CSE 417
Binary Search (pt 3)

UNIVERSITY *of* WASHINGTON

Reminders

- **HW1 is due today**
  - added a clarification on 1d
- **HW2 will be posted shortly**
  - coding HW: fitting an ML model using ternary search
  - start early! (might require some trial & error)

Outline for Today

> Binary search over the reals
> Ternary search over the reals
> Applications to ML

Binary search over the reals

- Above we considered $f : Z \to R$. What about $f : R \to R$?
- Standard problem in numerical analysis...
- But instead of inverting f, they want to find the *zeros of f*
  - these are equivalent problems:
    - to find t s.t. $f(t) = x$, just define $g(t) = f(t) - x$
    - $g(t) = 0$ means $f(t) = x$

Binary search over the reals

- New problem: when do we stop?
  - before, if f(t) < x, we can try f(t+1), f(t+2), …
  - now, we might need to try f(t+0.00000000001)

Input: A monotonically increasing function $f : R \rightarrow R$, a range [a, b], a number x in R, and <u>an error tolerance ε</u> in R

Output: number u in [a, b] such that:

- $f(t) <= x$ for all t in [a, u)
- $x < f(t)$ for all t in $[u + \varepsilon, b)$

Binary search over the reals

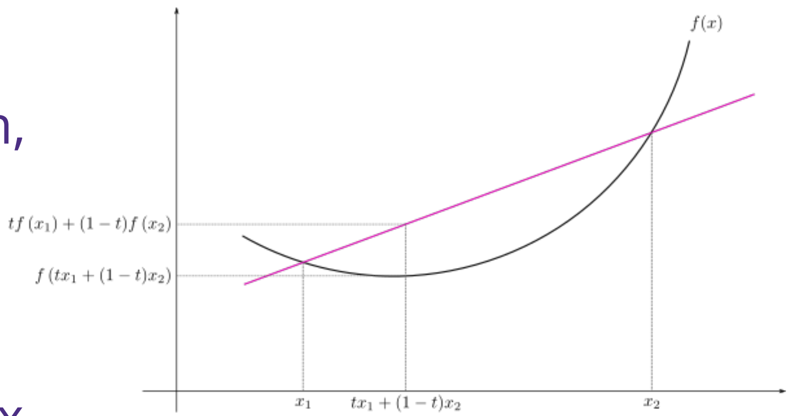
```
float u = a, v = b;

// Invariant: (f(s) <= x for s <= u) and (x < f(s) for s >= v)
while (v - u > eps) {
  float t = (u + v) / 2;
  if (f(t) <= x)
    u = m;
  else
    v = m;
}

return u;
```

floating point division

How to choose ε (*out of scope*)

- Want to choose ε so that $|f(t) - x|$ is small
- If f is differentiable, then $f(t + s) \approx f(t) + f'(t)\, s$
  - so $f(t+s) - f(t) \approx f'(t)\, s$
- If $f'(t) \le U$, for some U, and we want $|f(t+\varepsilon) - f(t)| < \delta$ then we can take $\varepsilon = \delta / U$
  - (this works if f is not differentiable provided that it is Lipschitz continuous)

Find minimum of a convex function



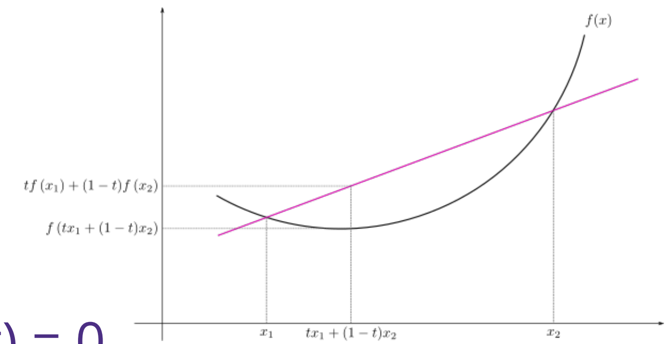
> Rather than find the zeros of function, we might want to *minimize* it

> This is always reasonable if f is convex
  - definition: $f((x_1 + x_2) / 2) <= (f(x_1) + f(x_2)) / 2$ for all x_1 & x_2

