GEOGG121: Methods
Inversion II: non-linear methods

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Lecture outline

- Non-linear models, inversion
  - The non-linear problem
  - Parameter estimation, uncertainty
  - Numerical approaches
  - Implementation
  - Practical examples

Reading

- Non-linear models, inversion
  - Gradient descent: Press et al. Numerical Recipes in C (1992) online version), Section 10.7 eg BFGS http://apps.nrbook.com/c/index.html
  - Conjugate gradient, Simplex, Simulated Annealing etc.: Press et al. Numerical Recipes in C (1992), ch. 10 http://apps.nrbook.com/c/index.html
  - Liang, S. (2004) Quantitative Remote Sensing of the Land Surface, ch. 8 (section 8.2).
  - Gershenfeld, N. (2002) The Nature of Mathematical Modelling, CUP

Non-linear inversion

- If we cannot phrase our problem in linear form, then we have non-linear inversion problem
- Key tool for <u>many</u> applications
  - Resource allocation
  - Systems control
  - (Non-linear) Model parameter estimation
    - AKA curve or function fitting: i.e. obtain parameter values that provide "best fit" (in some sense) to a set of observations
    - And estimate of parameter uncertainty, model fit

Options for Numerical Inversion

- Same principle as for linear
  - i.e. find minimum of some cost func. expressing difference between model and obs
  - We want some set of parameters (x*) which minimise cost function f(x) i.e. for some (small) tolerance δ > 0 so for all x

$$\left\| x - x^* \right\| \leq \delta$$

  - Where f(x*) ≤ f(x). So for some region around x*, all values of f(x) are higher (a <u>local minima</u> – may be many)
  - If region encompasses full range of x, then we have the <u>global minima</u>

Numerical Inversion

- Iterative numerical techniques
  - Can we differentiate model (e.g. adjoint)?
  - YES: Quasi-Newton (eg BFGS etc)
  - NO: Powell, Simplex, Simulated annealing, Artificial Neural Networks (ANNs), Genetic Algorithms (GAs), Look-up Tables (LUTs); Knowledge-based systems (KBS)

Errico (1997) What is an adjoint model?, BAMS, 78, 2577-2591
http://paoc2001.mit.edu/cmi/development/adjoint.htm

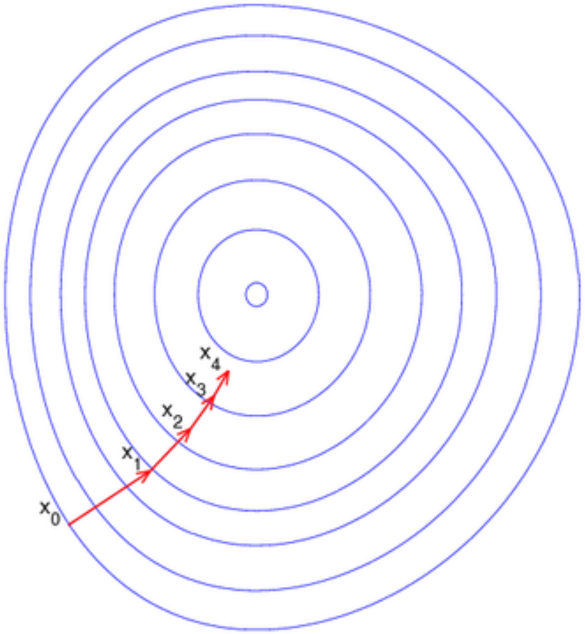
Today

- Outline principle of Quasi-Newton:
  - BFGS
- Outline principles when no differential:
  - Powell, Simplex, Simulated annealing
- V. briefly mention:
  - Artificial Neural Networks (ANNs)
  - Look-up Tables (LUTs) – v. useful brute force method

Errico (1997) What is an adjoint model?, BAMS, 78, 2577-2591
http://paoc2001.mit.edu/cmi/development/adjoint.htm

First order optimisation: gradient descent

- For multivariate function F(**x**) in neighbourhood of point a, F(**x**) decreases fastest if we move in direction of –ve gradient i.e. $-\nabla F(a)$
- If $b = a - \gamma \nabla F(a)$ for small enough step size γ, then F(**a**) ≥ F(**b**)
- And for sequence x_0, x_1, x_2 … x_n we have $x_{n+1} = x_n - \gamma_n \nabla F(x_n)$



http://en.wikipedia.org/wiki/Gradient_descent

Newton's method

- Construct a sequence x_n starting at x_0, converging to x^* where $f'(x^*) = 0$, the stationary point of f(x), by approximating as a quadratic….
- 2^{nd} order Taylor expansion around x_n (where $\Delta x = x - x_n$) is

$$f_T\left(x_n + \Delta x\right) = f_T\left(x\right) = f\left(x_n\right) + f'\left(x_n\right)\Delta x + \frac{1}{2} f''\left(x_n\right)\Delta x^2$$

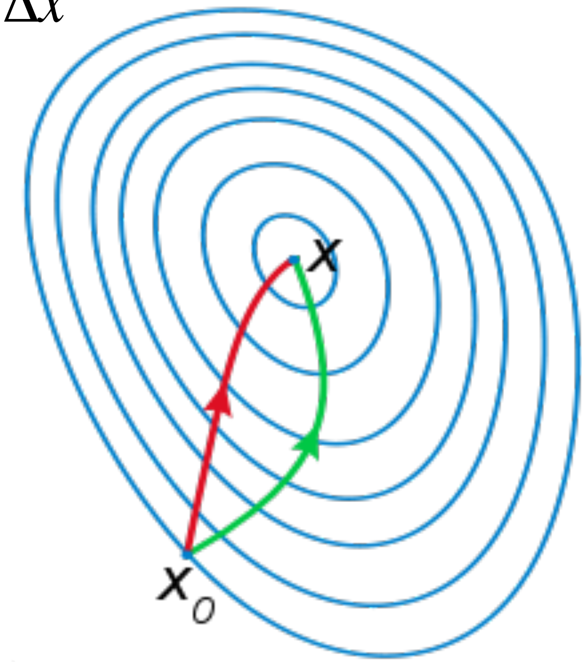
- Max where d(Δx)/dx = 0 i.e. for linear eqn

$$f'\left(x_n\right) + f''\left(x_n\right)\Delta x = 0$$

- So for sequence x_n

$$\Delta x = x - x_n = -\frac{f'\left(x_n\right)}{f''\left(x_n\right)}$$

- So $x_{n+1} = x_n - \dfrac{f'\left(x_n\right)}{f''\left(x_n\right)}, n = 0,1,\ldots$



Red: Newton
green: grad. descent

http://en.wikipedia.org/wiki/Newton%27s_method_in_optimization

Quasi-Newton methods…

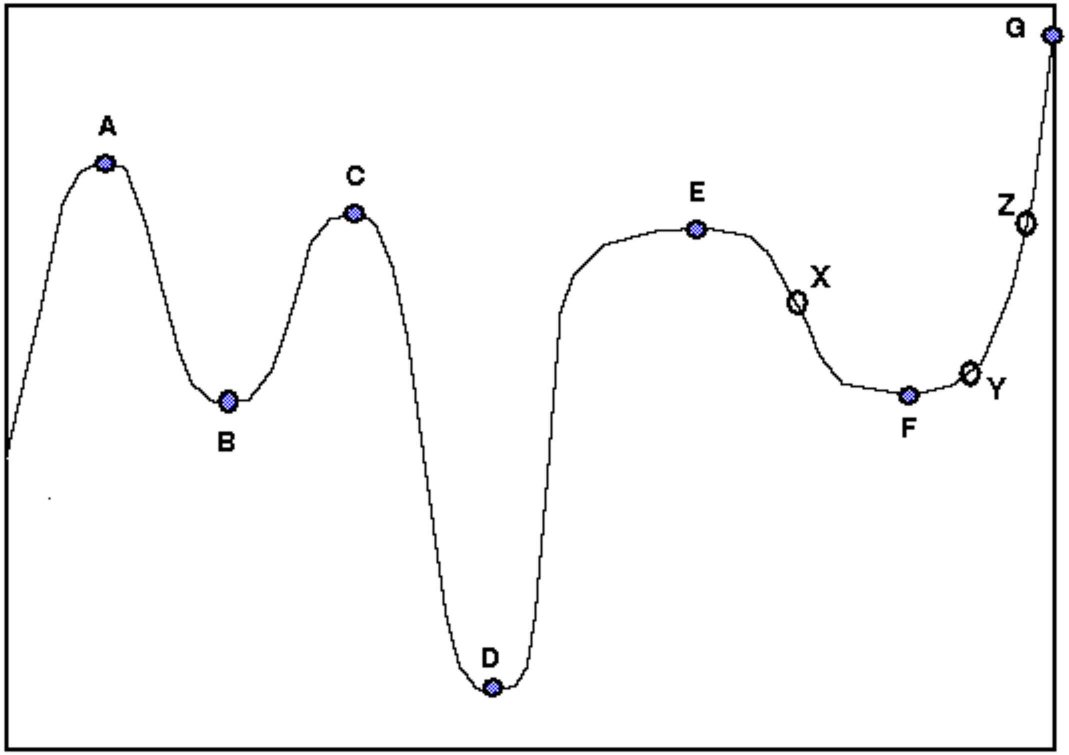
- Quasi-Newton: use Taylor approx also, but Hessian matrix of 2nd derivatives doesn't need to be computed
- Update Hessian by analysing successive derivatives instead

