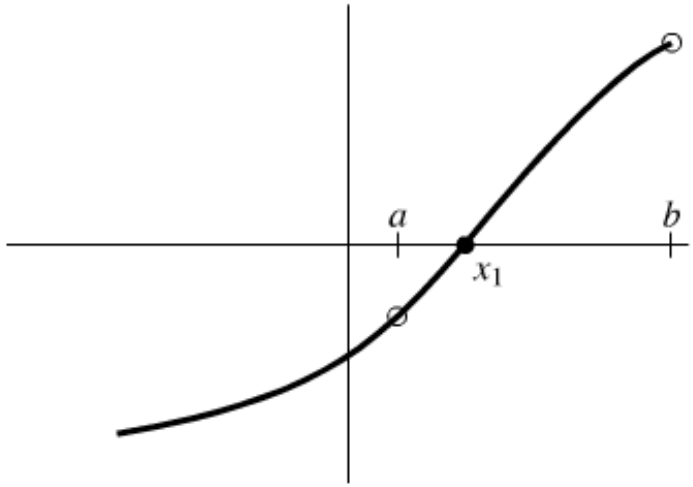
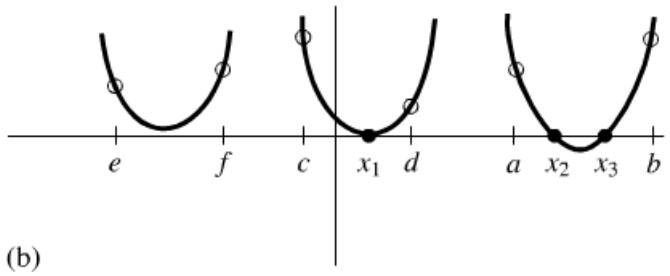
LECTURE 6: Nonlinear Equations and Optimization

- The topic is related to optimization (Lecture 8) so we cover solving nonlinear equations and 1-d optimization here
- $f(x) = 0$ (either in 1-d or many dimensions)
- In 1-d we can bracket the root and then find it, in many dims we cannot
- Bracketing in 1-d: if $f(x) < 0$ at a and $f(x) > 0$ at $b > a$ (or the other way around) and f(x) is continuous then there is a root at $a < x < b$



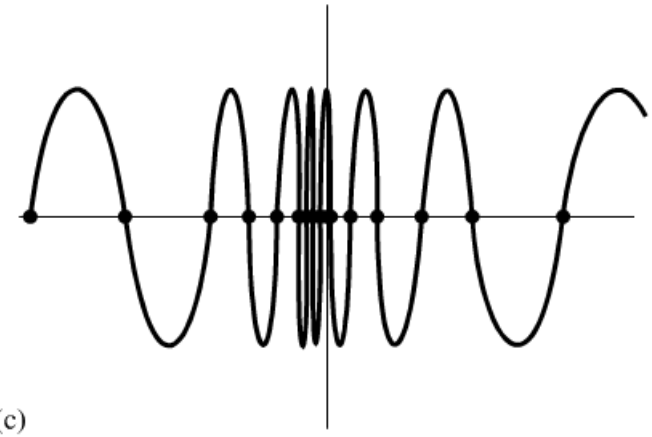
Other Situations:

- No roots or one or two roots but no sign change:



(b)

- Many roots: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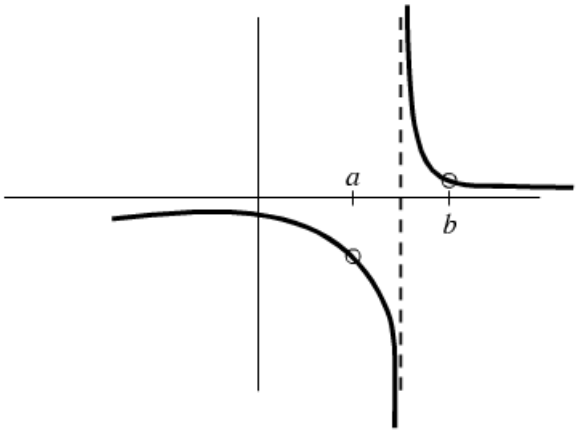
- Singularity:



(d)

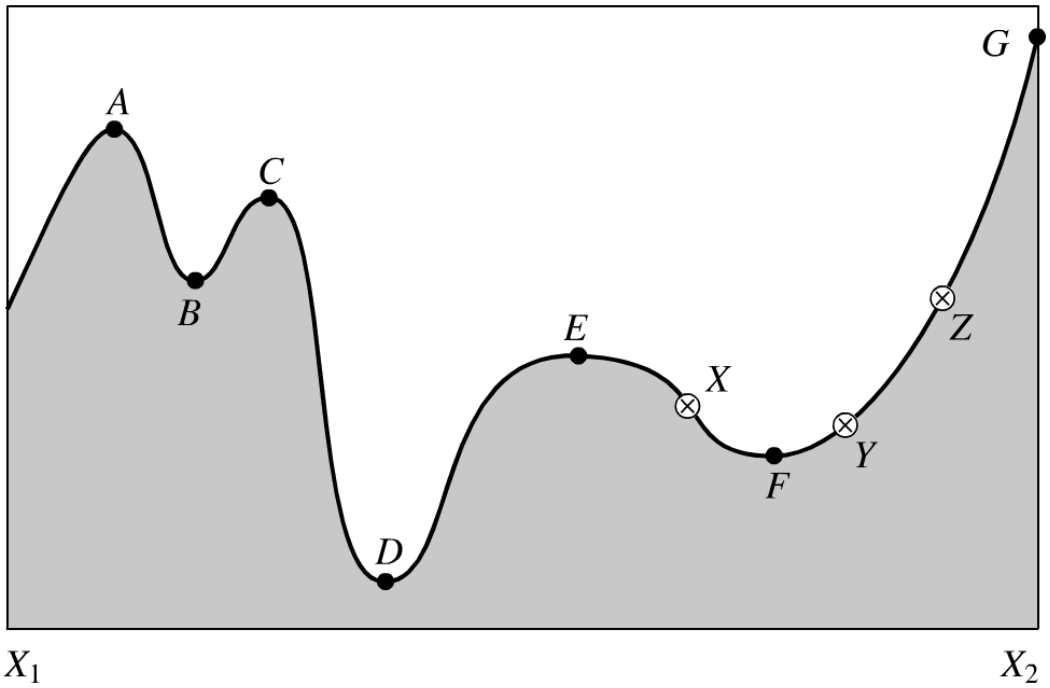
Bisection for Bracketing

- We can use bisection: divide interval by 2, evaluate at the new position, and choose left or right half-interval depending on where the function has opposite sign. Number of steps is $log_2[(b\text{-}a)/\varepsilon]$, where e is the error tolerance. The method must succeed.
- Error at next step is $\varepsilon_{n+1} = \varepsilon_n/2$, so converges linearly
- Higher order methods scale as $\varepsilon_{n+1} = c\varepsilon_n^m$, with $m > 1$

1-d Optimization: Local and Global Extrema, Bracketing

- Optimization: minimization or maximization
- In most cases only local minimum (B,D,F) or local maximum (A,C,E,G) can be found, difficult to prove they are global minimum (D) or global maximum (G)

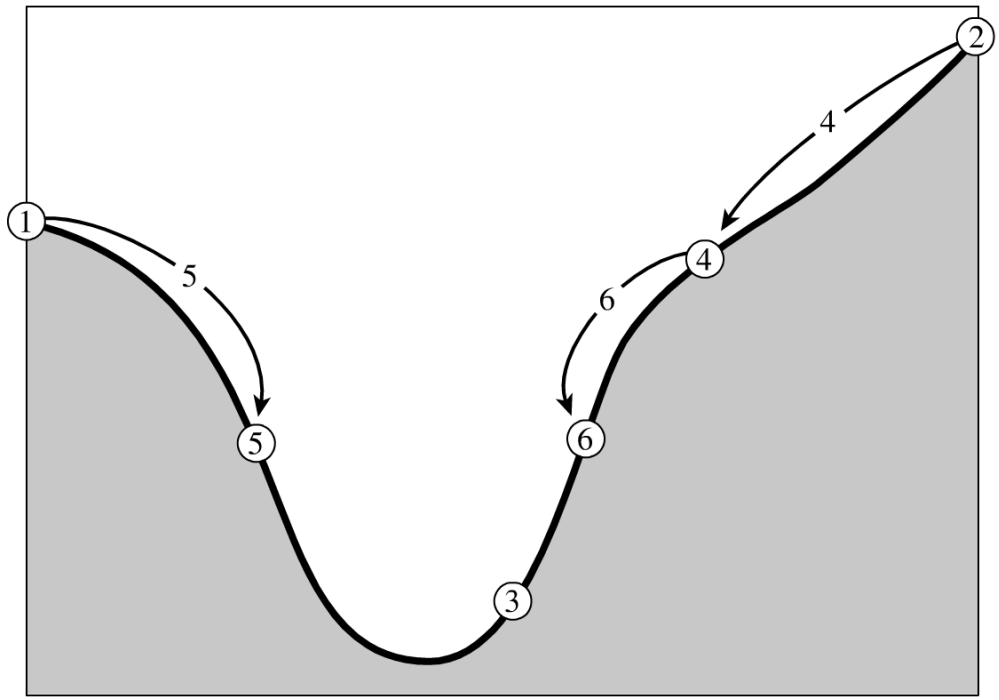
- We bracket a local minimum if we find $f(X) > f(Y)$ and $f(Z) > f(Y)$ for $X < Y < Z$.