Picture from en.wikipedia.org/wiki/Convex_function

Find minimum of a convex function

> Fact: differentiable function f is *convex* iff its derivative f' is *monotonically increasing*



> In particular, its minimum occurs where f'(t) = 0
> So we can minimize f by finding a zero of f'
  – hence, we can minimize a convex function using binary search
  – assuming that we can compute the derivative f'
    > (actually, weaker notions of derivatives would work here)
    > (e.g., a convex function is left-differentiable)

Example: minimize smoothed rank

- Minimize $f(t) = \log\det(X + t\,Y)$, where X and Y are matrices
  - this is $R \to R$ even though it operates on matrices (tables)
    - would not expect an analytical solution
  - it is also convex! (not easy to prove, but true)
  - would still need to compute f′ though (yuck!)
- $\log\det(A + \varepsilon I)$ is called the smoothed rank of the matrix
  - minimizing actual matrix rank is hard
  - this gives an efficiently computable approximation
  - applications to, e.g., low-dimension approximation of high-dimensional noisy data

Find minimum of a convex function

- That said, binary search is not the fastest algorithm
- The fastest algorithm is Newton's method
  - in fact, Newton's method is exponentially faster than binary search

- Cannot overstate the importance of an exponential speedup
  - that said, if binary search takes O(log n) iterations, then Newton's method takes O(log log n) iterations
  - in practice, the difference is not always important
  - importance is when n is exponentially large
    - then log n is polynomial, but log log n is actually small

Find minimum of a convex function

- Newton's method requires another derivative
  - so we would need the function to be twice differentiable
  - if our function is multi-variate, then the second derivative is a matrix
    - see the HW for an example where this would arise
  - sometimes that is too much to ask
- It is actually possible to find the minimum with *no derivatives…*

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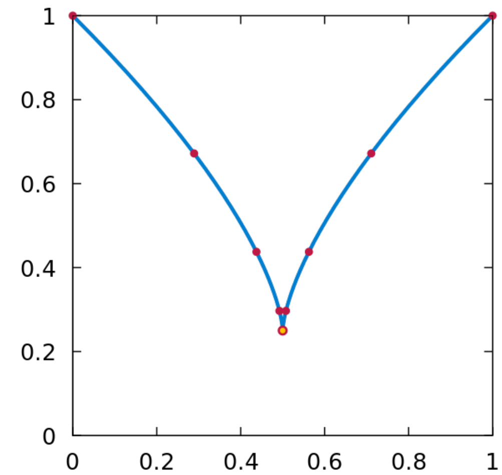
Ternary Search



Input: a *unimodal* function f : R → R, a range [a, b], and an error tolerance ε in R

- **unimodal** means it decreases *monotonically* and then increases
- slightly larger class than convex
  - functions can have cusps (see picture)

Picture from abcalculus.wikispaces.com/When+does+a+derivative+NOT+exist%3F

Ternary Search

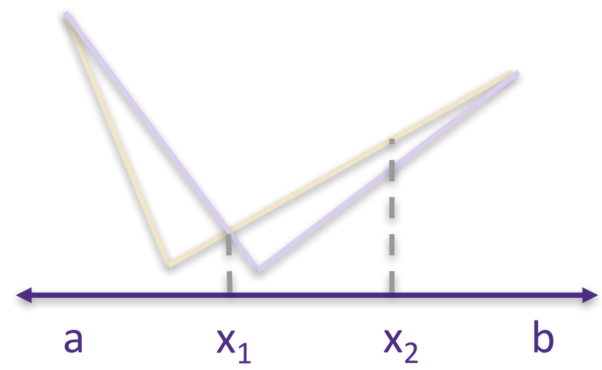
Input: a *unimodal* function $f : R \to R$, a range $[a, b]$, and an error tolerance ε in R

Output: number t in $[a, b]$ such that the minimum lies in $[t, t + \varepsilon]$