$$f_T\left(x_k + \Delta x\right) \approx f\left(x_k\right) + \nabla f\left(x_k\right)^T \Delta x + \frac{1}{2}\Delta x^T B \Delta x$$

- Where ∇f is the gradient and B is approx. to Hessian matrix
- So gradient of this approx is $\nabla f\left(x_k + \Delta x\right) \approx \nabla f\left(x_k\right) + B\Delta x$
- So set to zero i.e. $\Delta x = -B^{-1}\nabla f\left(x_k\right)$
- And choose B (Hessian approx.) to satisfy
- Various methods to choose/update B
  - eg BFGS (Broyden-Fletcher-Goldfarb-Shanno)
  - Iterative line searches using approx. to 2nd differential

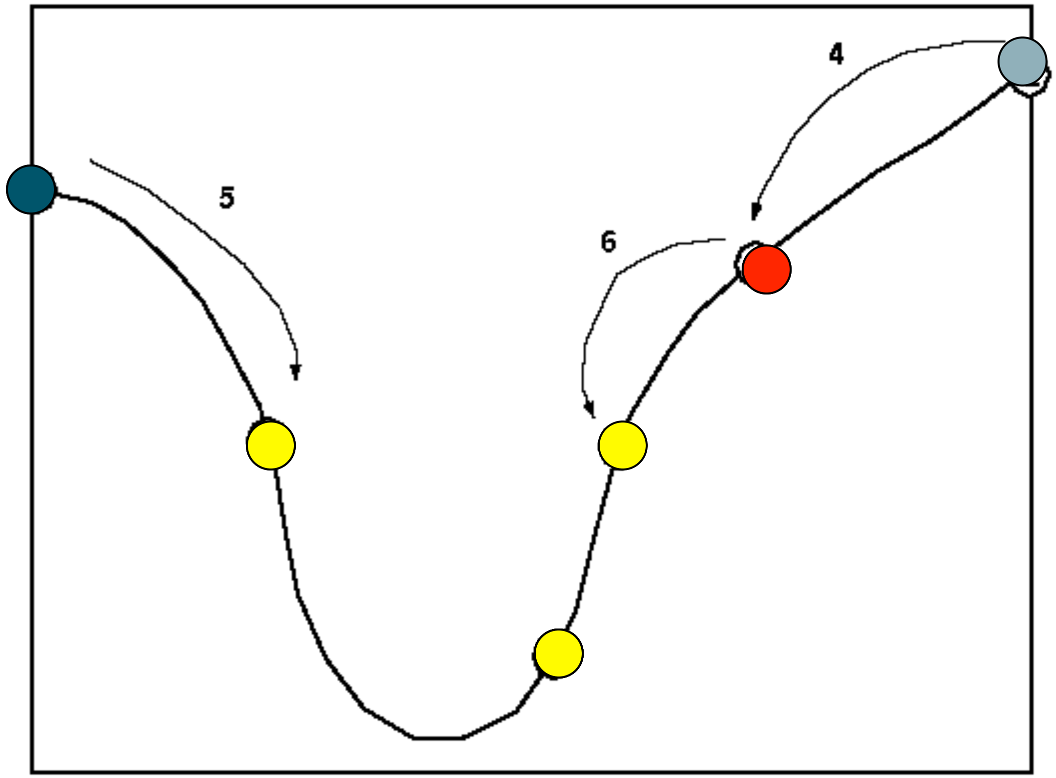
http://en.wikipedia.org/wiki/Quasi-Newton_method
http://en.wikipedia.org/wiki/BFGS_method

Methods without derivatives: local and global minima (general: optima)



Need starting point

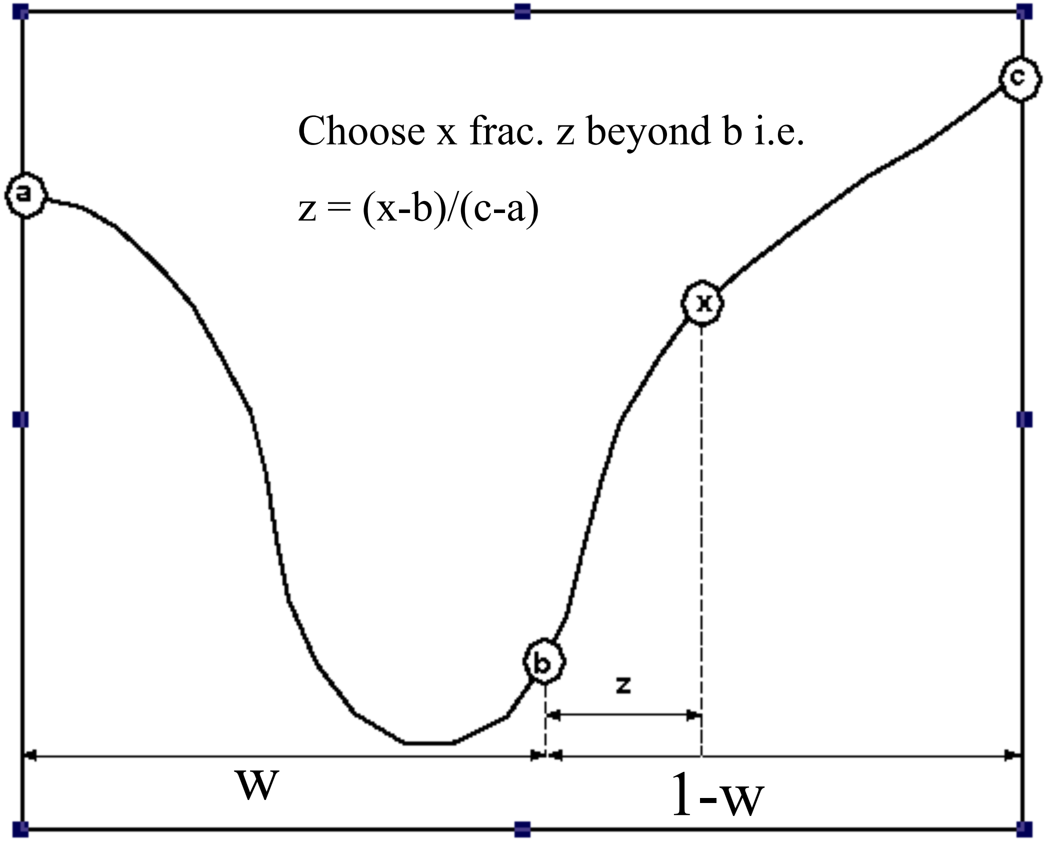
How to go 'downhill'?