Golden Ratio Search

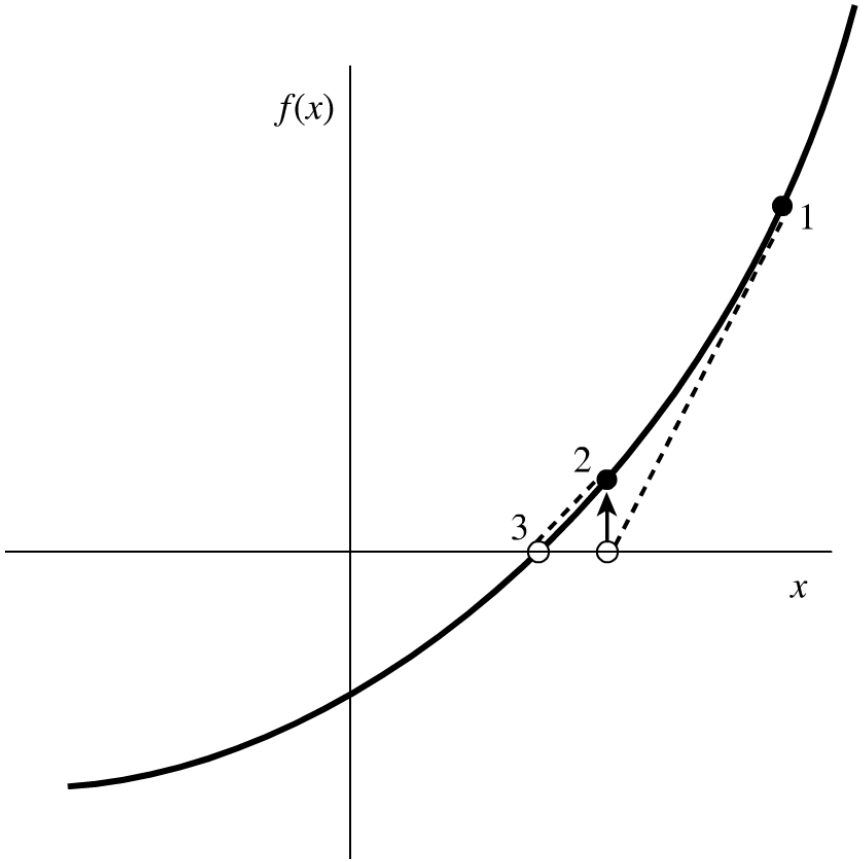
- Remember that we need a triplet of points to bracket $a < b < c$ such that $f(b)$ is less than $f(a)$ and $f(c)$
- Suppose w = $(b-a)/(c-a)$. We evaluate at x, define $(x-b)/(c-a) = z$. The next bracketing segment will be either w+z or 1-w.

To minimize the error choose these two to be equal: $z = 1 - 2w$.
But w was also chosen this way, so $z/(1-w) = w$,
and $w = (3-5^{1/2})/2 = 0.382$,
$1 - w = 0.618$,
Golden Ratio
$(1/0.618 = 1.618 = (1+5^{1/2})/2)$.

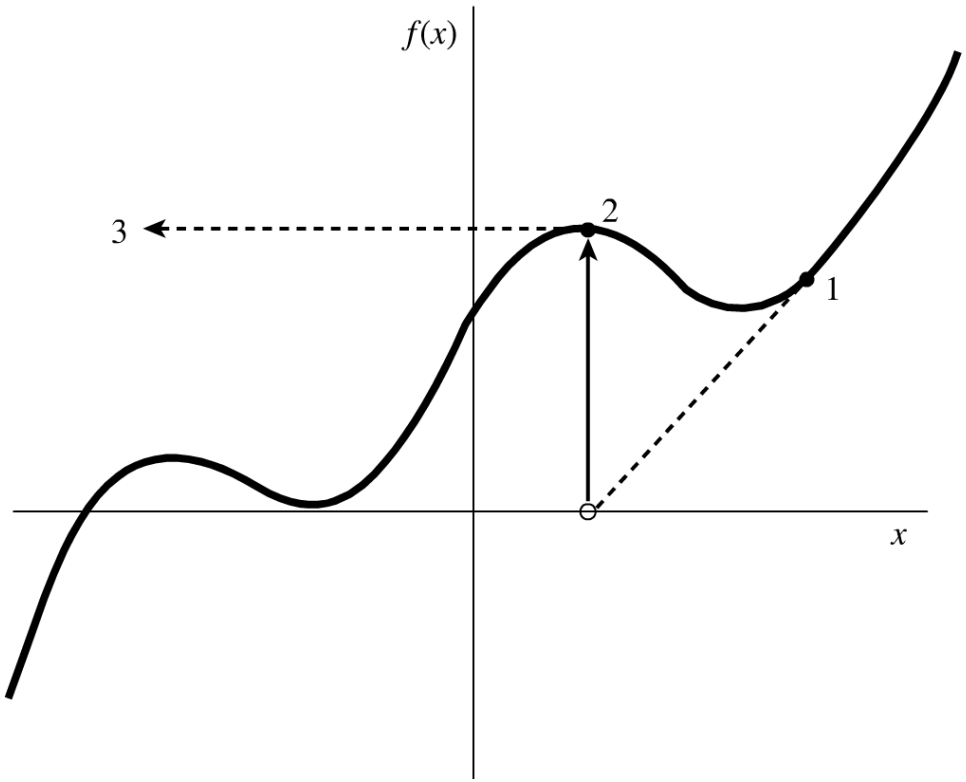


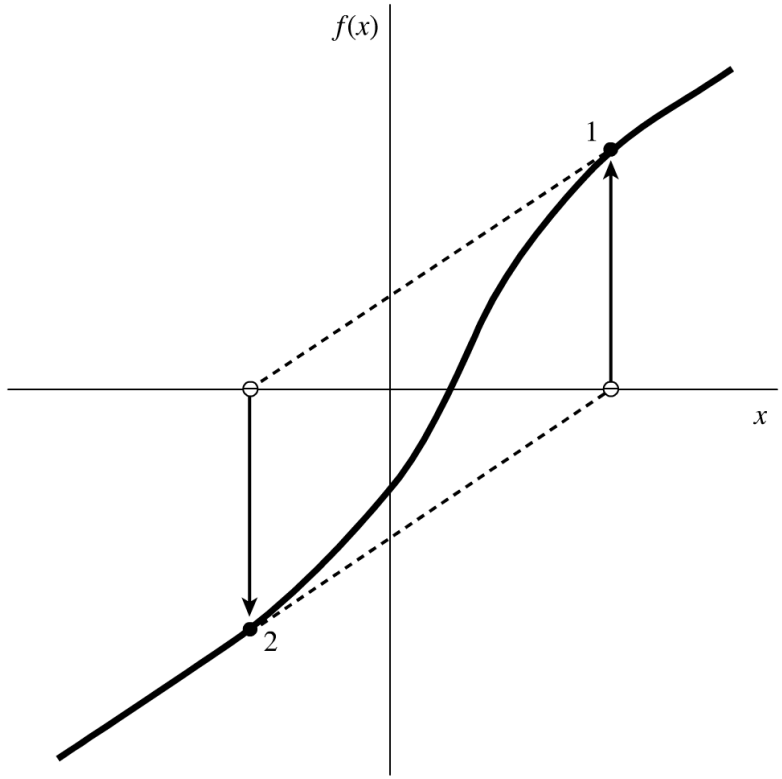
Newton(-Raphson) Method

- Most celebrated of all methods, we will use it extensively in higher dimensions
- Requires a gradient:
  $f(x+\delta) = f(x) + \delta f'(x) + \ldots$
- We want $f(x+\delta) = 0$, hence
  $\delta = -f(x)/f'(x)$
- Rate of convergence is quadratic (NR 9.4)
  $\varepsilon_{i+1} = \varepsilon_i^2 f''(x)/(2f'(x))$



Newton-Raphson is not Failure-free



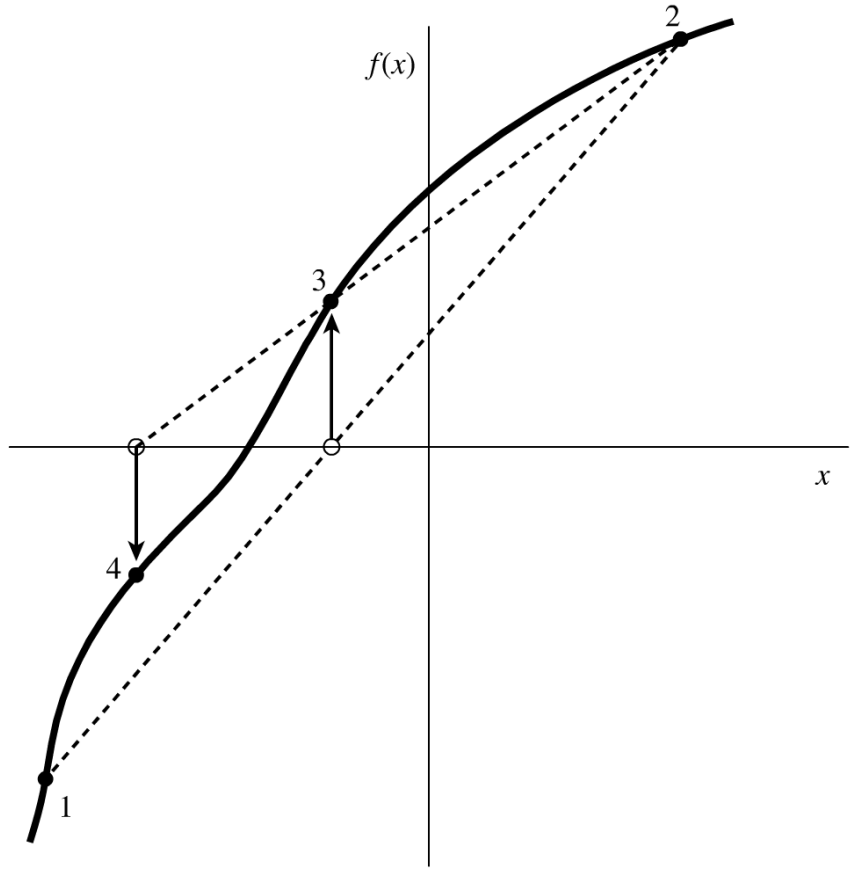


Newton-Raphson for 1-d Optimization

- Expand function to 2nd order (note: we did this already when expanding log likelihood)
- $f(x+\delta) = f(x) + \delta f'(x) + \delta^2 f''(x)/2 + \ldots$
- Expand its derivative $f'(x+\delta) = f'(x) + \delta f''(x) + \ldots$
- Extremum requires $f'(x+\delta) = 0$ hence $\delta = -f'(x)/f''(x)$
- This requires f'': Newton's optimization method
- In least square problems we sometimes only need f'^2: Gauss-Newton method (next lecture)