Ternary Search

Let $x_1 = a + (b - a) / 3$

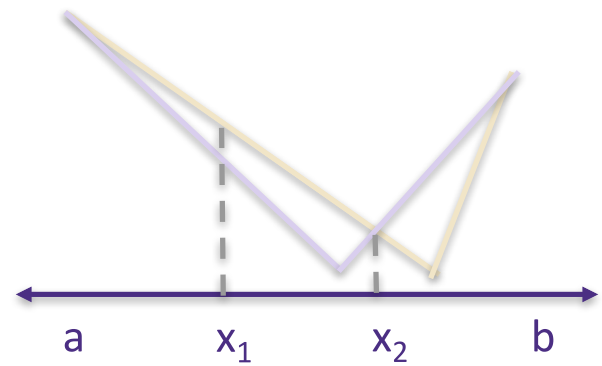
Let $x_2 = a + 2\,(b - a) / 3$



Idea: evaluate $f(x_1)$ and $f(x_2)$

> if $f(x_1) < f(x_2)$, then the minimum cannot be in $[x_2, b]$
  - function decreases then increases
  - if the minimum were in $[x_2, b]$, it would have decreased from x_1 to x_2

Ternary Search



Let $x_1 = a + (b - a) / 3$

Let $x_2 = a + 2 (b - a) / 3$

Idea: evaluate $f(x_1)$ and $f(x_2)$

> if $f(x_1) < f(x_2)$, then the minimum cannot be in $[x_2, b]$
  - function decreases then increases
  - if the minimum were in $[x_2, b]$, would have decreased from x_1 to x_2

> if $f(x_1) > f(x_2)$, then the minimum cannot be in $[a, x_1]$
  - if the minimum were in $[a, x_1]$, would have increased from x_1 to x_2

Ternary Search

- Each iteration removes 1/3 of the search space
  - if $f(x_1) < f(x_2)$, we eliminate $[x_2, b]$
  - if $(fx_1) > f(x_2)$, we eliminate $[a, x_1]$

- Reduced to (b – a) (2 / 3)^k after k iterations
- Done after $k = \log_{3/2}((b - a) / \varepsilon)$ iterations

- Takes $O(\log((b - a) / \varepsilon))$ time if evaluating f takes O(1)
  - in general, factor of $O(\log((b - a) / \varepsilon))$ increase in time versus time to evaluate f

“Binary Search” Most Broadly

- Binary and ternary search reduce search space by constant factor (1/2 or 2/3) on each iteration

- Any algorithm with that properly will take O(log(b – a)) iterations to reduce to interval of length 1
  - even a reduction to 99/100 of the size still works
  - since (b – a) (99/100)^k = 1 is true when
    $k = \log_{100/99} (b - a) = \log(b - a) / \log(100/99) = O(\log(b - a))$

“Binary Search” Most Broadly

- This is a general algorithm design approach:
  try to reduce size of search space by a constant fraction
  - some people consider this a type of “divide & conquer” algorithm
  - I think of it as a separate group, but whatever

- Other examples of algorithms within this paradigm
- Worth trying out when you’re looking for algorithms

"Binary Search" Most Broadly

- For me, the presence of monotonicity & unimodality are usually the best clues to look for
  - these only work in a subset of the cases
  - but they are the easiest to spot and arise most often
- In particular, key idea: *consider computing the inverse instead*
  - e.g., rather than trying to compute profit → hemming cost, compute hemming cost → profit
  - if it is monotonic, then you can invert with binary search

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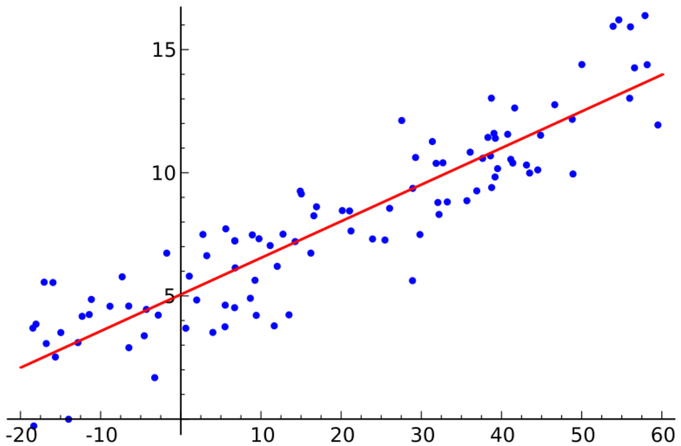
Model Fitting

- **Problem**: want to find the best description of the data

- Choose a model that you think should look like the data
  - describes the general shape
- Model usually has parameters
  - parameters give the exact function

- **Sub-problem**: find the choice of parameters that make the model best fit the data

Example: best fit line



> You think the data should be ~linear
  - not exactly linear due to measurement error etc.