Bracketing of a minimum: choose new points at each end closer to a minimum

Slow, but sure

How far to go 'downhill'? i.e. how to choose next points?



w=(b-a)/(c-a)

1-w=(c-b)/(c-a)

Choose:

z+w=1-w

For symmetry

Choose:

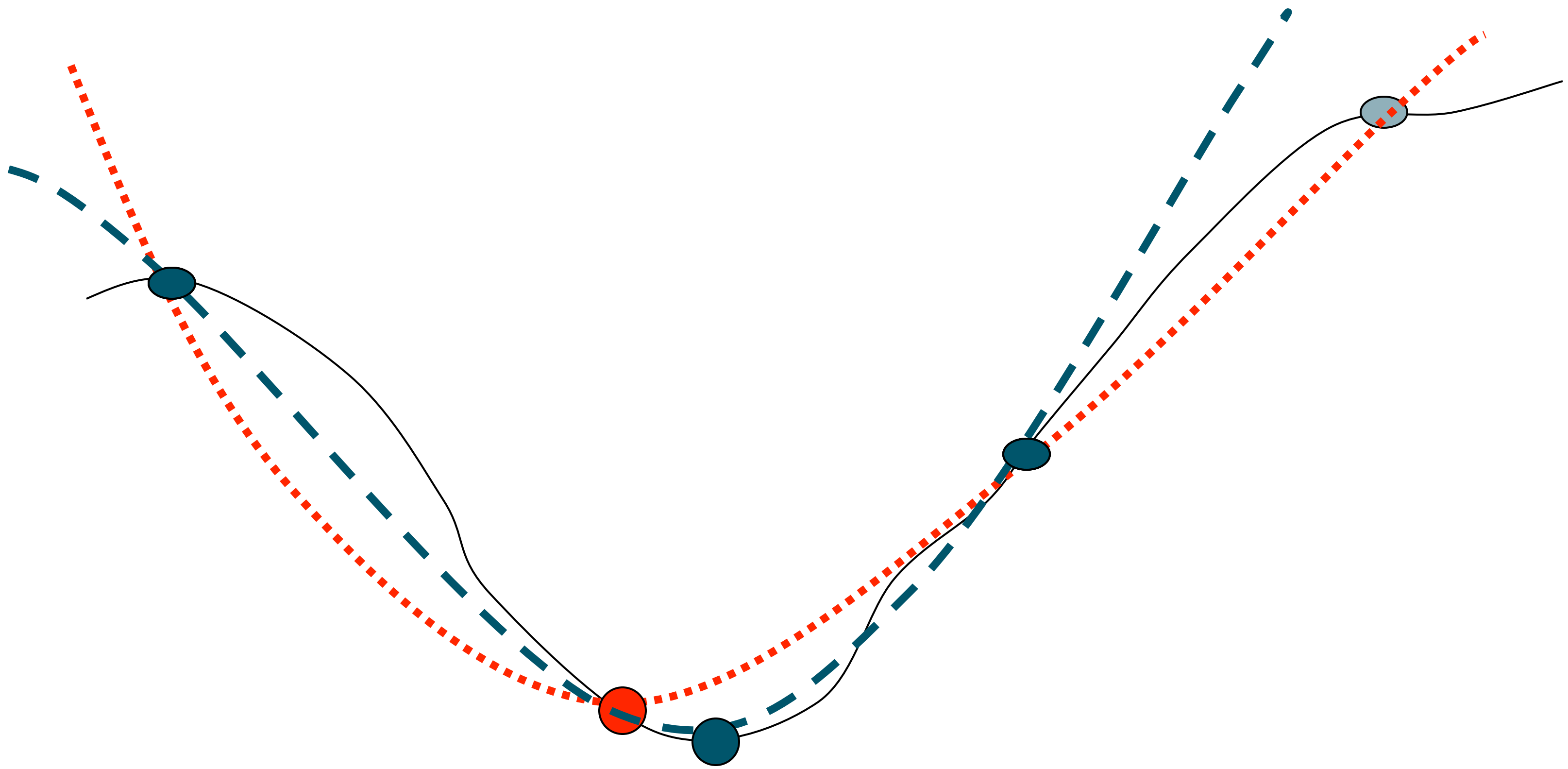
w=z/(1-w)

To keep proportions the same

z=w-w²=1-2w

0= w² -3w+1   Golden Mean Fraction =w=0.38197

Parabolic Interpolation



Inverse parabolic interpolation

More rapid

Brent's method

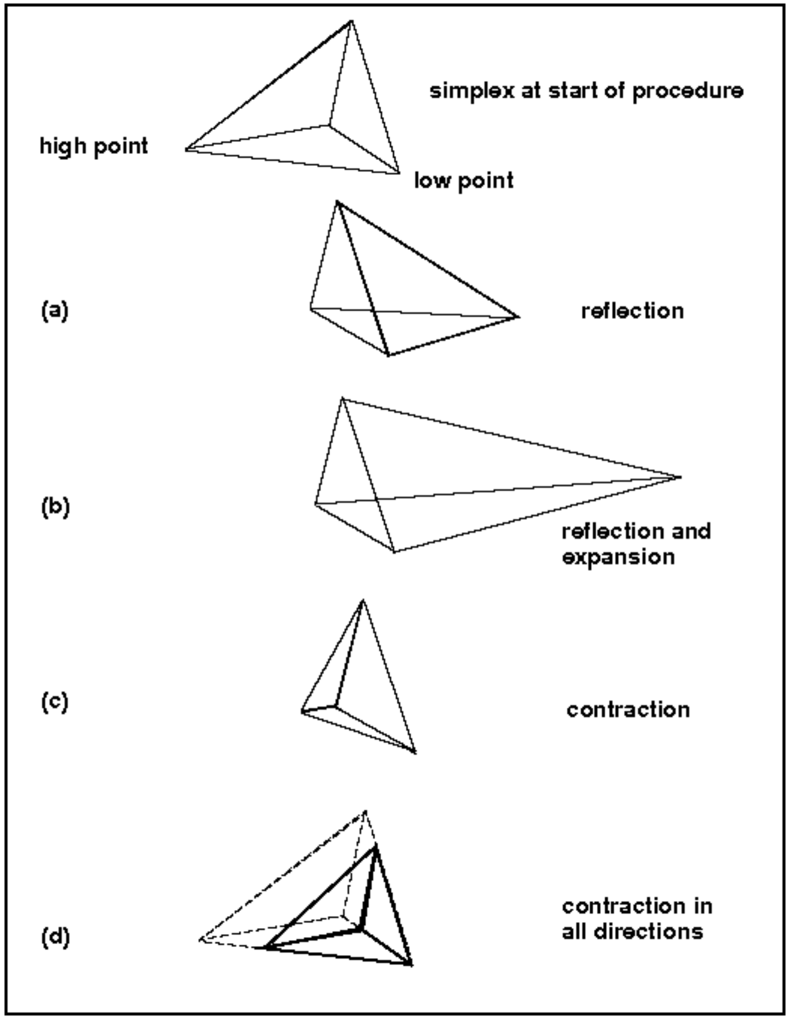
- Require 'fast' but robust inversion
- Golden mean search
  - Slow but sure
    - Use in unfavourable areas
- Use Parabolic method
  - when get close to minimum