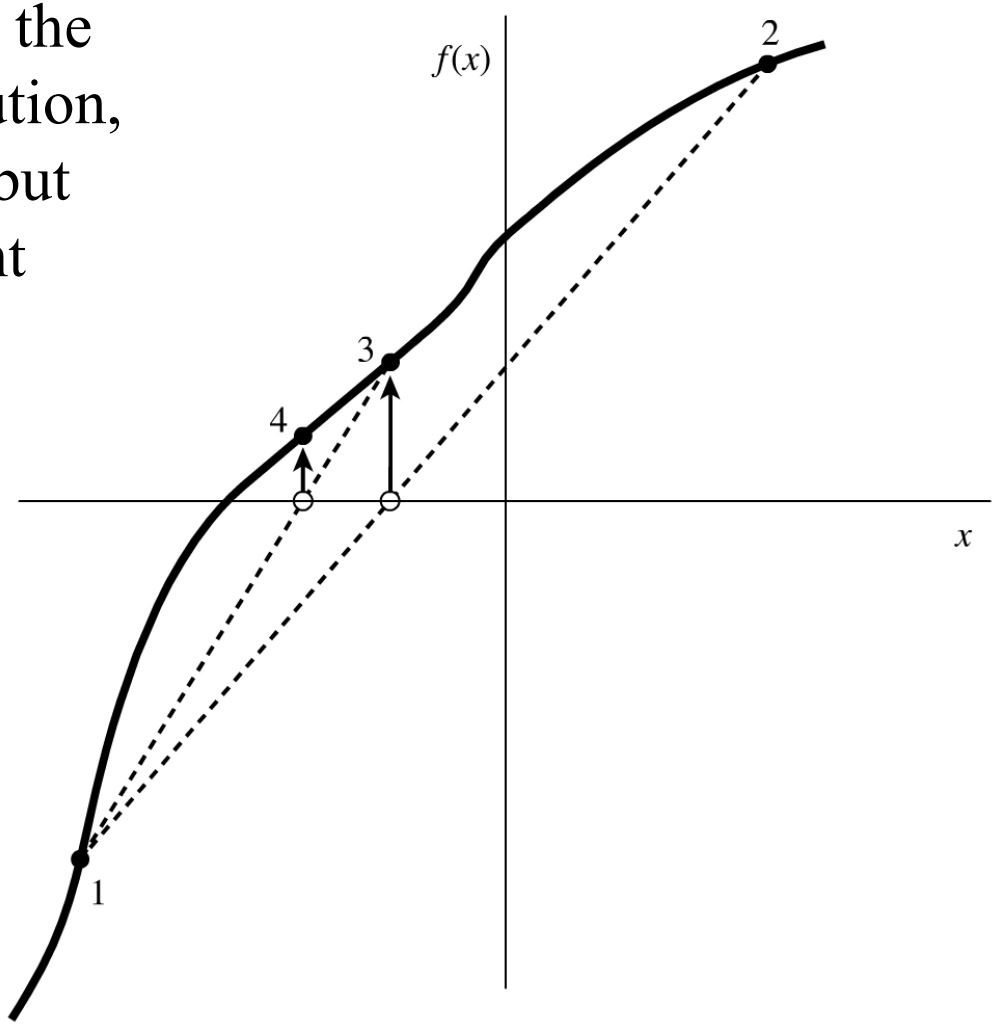
Secant Method for Nonlinear Equations

- Newton's method using numerical evaluation of a gradient defined across the entire interval:
  $f'(x_2) = [f(x_2)-f(x_1)]/(x_2-x_1)$
- $x_3 = x_2 - f(x_2)/f'(x_2)$
- Can fail, since does not always bracket
- $m = 1.618$ (golden ratio), a lot faster than bisection

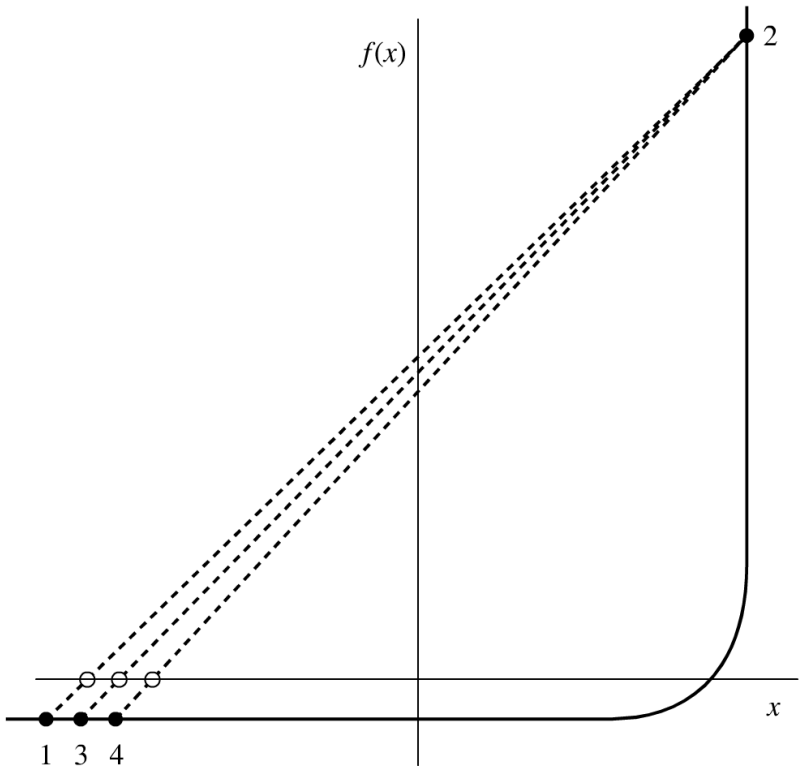


False Position Method for Nonlinear Equations

- Similar to secant, but keep the points that bracket the solution, so guaranteed to succeed, but with more steps than secant



Sometimes convergence can be slow

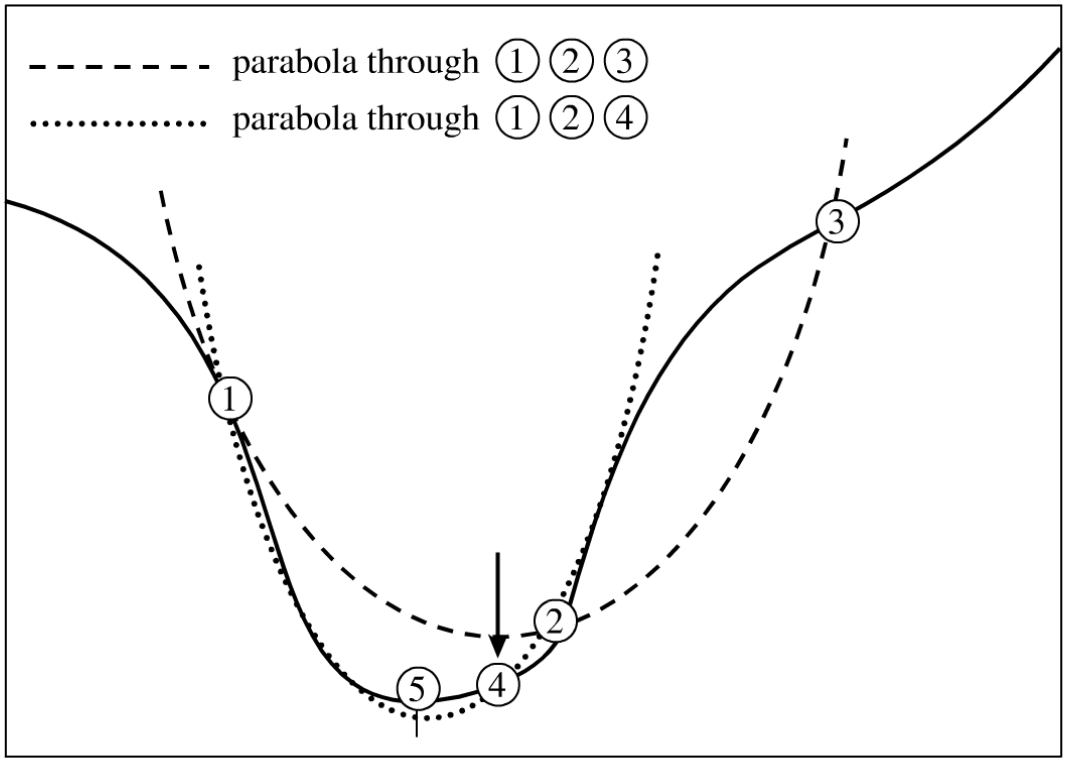


Better methods without derivatives such as Ridders or Brent's method combine these basic techniques: use these as default option and (optionally) switch to Newton once the solution is guaranteed for a higher convergence rate

Parabolic Method for 1-d Optimization

- Approximate the function of a, b, c as a parabola

$$x = b - \frac{1}{2}\frac{(b-a)^2[f(b)-f(c)] - (b-c)^2[f(b)-f(a)]}{(b-a)[f(b)-f(c)] - (b-c)[f(b)-f(a)]}$$