> Model: y ~ A x + B
  - parameter A: slope
  - parameter B: y-intercept

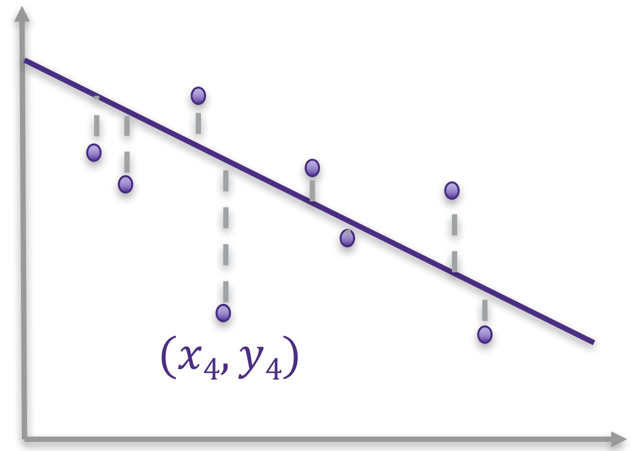
Picture from en.wikipedia.org/wiki/Linear_regression

Model Fitting

- Q: How do you find the best model parameters
- A: Choose the setting that minimizes / maximizes some function
  - for minimization, often called a ”loss function”

- Take an ML course for details on ways choose these
  - maximum likelihood
  - maximum a posteriori
  - regularization
  - etc.

Example: best fit line



- Model: y ~ A x + B

- Classical linear regression:
  Find A and B to minimize sum of squared errors:

$$\sum_i \left(y_i - (A\, x_i + B)\right)^2$$

Model Fitting

- There is a formula in this case, but not in general...
- Q: How do we fit the model?

- Note that the loss function is usually convex
  - counter-example: deep learning
- A: Newton's method

Minimizing *multivariate* convex function

- In contrast to earlier, this is never a function of one argument
  - even for linear regression, we have two parameters: A and B

- Newton's method generalizes well to multivariate functions
- However, it is not always used due to complexity
  - derivative of a multivariate function is a vector (the gradient)
  - second derivative is a matrix (the Hessian)
  - finding this matrix is work, both theoretical and computational
    - seen ML papers whose full contribution is giving formulas for the entries of the Hessian matrix of a model

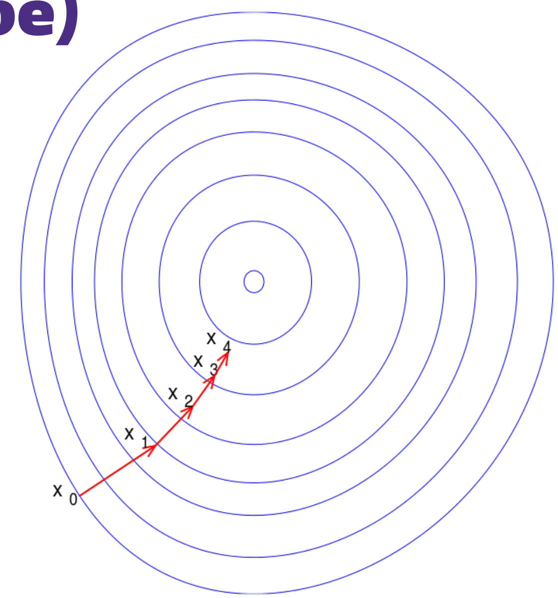
Minimizing *multivariate* convex function

- In contrast our earlier, this is never a function of one argument
  - even for linear regression, we have two parameters: A and B
- Common alternative is gradient descent...