http://apps.nrbook.com/c/index.html p402

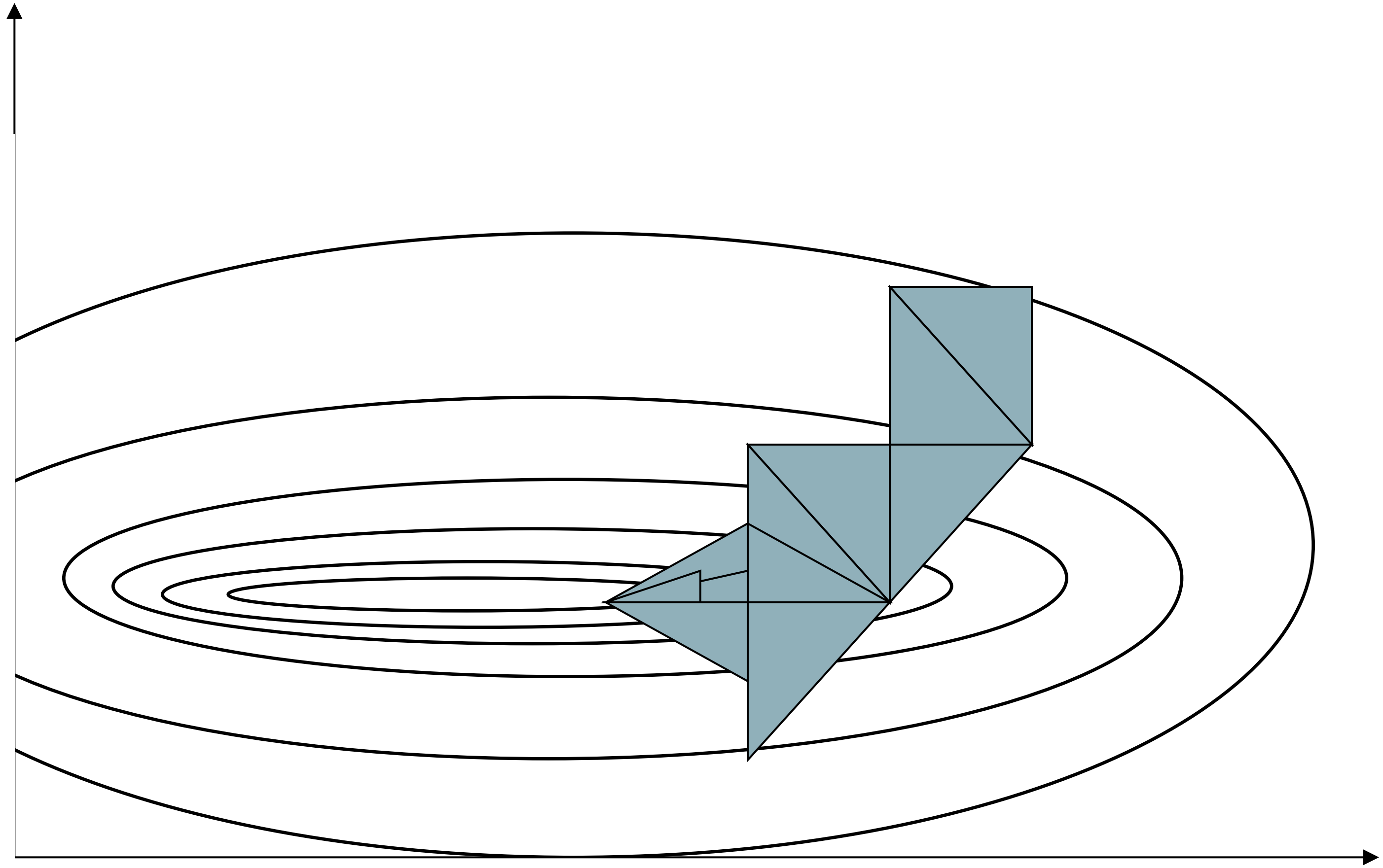
Multi-dimensional minimisation

- Use 1D methods multiple times
  - In which directions?
- Some methods for N-D problems
  - Simplex (amoeba)

Downhill Simplex



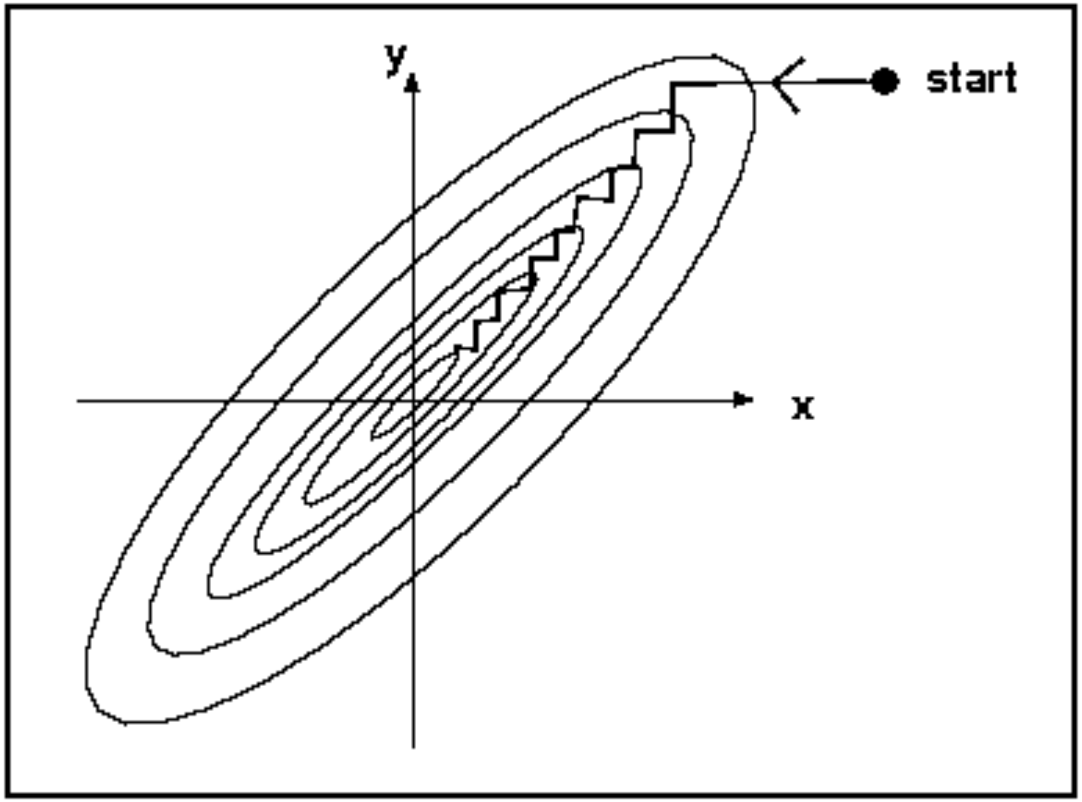
- Simplex:
  - Simplest N-D
    - N+1 vertices
- Simplex operations:
  - a reflection away from the high point
  - a reflection and expansion away from the high point
  - a contraction along one dimension from the high point
  - a contraction along all dimensions towards the low point.
- Find way to minimum