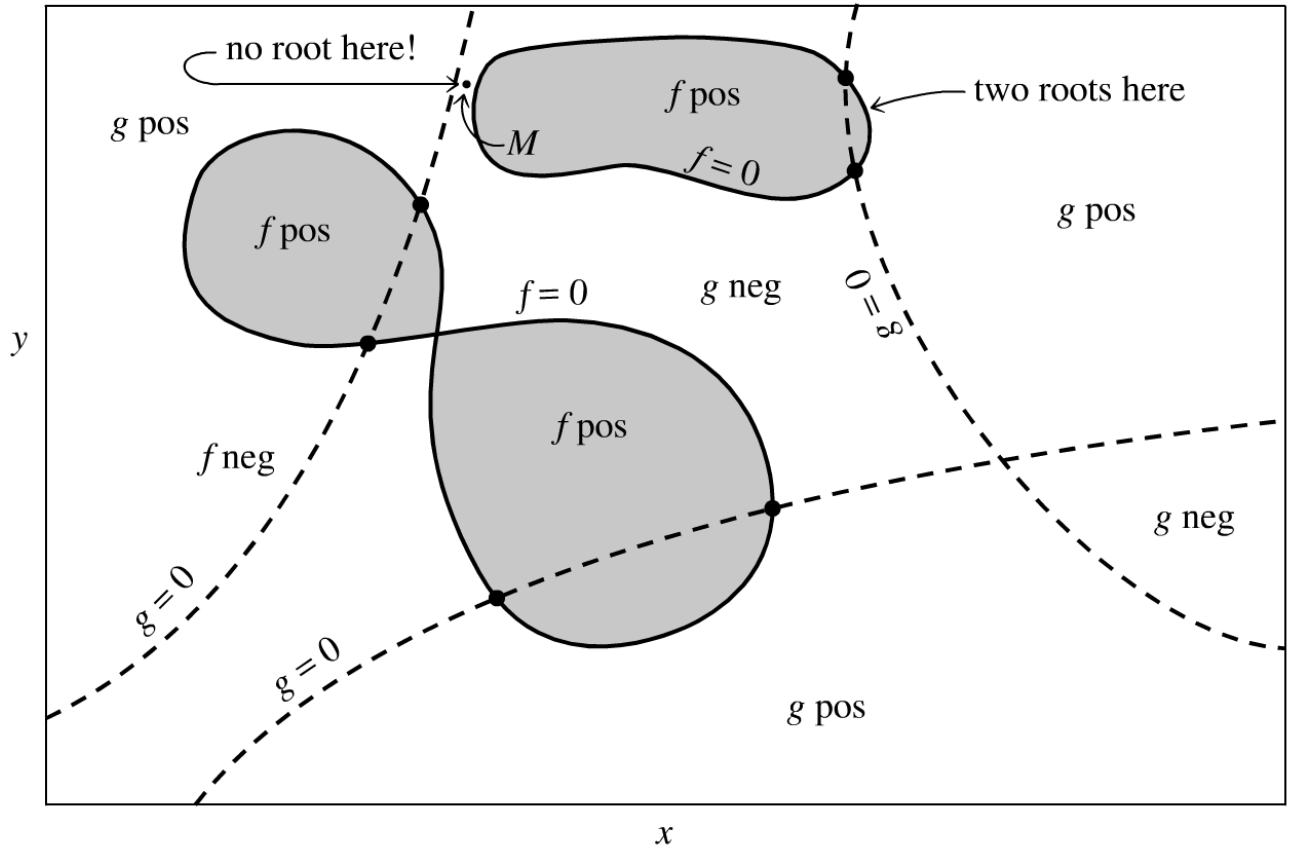


Gradient Descent in 1-d

- Suppose we do not have f'', but we have f': so we know the direction of function descent. We can take a small step in that direction: $\delta = -\eta f'(x)$. We must choose the sign of η to descend (if minimum is what we want) and it must be small enough not to overshoot.
- We can make a secant version of this method by evaluating gradient with finite difference: $f'(x_2) = [f(x_2)-f(x_1)]/(x_2-x_1)$

Nonlinear Equations in Many Dimensions

- $f(x,y) = 0$ and $g(x,y) = 0$: but the two functions f and g are unrelated, so it is difficult to look for general methods that will find all solutions



Newton-Raphson in Higher Dimensions

- Assume N functions

$$F_i(x_0, x_1, \ldots, x_{N-1}) = 0 \qquad i = 0, 1, \ldots, N-1.$$

- Taylor expand $F_i(\mathbf{x} + \delta\mathbf{x}) = F_i(\mathbf{x}) + \sum_{j=0}^{N-1} \frac{\partial F_i}{\partial x_j} \delta x_j + O(\delta\mathbf{x}^2).$
- Define Jacobian $J_{ij} \equiv \frac{\partial F_i}{\partial x_j}$
- In matrix notation $\mathbf{F}(\mathbf{x} + \delta\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J} \cdot \delta\mathbf{x} + O(\delta\mathbf{x}^2).$
- Setting $\mathbf{F}(\mathbf{x} + \delta\mathbf{x}) = 0$, we find $\mathbf{J} \cdot \delta\mathbf{x} = -\mathbf{F}$.
- This is a matrix equations: solve with LU
- Update $\mathbf{x}_{\rm new} = \mathbf{x}_{\rm old} + \delta\mathbf{x}$ and iterate again

Globally Convergent Methods and Secant Methods

- If quadratic approximation in N-R method is not accurate taking a full step may make the solution worse. Instead one can do a line search backtracking and combine it with a descent direction (or use a thrust region).
- When derivatives are not available we can approximate them: multi-dimensional secant method (Broyden's method).
- Both of these methods have clear analogies in optimization and since the latter is more important for data science we will explain the concepts in optimization lecture next.

Relaxation Methods

- Another class of methods solving $x = f(x)$
- Take $x = 2\text{-}e^{-x}$, start at $x_0 = 1$ and evaluate
  $f(x_0) = 2\text{-}e^{-1} = 1.63 = x_1$
- Now use this solution again: $f(x_1) = 2\text{-}e^{-1.63} = 1.80 = x_2$
- Correct solution is $x = 1.84140\ldots$
- If there are multiple solutions which one one converges to depends on the starting point
- Convergence is not guaranteed: suppose x^0 is exact solution:
  $x_{n+1} = f(x_n) = f(x^0) + (x_n\text{-}x^0)f'(x^0) + \ldots$ since $x^0 = f(x^0)$ we get
  $x_{n+1}\text{-}x^0 = f'(x^0)(x_n\text{-}x^0)$ so this converges if $|f'(x^0)| < 1$
- When this is not satisfied we can try to invert the equation to get $u = f^{-1}(u)$ so that $|f'^{-1}(u)| < 1$

Relaxation Methods in Many Dimensions

- Same idea: write equations as $x = f(x,y)$ and $y = g(x,y)$, use some good starting point and see if you converge
- Easily generalized to N variables and equations
- Simple, and (sometimes) works!
- Again impossible to find all the solutions unless we know something about their structure

Over-relaxation

- We can accelerate the convergence:
- $\Delta x_n = x_{n+1} - x_n = f(x_n) - x_n$
- $x_{n+1} = x_n + (1+\omega)Dx_n$
- if $\omega = 0$ this is relaxation method
- If $\omega > 0$ this is over-relaxation method
- No general theory for how to select ω : trial and error

Optimization in many dimensions

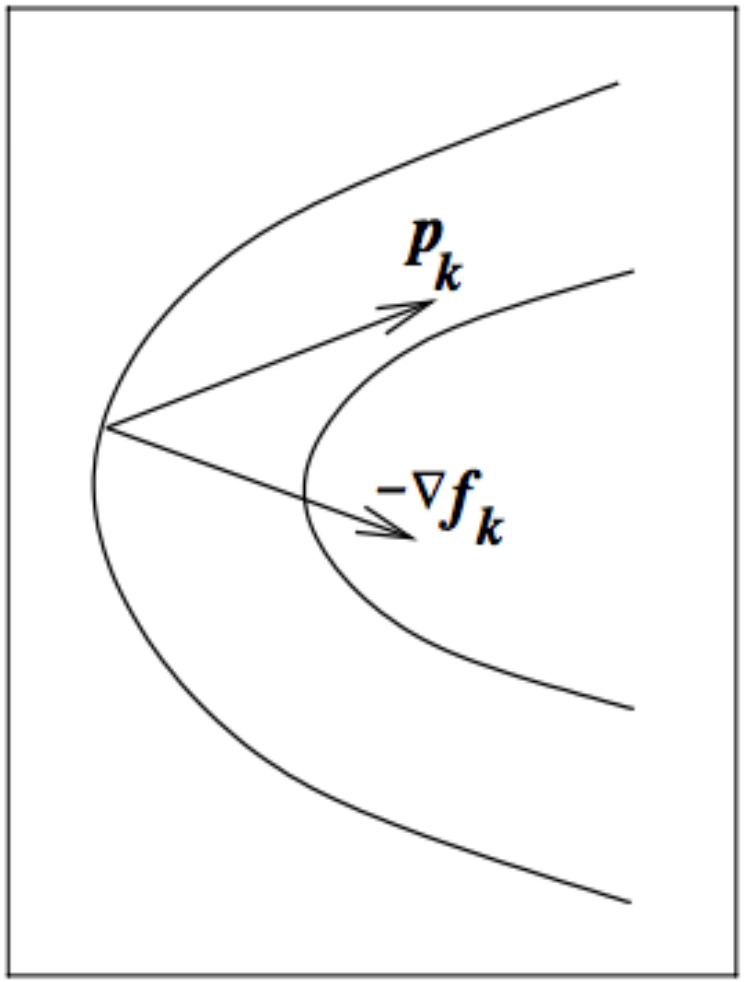
- Optimization (maximization/minimization) is of huge importance in data analysis and is the basis for recent breakthroughs in machine learning and big data
- A lot of it is application dependent and there is a vast number of methods developed: we cannot cover them all in this lecture
- Broadly can be divided into 1^{st} order (derivatives are available, but not Hessian) and 2^{nd} order (approximate Hessian or full Hessian evaluation)
- 0^{th} order: no gradients available: use finite difference to get the gradient or use downhill simplex (Nelder & Mead method). Very slow and we will not discuss them here.

Preparation of Parameters

- Often the parameters are not unconstrained: they may be positive (or negative), or bounded to an interval
- First step is to make optimization unconstrained: map the parameter to a new parameter that is unbounded. For example, if a variable is positive, $x > 0$, use $z = log(x)$ instead of x.
- One can also change the prior so that it reflects the original prior: $p_{pr}(z)dz = p_{pr}(x)dx$
- If $x > 0$ has uniform prior in x then $p_{pr}(z) = dx/dz = x = e^z$

General Strategy

- We want to descend down a function $J(a)$ (if minimizing) using iterative sequence of steps at a_t. For this we need to choose a direction p_t and move in that direction: $J(a_t+\eta p_t)$
- A few options: fix η
- line search: vary η until $J(a_t+\eta p_t)$ is minimized
- Trust region: construct an approximate quadratic model for J and minimize it but only within trust region where quadratic model is approximately valid



Line Search Directions and Backtracking

- Gradient descent: Gradient $-\nabla_a J(a,x_t)$
- Newton: Inverse Hessian H^{-1} times gradient
  $-H^{-1}\ \nabla_a J(a)$
- Quasi-Newton: approximate H^{-1} with B^{-1} (SR1 and BFGS)
- Nonlinear conjugate gradient:
  $p_t = -\nabla_a J(a,x_t) + \beta_t p_{t-1}$, where p_{t-1} and p_t are conjugate
- Step length with backtracking: choose first proposed length
- If it does not reduce the function value reduce it by some factor, check again
- Repeat until step length is ε, at that point switch to gradient descent

Trust Region Method

- Multi-dim parabola method: define approximate quadratic function, but limit the step

