar{f}(x)$ with the following properties

$f(x)$		$\bar{f}(x)$
minimum	$\leftrightarrow$	saddle point
saddle point	$\leftrightarrow$	minimum

  - the function $\bar{f}(x)$ is said to be the image function of $f(x)$
- We may locate a saddle point of $f(x)$ by minimizing $\bar{f}(x)$!
  - a trivial example:



- In general, we cannot construct an image function—it may not even exist
  - however, we know its gradient and Hessian
  - this is sufficient for second-order optimizations

Trust-region image minimization

- The gradient and Hessians of a function f and its image $\bar{f}$ are related as

$$\phi(x) = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}, \quad \lambda(x) = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

$$\bar{\phi}(x) = \begin{bmatrix} -\phi_1 \\ \phi_2 \end{bmatrix}, \quad \bar{\lambda}(x) = \begin{bmatrix} -\lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

- To minimize $\bar{f}(x)$, we must use the trust-region method—line search is impossible
- The level-shifted Newton step for the image function is now given by

$$s(\mu) = -(\bar{H}_c - \mu 1)^{-1}\bar{g}_c = -\frac{\bar{\phi}_1}{\bar{\lambda}_1 - \mu}\vec{v}_1 - \frac{\bar{\phi}_2}{\bar{\lambda}_2 - \mu}\vec{v}_2$$

$$= -\frac{\phi_1}{\lambda_1 + \mu}\vec{v}_1 - \frac{\phi_2}{\lambda_2 - \mu}\vec{v}_2$$

  - a simple sign change in the level-shift parameter μ for one mode
  - the level-shifted Newton method maximizes this mode and minimize all others
- Trust-region image minimization is typically applied to the lowest Hessian mode
  - robust but not selective