http://apps.nrbook.com/c/index.html p408

Direction Set (Powell's) Method

- Multiple 1-D minimsations
  - Inefficient along axes



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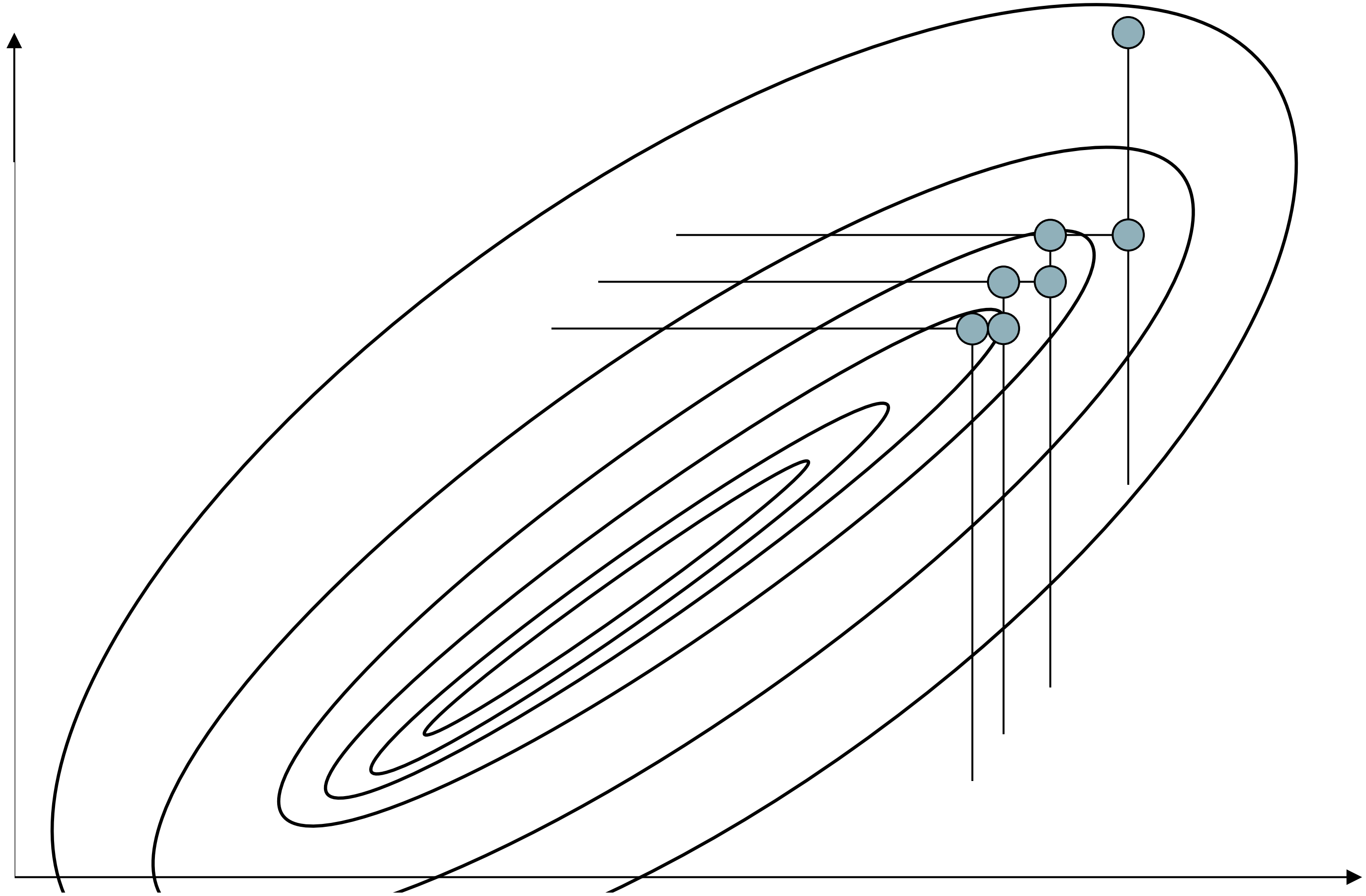
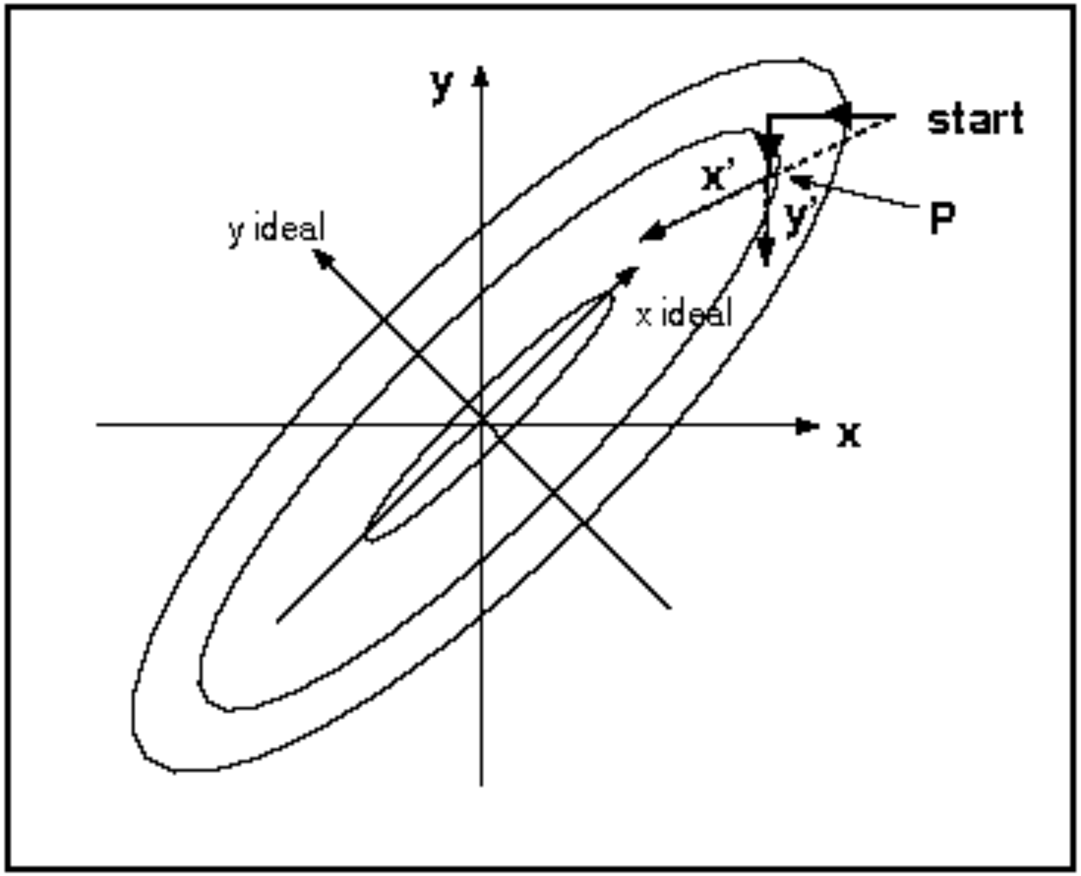
Powell

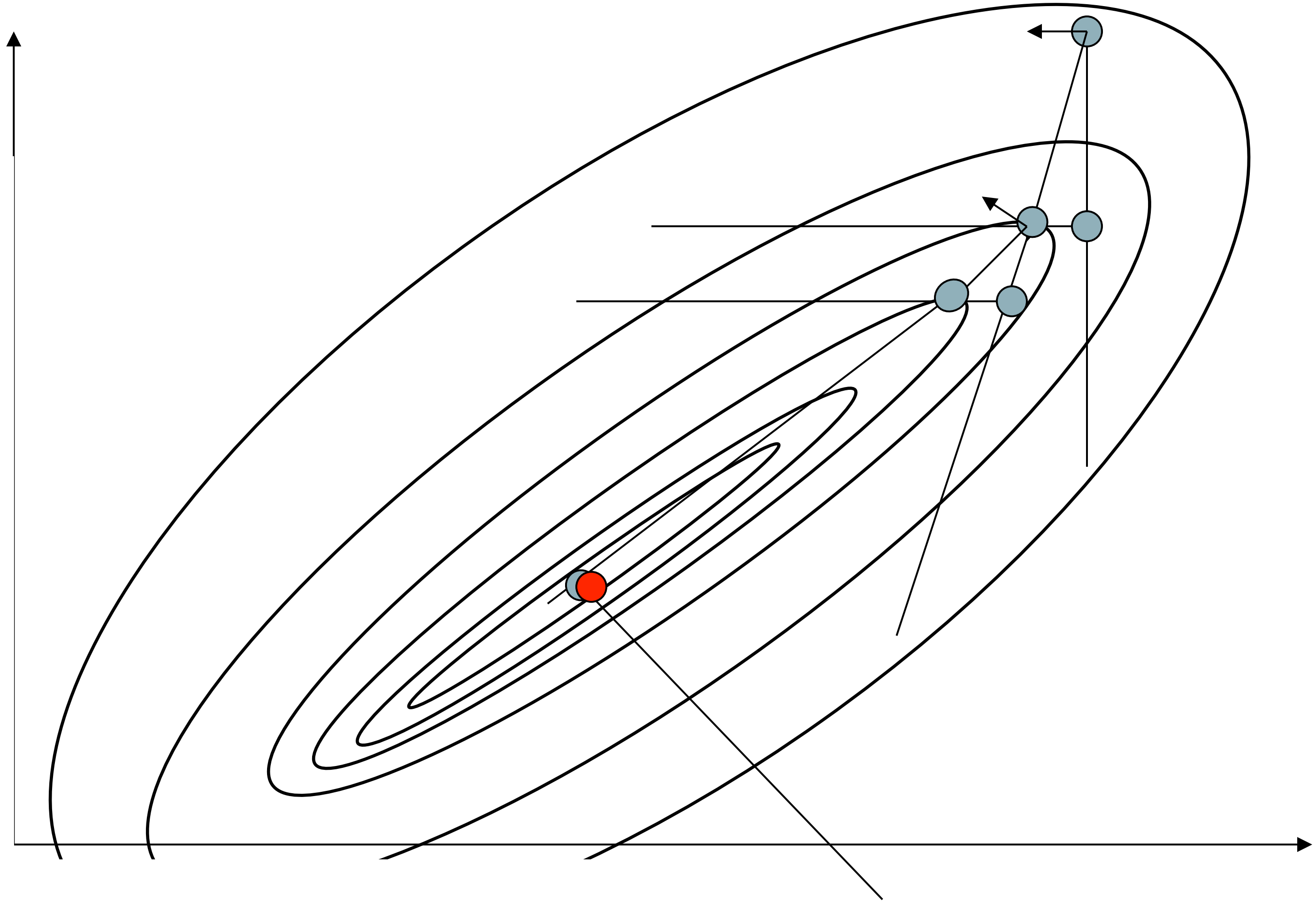


Direction Set (Powell's) Method

- Use conjugate directions
  - Update primary & secondary directions
- Issues
  - Axis covariance