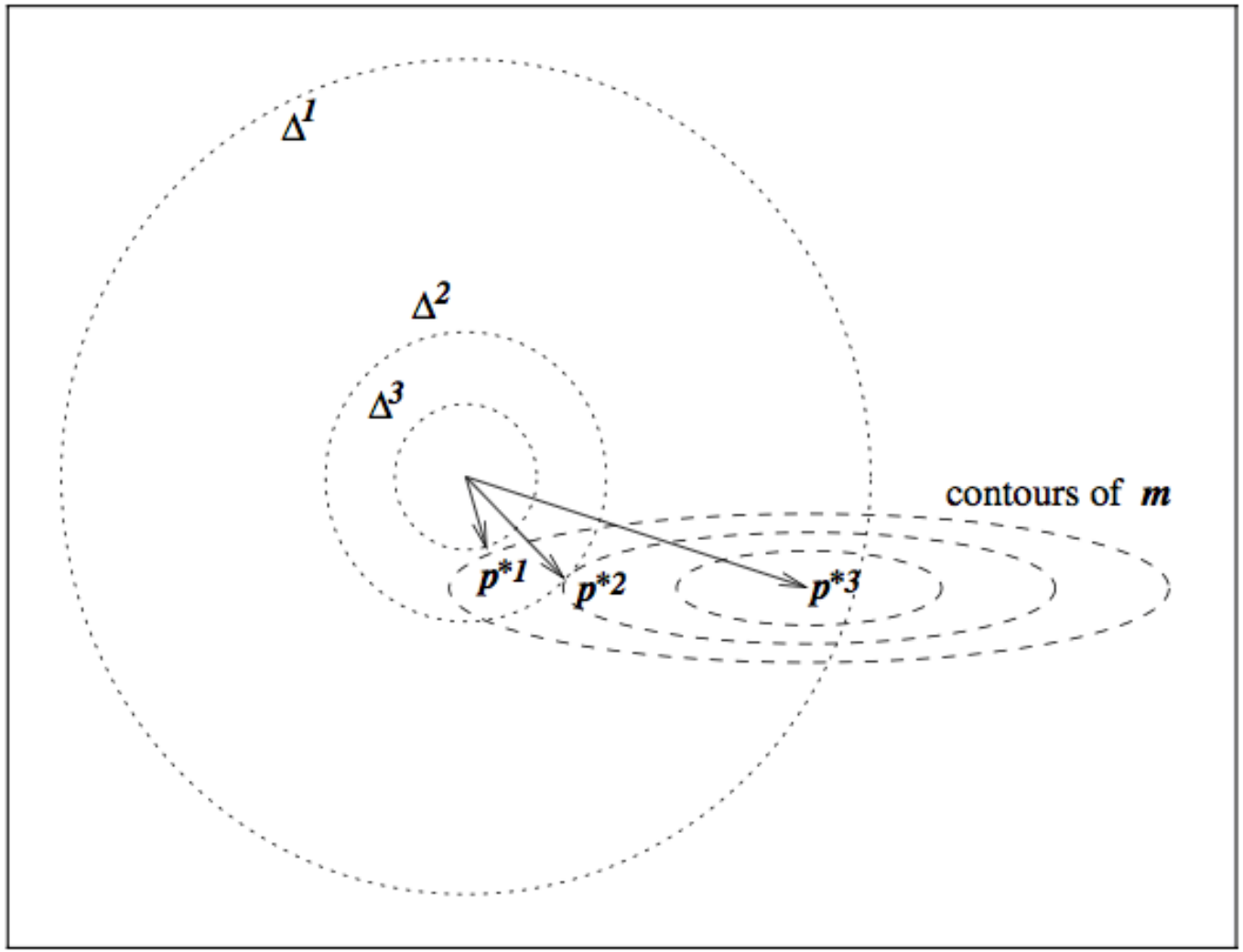
$$\min_{p\in\mathbb{R}^n} m_k(p) = f_k + g_k^T p + \tfrac{1}{2} p^T B_k p \qquad \text{s.t. } \|p\| \le \Delta_k$$

- Here Δ_k is trust region radius
- Evaluate at previous iteration and compare the actual reduction to predicted reduction

$$\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}$$

- If ρ_k around 1 we can increase Δ_k
- If close to 0 or negative we shrink Δ_k

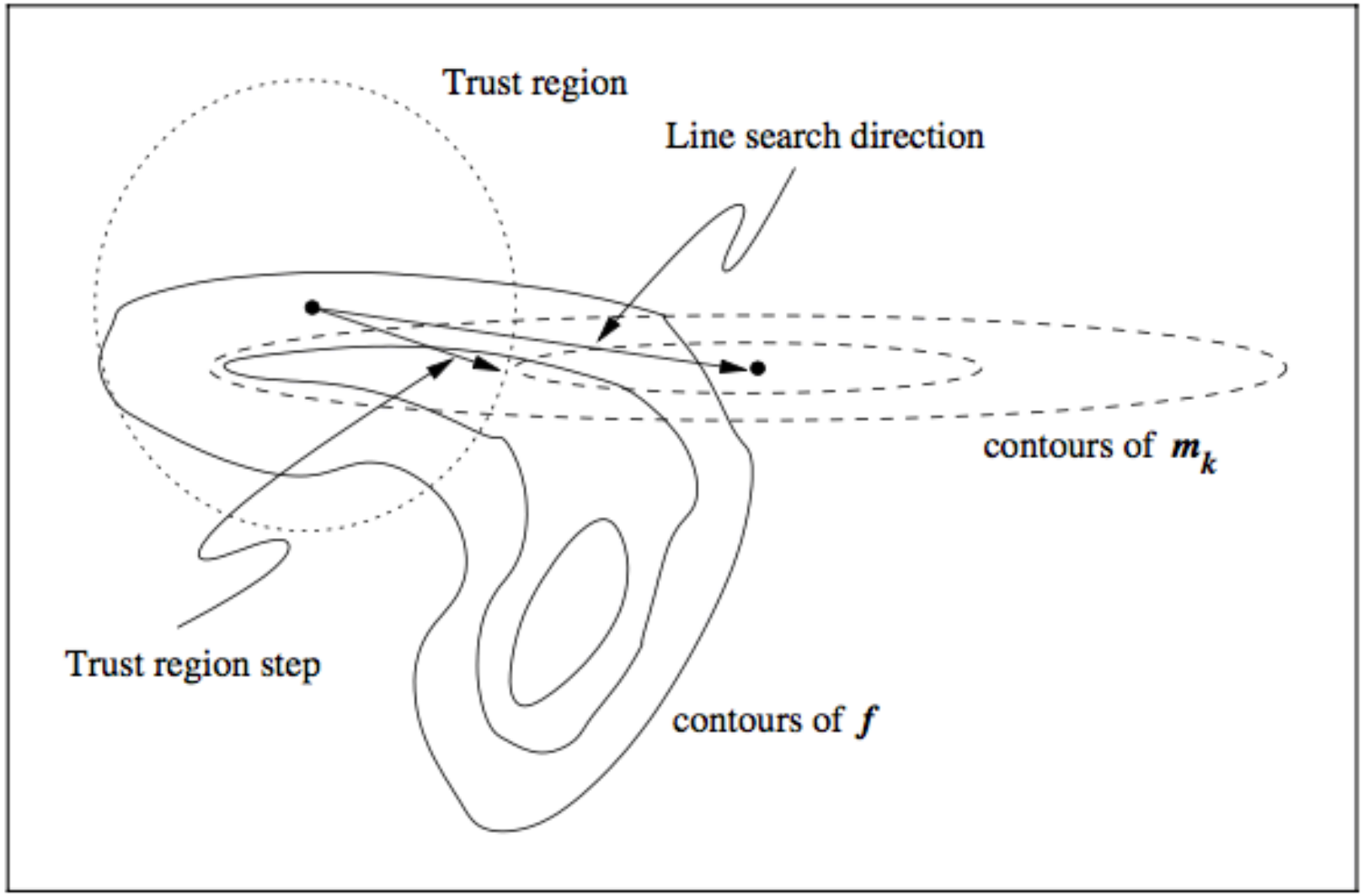
- If trust region covers *m* center step there
- Otherwise direction of step changes



Constrained Optimization: Lagrange Multiplier Method

- If the center of m is inside trust region step there
- Otherwise we must solve constrained optimization
- We solve this optimization with Lagrange multiplier method: minimize $f + g^T p + p^T B p + \lambda\,(p^2 - \Delta^2)$ with respect to p and λ. Gradient w.r.t. λ gives the constraint $p^2 = \Delta^2$, thus the constraint is automatically satisfied. This determines the value of λ.
- Minimization with respect to p now includes λp^2
- As a result the step direction is not towards center of m when trust region does not cover it: see picture on next slide

Line Search vs. Trust Region



1st Order: Gradient Descent

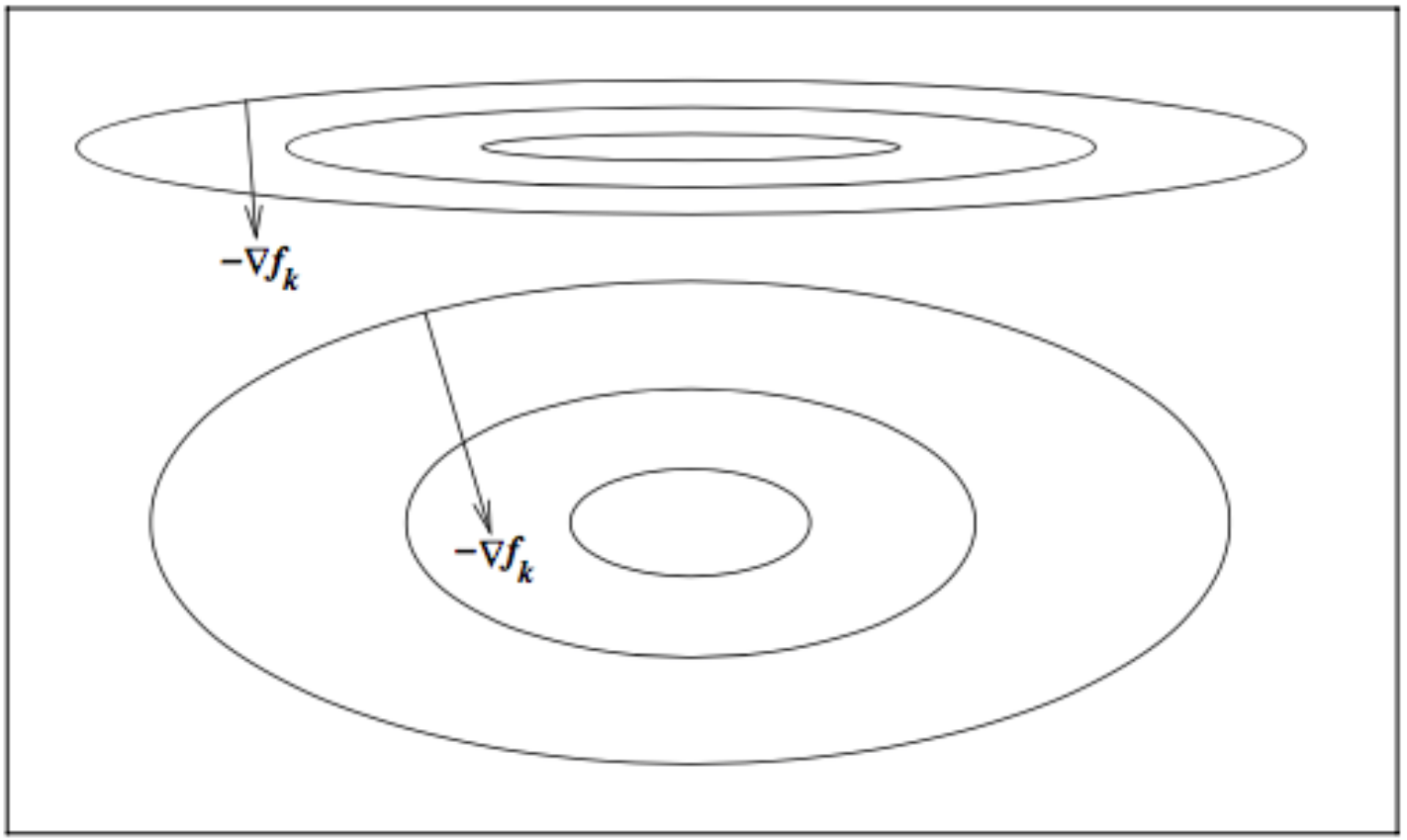
- We have a vector of parameters a and a scalar loss (cost) function $J(a,x,y)$ which is a function of a data vector (x,y) we want to optimize (say minimize). This could be a nonlinear least square loss function: $J = \chi^2$

$$\chi^2(\mathbf{a}) = \sum_{i=0}^{N-1} \left[\frac{y_i - y(x_i|\mathbf{a})}{\sigma_i} \right]^2$$