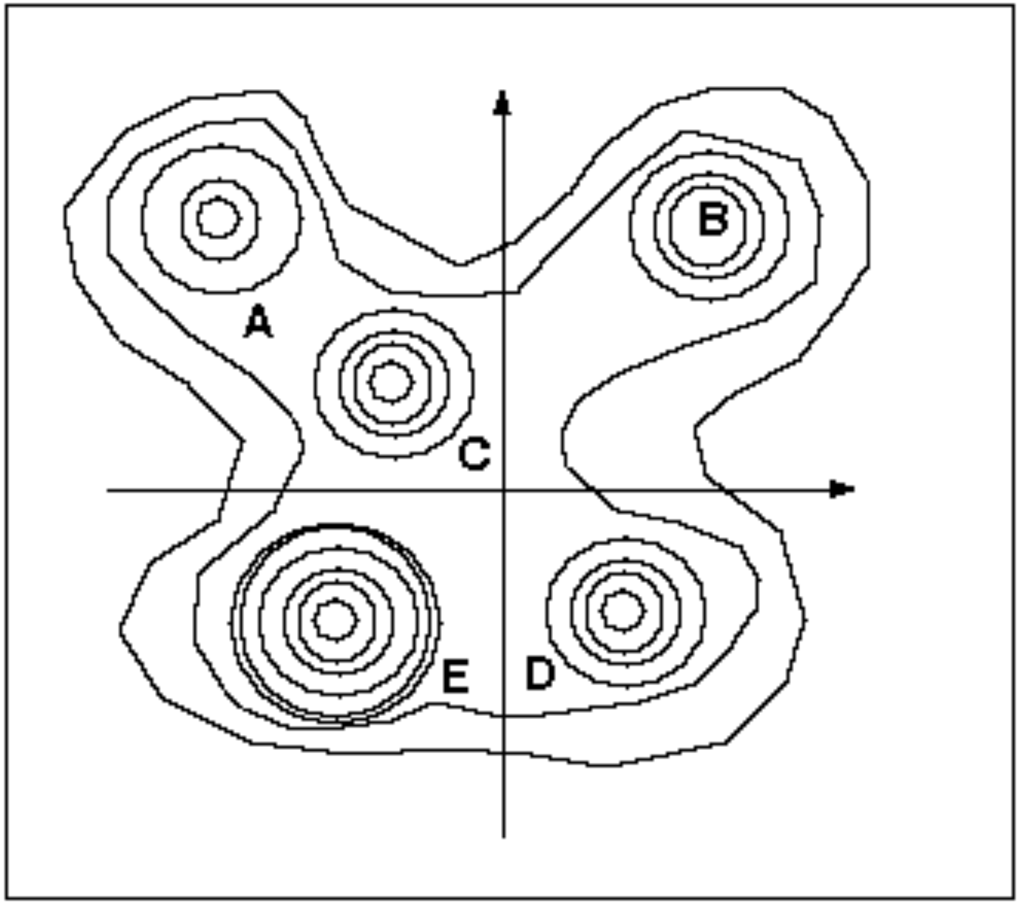
Powell



Simulated Annealing

- Previous methods:
  - Define start point
  - Minimise in some direction(s)
  - Test & proceed
- Issue:
  - Can get trapped in local minima i.e. CAN'T GO UPHILL!
- Solution (?)
  - Need to restart from different point
  - OR – allow chance of uphill move

Simulated Annealing



Simulated Annealing

- **Annealing**
  - Thermodynamic phenomenon
  - ‘slow cooling’ of metals or crystalisation of liquids
  - Atoms ‘line up’ & form ‘pure cystal’ / Stronger (metals)
  - Slow cooling allows time for atoms to redistribute as they lose energy (cool)
  - **Low energy state**
- **Quenching**
  - ‘fast cooling’
  - Polycrystaline state

Simulated Annealing

- Simulate ‘slow cooling’
- Based on Boltzmann probability distribution: $\Pr(E) \propto e^{-\frac{E}{kT}}$

- k – constant relating energy to temperature
- System in thermal equilibrium at temperature T has distribution of energy states E
- All (E) states possible, but some more likely than others
- Even at low T, small probability that system may be in higher energy state (uphill)

http://apps.nrbook.com/c/index.html p444

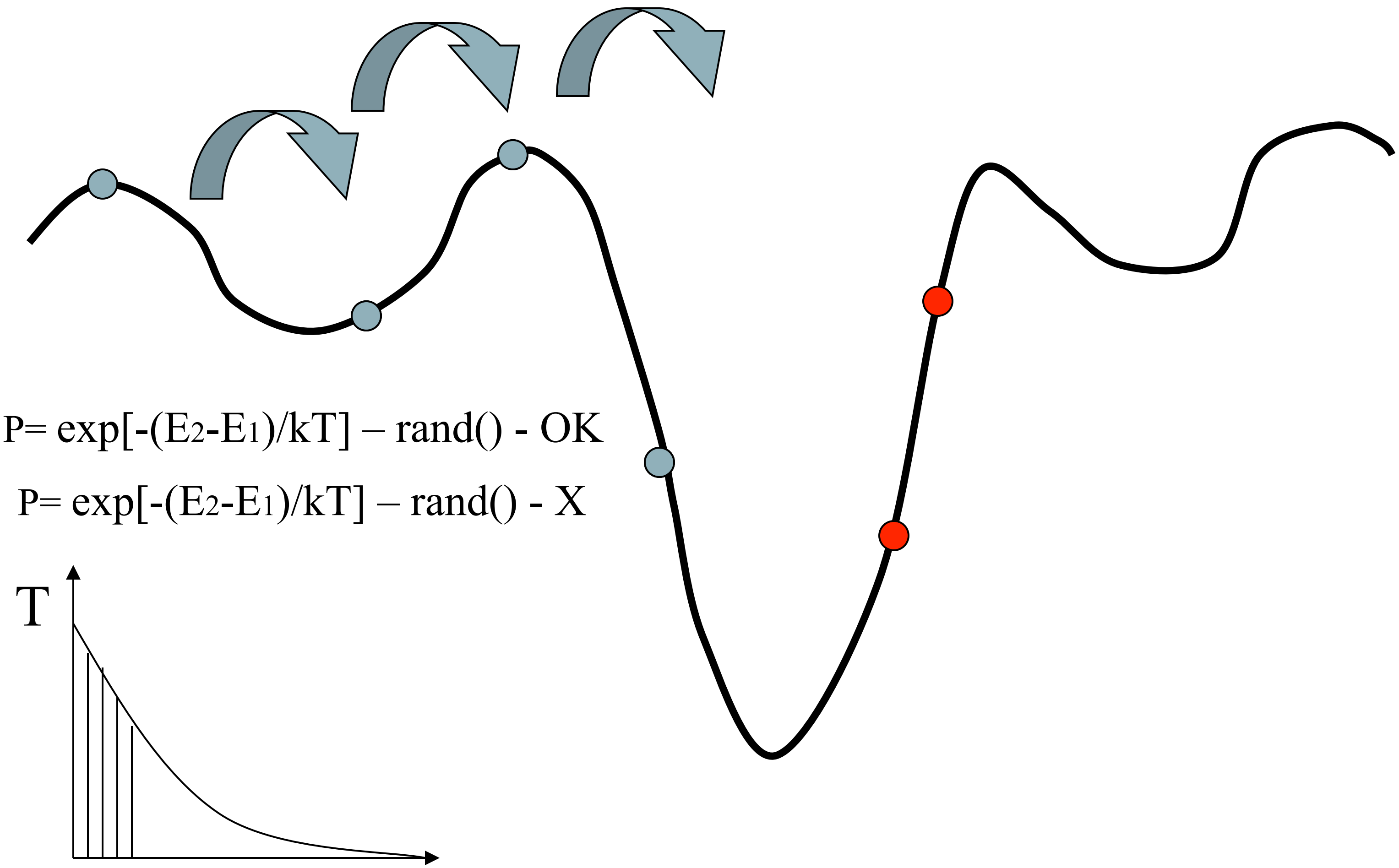
Simulated Annealing

- Use analogy of energy to RMSE
- As decrease ‘temperature’, move to generally lower energy state
- Boltzmann gives distribution of E states
  - So some probability of higher energy state
    - i.e. ‘going uphill’
  - Probability of ‘uphill’ decreases as T decreases

Implementation

- System changes from E_1 to E_2 with probability $\exp[-(E_2-E_1)/kT]$
  - If($E_2 < E_1$), P>1 (threshold at 1)
    - System **will** take this option
  - If($E_2 > E_1$), P<1
    - Generate random number
    - System **may** take this option
    - Probability of doing so decreases with T

Simulated Annealing



$P = \exp[-(E_2-E_1)/kT] - \text{rand}()$ - OK

$P = \exp[-(E_2-E_1)/kT] - \text{rand}()$ - X

T

Simulated Annealing

- Rate of cooling very important
- Coupled with effects of k
  - $\exp[-(E_2-E_1)/kT]$
  - So 2xk equivalent to state of T/2
- Used in a range of optimisation problems where we value a global minimum over possible local minima ‘nearly’ as good

SA deprectaed in scipy: replaced by basinhopping

- Similar to SA. Each iteration involves
  - Random perturbation of coords (location on error surface)
  - Local minimization – find best (lowest) error locally
  - Accept/reject new position based on function value at that point
- Acceptance test is Metropolis criterion from Monte Carlo (Metropolis-Hastings) methods.
  - MH is more generally used to generate random samples from a prob. distribution from which direct sampling is difficult (maybe we don’t know what it looks like)
  - Approximate distribution, compute integral. See MCMC (Markov Chain Monte Carlo) next week

See Asenjo et al. (2013) from http://www-wales.ch.cam.ac.uk/

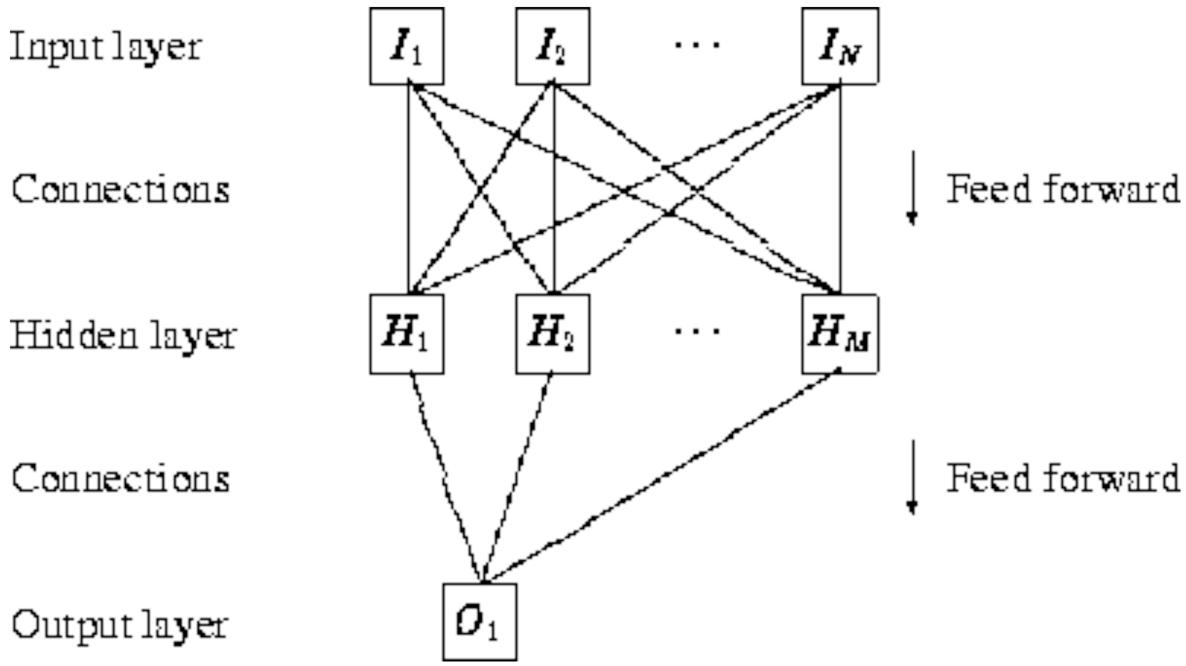
(Artificial) Neural networks (ANN)

- Another ‘Natural’ analogy
  - Biological NNs good at solving complex problems
  - Do so by ‘training’ system with ‘experience’
  - Potentially slow but can GENERALISE

http://en.wikipedia.org/wiki/Artificial_neural_network
http://www.doc.ic.ac.uk/~nd/surprise_96/journal/vol4/cs11/report.html
Gershenson, C. (2003) http://arxiv.org/pdf/cs/0308031

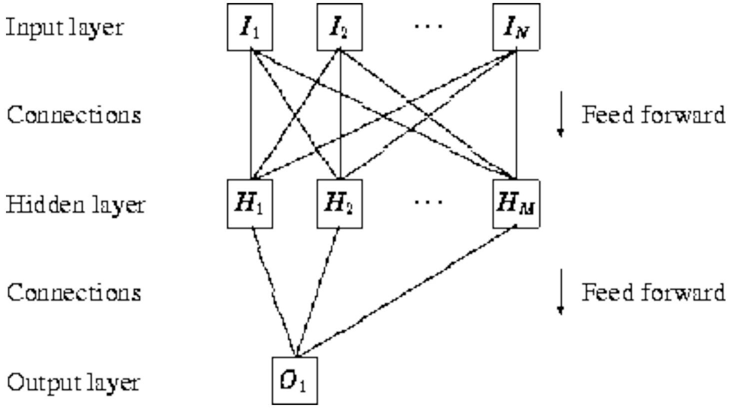
(Artificial) Neural networks (ANN)

- ANN architecture



(Artificial) Neural networks (ANN)

- ‘Neurons’
  - have 1 output but many inputs
  - Output is weighted sum of inputs
  - Threshold can be set
    - Gives non-linear response



(Artificial) Neural networks (ANN)

- Training
  - Initialise weights for all neurons
  - Present input layer with e.g. spectral reflectance
  - Calculate outputs
  - Compare outputs with e.g. biophysical parameters
  - Update weights to attempt a match
  - Repeat until all examples presented

(Artificial) Neural networks (ANN)

- Use in this way for model inversion
- Train other way around for forward model
- Also used for classification and spectral unmixing
  - Again – train with examples
- ANN has ability to generalise from input examples
- Definition of architecture and training phases critical
  - Can ‘over-train’ – too specific
  - Similar to fitting polynomial with too high an order
- Many ‘types’ of ANN – feedback/forward

(Artificial) Neural networks (ANN)

- In essence, trained ANN is just a (essentially) (highly) non-linear response function
- Training (definition of e.g. inverse model) is performed as separate stage to application of inversion
  - Can use complex models for training
- Many examples in remote sensing
- Issue:
  - How to train for arbitrary set of viewing/illumination angles? – not solved problem

Genetic (or evolutionary) algorithms (GAs)

- Another ‘Natural’ analogy
- Phrase optimisation as ‘fitness for survival’
- Description of state encoded through ‘string’ (equivalent to genetic pattern)
- Apply operations to ‘genes’
  - Cross-over, mutation, inversion

http://en.wikipedia.org/wiki/Genetic_algorithms
http://www.obitko.com/tutorials/genetic-algorithms/index.php
http://www.rennard.org/alife/english/gavintrgb.html
http://code.activestate.com/recipes/199121-a-simple-genetic-algorithm/

Genetic (or evolutionary) algorithms (GAs)

- Encode N-D vector representing current state of model parameters as string
- Apply operations:
  - E.g. mutation/mating with another string
  - See if mutant is ‘fitter to survive’ (lower RMSE)
  - If not, can discard (die)