- (Batch) gradient descent updates all the variables at once: $\delta a = - \eta \nabla_a J(a)$: in ML. η is called learning rate
- It gets stuck on saddle points, where gradient is 0 everywhere (see animation later)

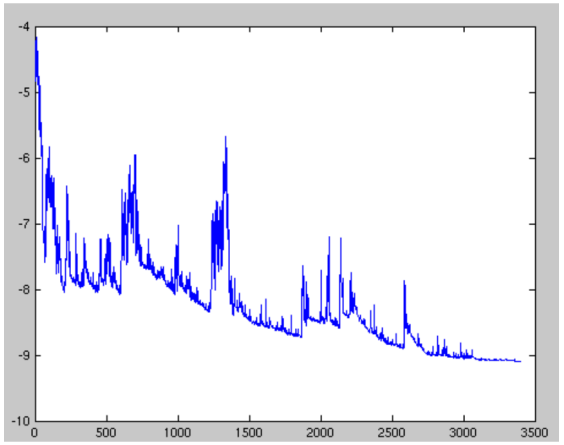
Scaling

- Change variables to make surface more circular
- Example: change of dimensions



Stochastic Gradient Descent

- Stochastic gradient descent: do this just for one data pair x_i, y_i: $\delta a = -\eta \nabla_a J(a, x_i, y_i)$
- This saves on computational cost, but is noisy, so one repeats it by randomly choosing data i
- Has large fluctuations in the cost function

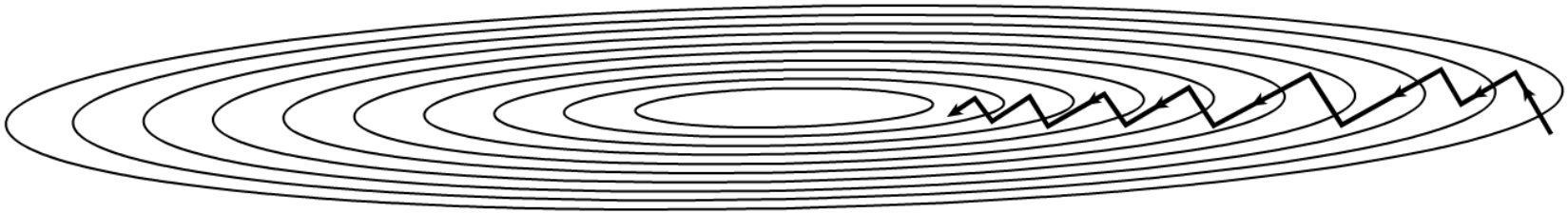


- This is potentially a good thing: it may avoid getting stuck in the local minima (or saddle points)
- Learning rate is slowly reduced
- Has revolutionized machine learning

Mini-batch Stochastic Gradient

- Mini-batch takes advantage of hardware and software implementations where a gradient w.r.t. to a number of data points can be evaluated as fast as a single data (e.g. mini-batch of $N = 256$)
- Challenges of (stochastic) gradient descent: how to choose learning rate (in 2nd order methods this is given by Hessian)
- Ravines:

Ravines

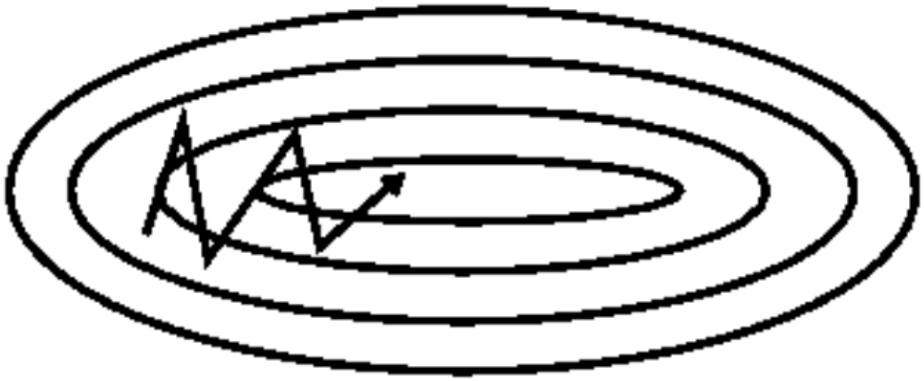


(a)

(b)

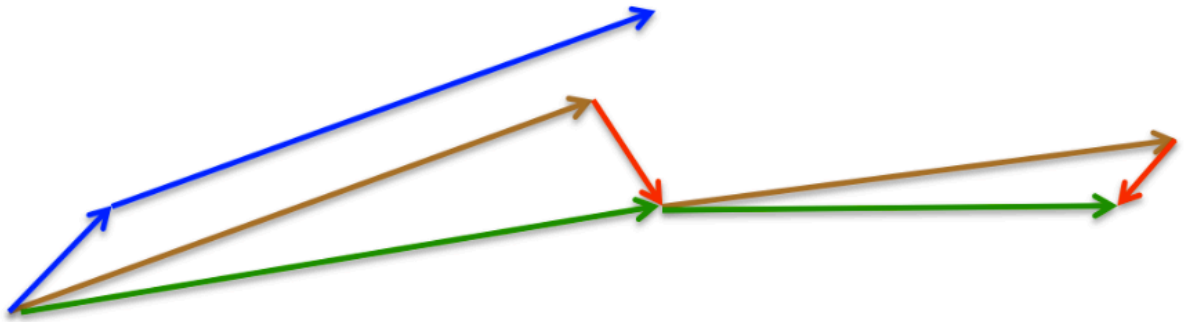
Adding Momentum: Rolling down the hill

- We can add momentum and mimic a ball rolling down the hill
- Use previous update as the direction
- $v_t = \gamma v_{t-1} + \eta \nabla_a J(a)$, $da = -v_t$ with γ of order 1 (e.g. 0.9)
- Momentum increases for directions where gradient does not change



Nesterov Accelerated Gradient

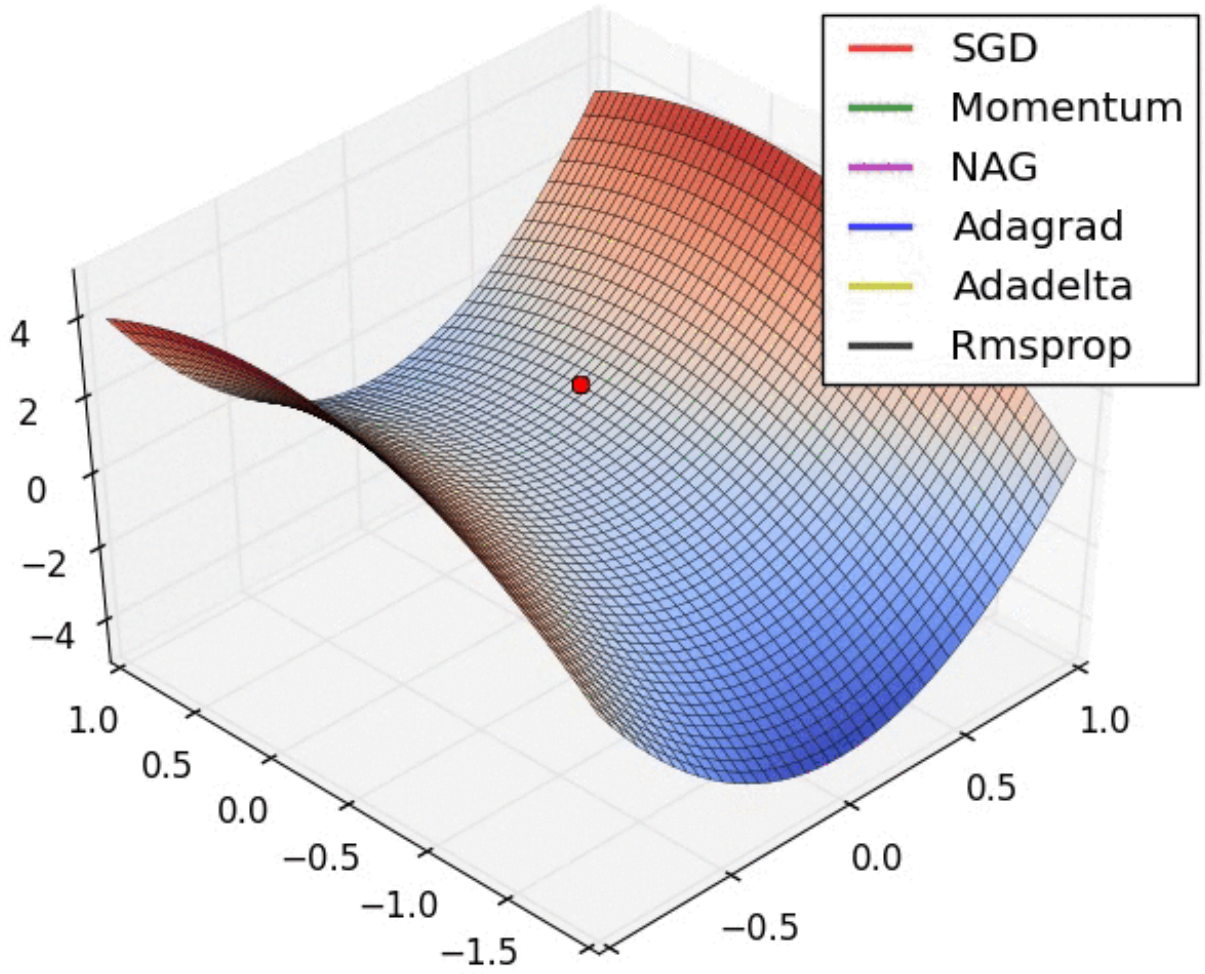
- We can predict where to evaluate next gradient using previous velocity update
- $v_t = \gamma v_{t-1} + \eta \nabla_a J(a - \gamma v_{t-1})$, $\delta a = -v_t$
- Momentum (blue) vs NAG (brown+red=green)