Genetic (or evolutionary) algorithms (GAs)

- **General operation**:
  - Populate set of chromosomes (strings)
  - Repeat:
    - Determine fitness of each
    - Choose best set
    - Evolve chosen set
      - Using crossover, mutation or inversion
  - Until a chromosome found of suitable fitness

Genetic (or evolutionary) algorithms (GAs)

- Differ from other optimisation methods
  - Work on coding of parameters, not parameters themselves
  - Search from population set, not single members (points)
  - Use ‘payoff’ information (some objective function for selection) not derivatives or other auxilliary information
  - Use probabilistic transition rules (as with simulated annealing) not deterministic rules

Genetic (or evolutionary) algorithms (GAs)

- Example operation:
  1. Define genetic representation of state
  2. Create initial population, set t=0
  3. Compute average fitness of the set
     - Assign each individual normalised fitness value
     - Assign probability based on this
  4. Using this distribution, select N parents
  5. Pair parents at random
  6. Apply genetic operations to parent sets
     - generate offspring
     - Becomes population at t+1
  7. Repeat until termination criterion satisfied

Genetic (or evolutionary) algorithms (GAs)

- Flexible and powerful method
- Can solve problems with many small, ill-defined minima
- May take huge number of iterations to solve
- Again, use only in particular situations

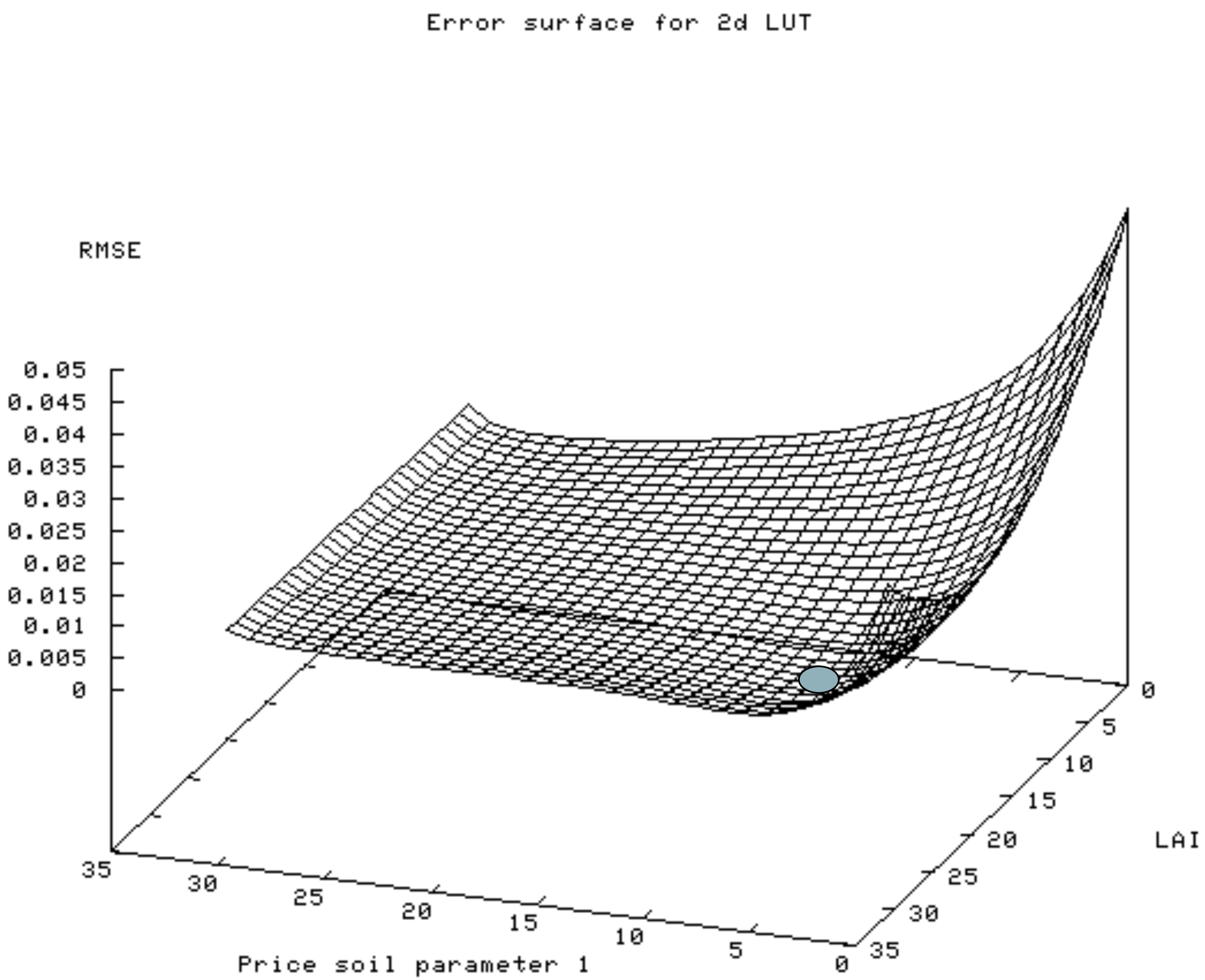
LUT Inversion

- Sample parameter space
- Calculate RMSE for each sample point
- Define best fit as minimum RMSE parameters
  - Or function of set of points fitting to a certain tolerance
- Essentially a sampled ‘exhaustive search’

http://en.wikipedia.org/wiki/Lookup_table
Gastellu et al. (2003) http://ferrangascon.free.fr/publicacions/gastellu_gascon_esteve-2003-RSE.pdf

LUT Inversion

- Issues:
  - May require large sample set
  - Not so if function is well-behaved
    - In some cases, may assume function is locally linear over large (linearised) parameter range
    - Use linear interpolation
  - May limit search space based on some expectation
    - E.g. some loose relationship between observed system & parameters of interest
    - Eg for remote sensing canopy growth model or land cover map
    - Approach used for operational MODIS LAI/fAPAR algorithm (Myneni et al)
    - http://modis.gsfc.nasa.gov/data/atbd/atbd_mod15.pdf


Error surface for 2d LUT
RMSE
0.05
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
35
30
25
20
15
10
5
0
Price soil parameter 1
0
5
10
15
20
25
30
35
LAI

LUT Inversion

- Issues:
  - As operating on stored LUT, can pre-calculate model outputs
    - Don’t need to calculate model ‘on the fly’ as in e.g. simplex methods
    - Can use complex models to populate LUT
      - E.g. of Lewis, Saich & Disney using 3D scattering models (optical and microwave) of forest and crop
  - Error in inversion may be slightly higher if (non-interpolated) sparse LUT
    - But may still lie within desirable limits
  - Method is simple to code and easy to understand
    - essentially a sort operation on a table

http://www2.geog.ucl.ac.uk/~mdisney/igarss03/FINAL/saich_lewis_disney.pdf

Summary: options for non-linear inversion

- Gradient methods
  - Newton (1^{st}, 2^{nd} derivs.,), Quasi-N (approx. 2^{nd} derivs eg BFGS) etc.
- Non-gradient, ‘traditional’ methods:
  - Powell, AMOEBA
    - Complex to code
      - though library functions available
    - Can easily converge to local minima
      - Need to start at several points
    - Calculate canopy reflectance ‘on the fly’
      - Need fast models, involving simplifications
    - Not felt to be suitable for operationalisation

Summary: options for non-linear inversion

- **Simulated Annealing**
  - Slow & need to define annealing schedule
  - BUT can deal with local minima
- **ANNs**
  - Train ANN from model (or measurements) to generalises as non-linear model
  - Issues of variable input conditions
  - Can train with complex models
- **GAs**
  - Novel approach, suitable for highly complex inversion problems
  - Can be very slow
  - Not suitable for operationalisation

Summary

- **LUT**
  - Simple ‘brute force’ method
    - Sorting, few/no assumptions about model behaviour
  - Used more and more widely for operational model inversion
    - Suitable for ‘well-behaved’ non-linear problems
  - Can operationalise
  - Can use arbitrarily complex models to populate LUT
  - Issue of LUT size
    - Can use additional information to limit search space
    - Can use interpolation for sparse LUT for ‘high information content’ inversion