- See https://arxiv.org/abs/1603.04245 for theoretical justification of NAG based on a Bregman divergence Lagrangian

Adagrad, Adadelta, Rmsprop, ADAM, …

- Make the learning rate h dependent on a_i
- Use past gradient information to update h
- Example ADAM: ADAptive Momentum estimation
- $m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t \qquad g_t = \nabla_a J(a)$
- $v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
- bias correction: $m_t' = m_t/(1-\beta_1)$, $v_t' = v_t/(1-\beta_2)$
- Update rule: $\delta a = -\eta/(v_t'^{1/2} + \varepsilon)$
- Recommended values $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\varepsilon = 10^{-8}$
- The methods are empirical (show animation)


SGD
Momentum
NAG
Adagrad
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2
0
−2
−4
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0.0
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−1.0
−1.5
1.0
0.5
0.0
−0.5

2nd Order Method: Newton

- We have seen that there is no natural way to choose learning rate in 1st order methods
- But Newton's method provides a clear answer what the learning rate should be:
- $J(a+\delta a) = J(a) + \delta a \nabla_a J(a) + \delta a \delta a' \nabla_a \nabla_{a'} J(a)/2 \ldots$
- Hessian $H_{ij} = \nabla_{a\_i} \nabla_{a\_j} J(a)$
- At the extremum we we want $\nabla_a J(a) = 0$ so a Newton update step is $\delta a = -H^{-1} \nabla_a J(a)$
- We do not need to guess the learning rate
- We do need to evaluate Hessian and invert it (or use LU): expensive in many dimensions!
- In many dimensions we use iterative schemes to solve this problem

Quasi-Newton

- Computing Hessian and inverting it is expensive, but one can approximate it with a low rank tensor
- Symmetric rank 1 (SR1) $s_k = x_{k+1} - x_k, \qquad y_k = \nabla f_{k+1} - \nabla f_k$

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k} \qquad B_{k+1} s_k = y_k$$

- BFGS (rank 2 update, positive definite)

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$$

- Inverse (Woodburry formula)

$$B_{k+1}^{-1} = \left(I - \rho_k s_k y_k^T\right) B_k^{-1} \left(I - \rho_k y_k s_k^T\right) + \rho_k s_k s_k^T, \qquad \rho_k = \frac{1}{y_k^T s_k}$$

L-BFGS

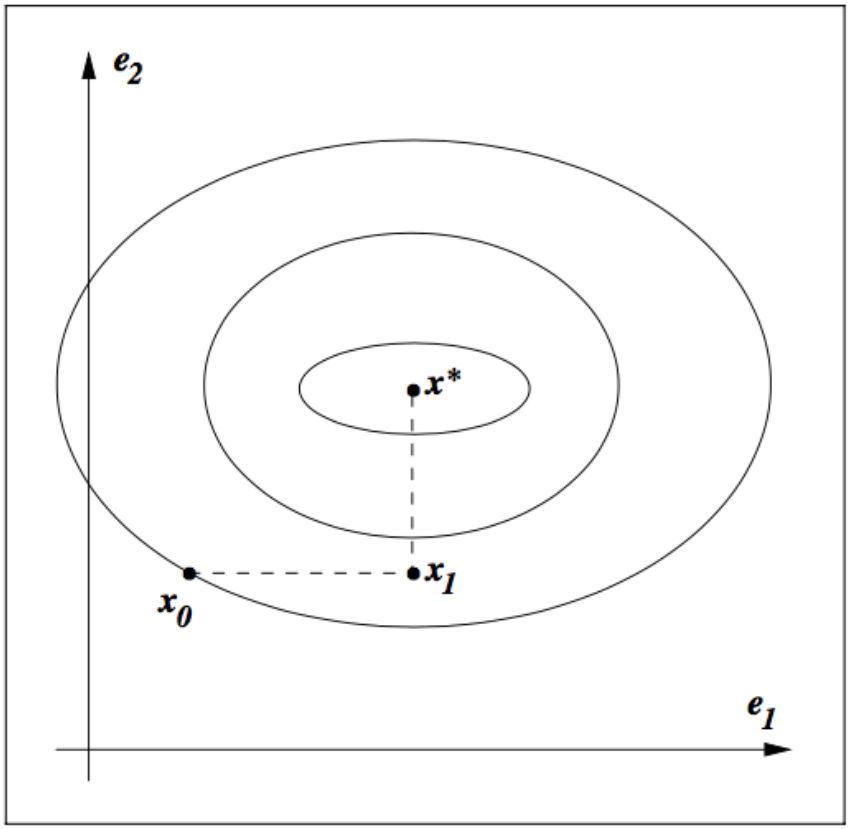
- For large problems this gets too expensive. Limited memory BFGS updates only based on last N iterations (N of order 10-100)
- In practice increasing N often does not improve the results
- Historical note: quasi-Newton methods originate from W.C. Davidon's work in 1950s, a physicist at Argonne national lab.

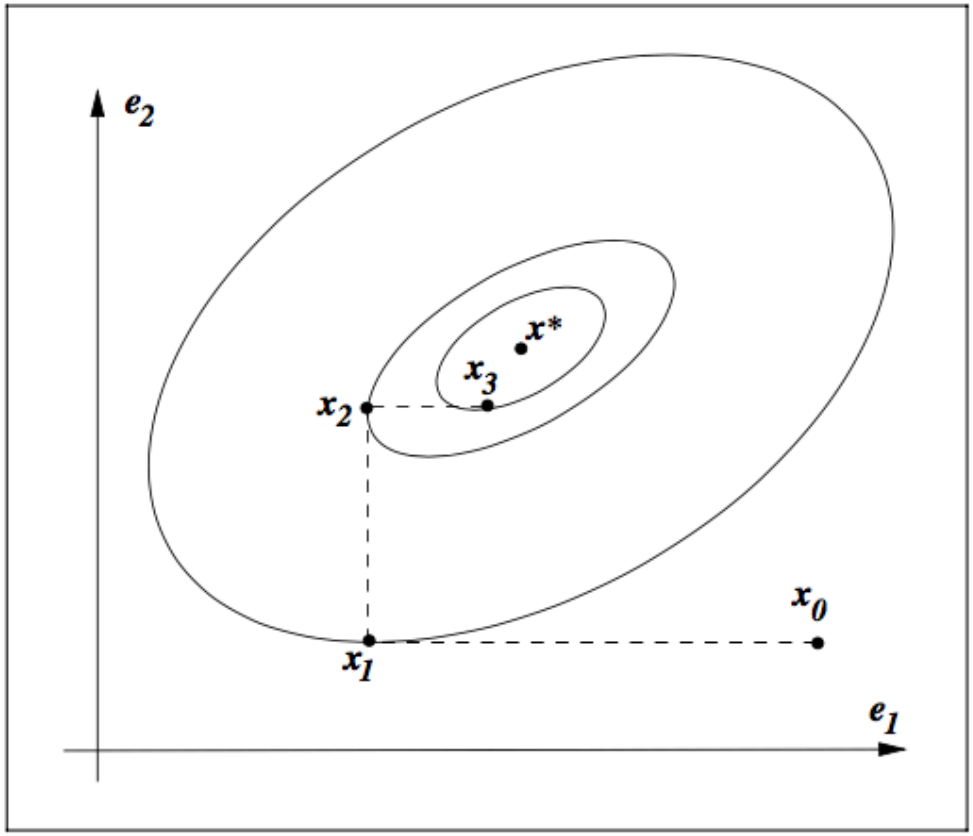
Linear Conjugate Direction

- Is an iterative method to solve $\mathbf{Ax} = \mathbf{b}$ (so belongs to linear algebra)
- Can be used for optimization: min $\mathbf{J} = \mathbf{x}^T\mathbf{Ax} - \mathbf{b}^T\mathbf{x}$
- Conjugate vectors: $\mathbf{p}_i\mathbf{A}\mathbf{p}_j = 0$ for all i, j not equal i
- Construction similar to Gram-Schmidt (QR), where A plays the role of scalar product norm: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k\mathbf{p}_k$ where $\alpha_k = -\boldsymbol{r}_k^T\boldsymbol{p}_k/(\boldsymbol{p}_k^T\boldsymbol{A}\boldsymbol{p}_k)$ and $\boldsymbol{r}_k = \boldsymbol{A}\boldsymbol{x}_k - \boldsymbol{b}$
- Essentially we are taking a dot product (with **A** norm) of the vector with previous vectors to project it perpendicular to previous vectors
- Since the space is N-dim after N steps we have spanned the full space and converged to true solution, $r_N = 0$.

Conjugate Direction

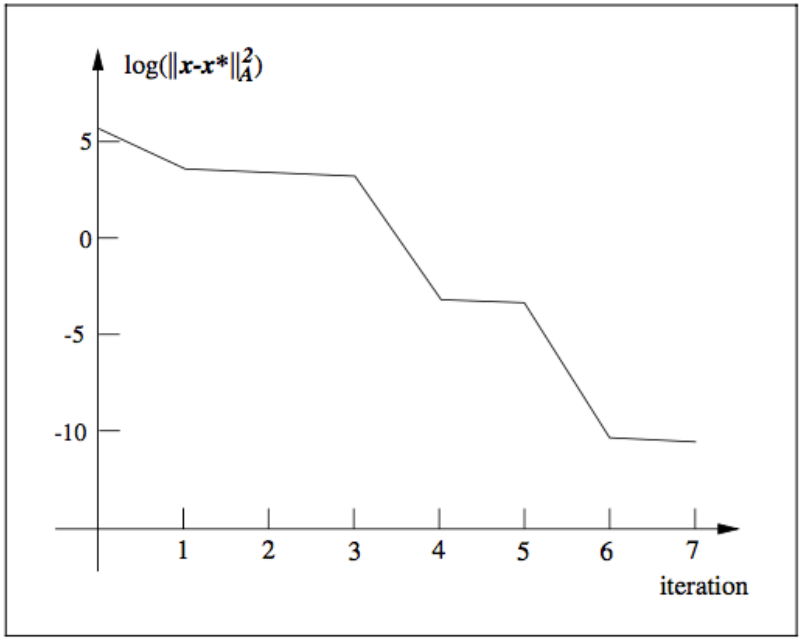
- If we have the matrix **A** in diagonal form so that basis vectors are orthogonal we can find the minimum trivially along the axes, otherwise not





Linear Conjugate Gradient

- Computes $\mathbf{p}_k$ from $\mathbf{p}_{k-1}$
- We want the step to be linear combination of residual $-\mathbf{r}_k$ and previous direction $\mathbf{p}_{k-1}$
- $\mathbf{p}_k = -\mathbf{r}_k + \beta_k \mathbf{p}_{k-1}$ premultiply by $\mathbf{p}^T_{k-1}\mathbf{A}$
- $\beta_k = (\mathbf{r}_k \mathbf{A} \mathbf{p}_{k-1})/(\mathbf{p}^T_{k-1}\mathbf{A}\mathbf{p}_{k-1})$ imposing $\mathbf{p}^T_{k-1}\mathbf{A}\mathbf{p}_k = 0$
- Converges rapidly for similar eigenvalues, not so much if condition number is high



Preconditioning

- Tries to improve condition number of **A** by multiplying by another matrix **C** that is simple

$$\hat{x} = Cx.$$

$$\hat{\phi}(\hat{x}) = \tfrac{1}{2}\hat{x}^T(C^{-T}AC^{-1})\hat{x} - (C^{-T}b)^T\hat{x}$$

$$(C^{-T}AC^{-1})\hat{x} = C^{-T}b$$

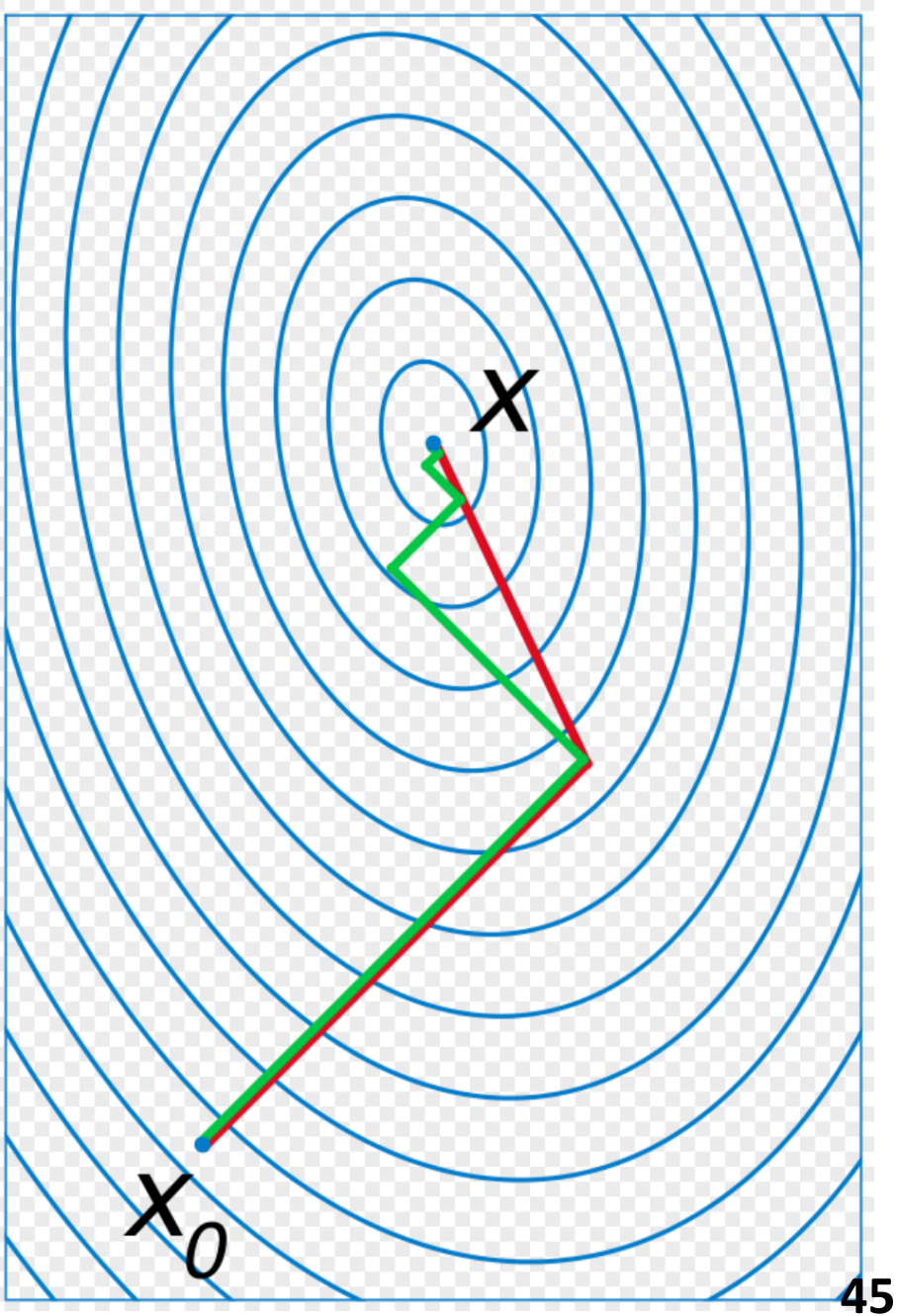
- We wish to reduce condition number of $C^{-T}AC^{-1}$
- Example: incomplete Cholesky $\mathbf{A} = \mathbf{L}\mathbf{L}^T$ by computing only a sparse **L**
- Preconditioners are very problem specific

Nonlinear Conjugate Gradient

- Replace $\mathbf{a_k}$ with line search that minimizes $\mathbf{J}$, and use $\mathbf{x_{k+1}} = \mathbf{x_k} + \mathbf{a_k p_k}$
- Replace $\mathbf{r_k} = \mathbf{A x_k} - \mathbf{b}$ with gradient of $\mathbf{J}$: $\bigtriangledown_a \mathbf{J}$
- This is Fletcher-Reeves version, Polak-Ribiere modifies β
- CG is one of the most competitive methods, but requires the Hessian to have low condition number
- Typically we do a few CG steps at each k, then move on to a new gradient evaluation

CG vs. Gradient Descent

- In 2-d CG has to converge in 2 steps



Gauss-Newton for Nonlinear Least Squares

$$\chi^2(\mathbf{a}) = \sum_{i=0}^{N-1} \left[\frac{y_i - y(x_i|\mathbf{a})}{\sigma_i} \right]^2$$

$$\frac{\partial \chi^2}{\partial a_k} = -2 \sum_{i=0}^{N-1} \frac{[y_i - y(x_i|\mathbf{a})]}{\sigma_i^2} \frac{\partial y(x_i|\mathbf{a})}{\partial a_k} \qquad k = 0, 1, \ldots, M-1$$

$$\frac{\partial^2 \chi^2}{\partial a_k \partial a_l} = 2 \sum_{i=0}^{N-1} \frac{1}{\sigma_i^2} \left[\frac{\partial y(x_i|\mathbf{a})}{\partial a_k} \frac{\partial y(x_i|\mathbf{a})}{\partial a_l} - [y_i - y(x_i|\mathbf{a})] \frac{\partial^2 y(x_i|\mathbf{a})}{\partial a_l \partial a_k} \right]$$

$$\beta_k \equiv -\frac{1}{2} \frac{\partial \chi^2}{\partial a_k} \qquad \alpha_{kl} \equiv \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_k \partial a_l} \qquad \sum_{l=0}^{M-1} \alpha_{kl} \, \delta a_l = \beta_k$$

$$\alpha_{kl} = \sum_{i=0}^{N-1} \frac{1}{\sigma_i^2} \left[\frac{\partial y(x_i|\mathbf{a})}{\partial a_k} \frac{\partial y(x_i|\mathbf{a})}{\partial a_l} \right]$$

Line search in direction δa

We drop 2nd term in Hessian because residual $r = y_i - y$ is small, fluctuates around 0 and because y'' may be small (or zero for linear problems)

Gauss-Newton + Trust Region = Levenberg-Marquardt Method

- Solving $\mathbf{A}^T\mathbf{A}\delta\mathbf{a} = \mathbf{A}^T\mathbf{b}$ is equivalent to minimize $|\mathbf{A}\delta\mathbf{a}-\mathbf{b}|^2$
- if trust region is within the solution just solve this equation
- If not we need to impose $||\delta\mathbf{a}||=\Delta_k$
- Lagrange multiplier minimization equivalent to $(\mathbf{A}^T\mathbf{A}+ \lambda I)\ \delta\mathbf{a} = \mathbf{A}^T\mathbf{b}$ and $\lambda(\Delta-||\delta\mathbf{a}||) = 0$
- For small λ this is Gauss-Newton (use close to minimum), for large λ this is steepest descent (use far from minimum)
- A good method for nonlinear least squares

Summary

- Optimization one of key numerical methods of modern data analysis. Typical examples are nonlinear least square problem and ML parameters (e.g. neural networks etc.)
- If at this point you are confused which methods you should use you are not alone: it depends on application and often the best way to answer is to try
- Some general guidances: if there is a lot of parameters (e.g. ML) and likelihood evaluations are cheap then use 1st order methods

Summary

- If the data is independent and there is a lot of data then use stochastic 1st order methods, e.g. ADAM
- If the likelihood evaluation is slow and number of parameters low use Newton or Gauss-Newton (e.g. Levenberg-Marquardt)
- If likelihood slow and number of parameters large use approximate Newton or Gauss-Newton (e.g. Steihaug with nonlinear CG), or use quasi-Newton (e.g. L-BFGS)
- Choosing a method is not enough: you also need to choose line search method (e.g. backtracking, Wolfe conditions) or trust region determination
- Typically these methods only find local minimum. Non-convex problems are hard: we will look at some stochastic methods (e.g. simulated annealing) in next lecture

Literature

- *Numerical Recipes*, Press et al., Chapter 9, 10, 15
- *Computational Physics,* M. Newman, Chapter 6
- Nocedal and Wright, Optimization
- https://arxiv.org/abs/1609.04747