Gradient Descent (~out of scope)

- Gradient = direction of steepest ascent
- -Gradient = direction of steepest decline

- Minimize loss function by stepping along –gradient
  - re-compute gradient after each step
  - decrease step size on each iteration
  - see numerical analysis or ML class for more…



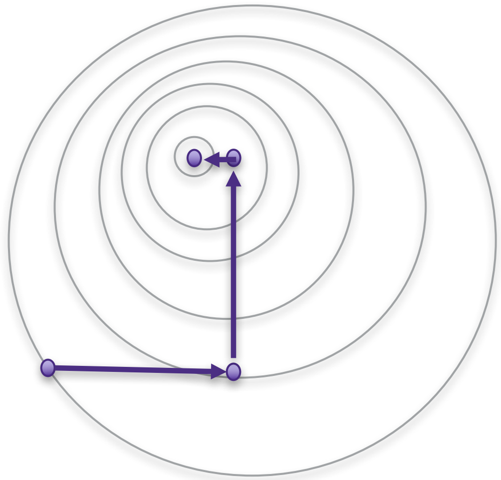
Picture from en.wikipedia.org/Gradient_descent

Gradient Descent (~out of scope)

- Gradient descent is widely used
- Newton's method may be faster
  - fewer iterations but more work per iteration
- also function must be twice differentiable...
  - not all loss functions even differentiable once!
    - see HW2 for an example

Coordinate Descent

- Only try stepping along coordinate axes



- Only trying to change one parameter at a time
  - loss function with **all parameters but one fixed**
  - *convex* function of one parameter
    - still convex since the loss function is convex
  - can minimize it using ternary search

Coordinate Descent for Model Fitting

start with an initial model

- maybe all zeros or random

repeat until it "stops changing much":

  for each parameter of the model:

    choose new value for the parameter that minimizes the loss function with all other parameters fixed

Coordinate Descent for Linear Regression

Either changing A or B

Minimizing function of the form:

$$f_B(A) := \sum_i \big(y_i - (A\,x_i + B)\big)^2$$

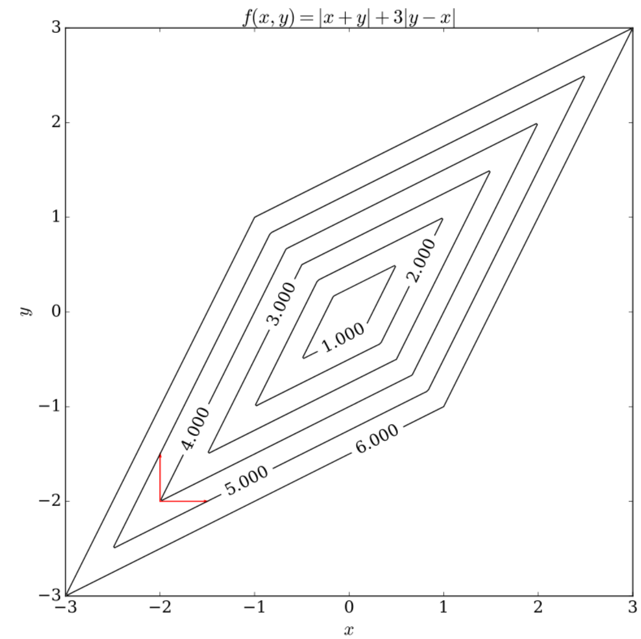
$$g_A(B) := \sum_i \big(y_i - (A\,x_i + B)\big)^2$$

B is fixed in first definition

A is fixed in second one

Coordinate Descent

> **Warning**: coordinate descent does not work for all functions
  - function can appear minimum along both axes BUT not be a true minimum
  - e.g., point (-2, -2) in picture



Picture from en.wikipedia.org/wiki/Coordinate_descent

Coordinate Descent

- Works for functions of the form $f(x_1, .., x_n) + g(x_1, ..., x_n)$ where
  - f is convex and differentiable
  - g is separable: $g(x_1, \dots, xn) := \sum_i g_i(xi)$ with each g_i convex
- In particular, it works for this function:

$$\sum_i \left(y_i - (A\, x_i + B)\right)^2 + |A| + |B|$$

- We will use this in HW2
  - (separable part is an "L1 regularization term"... they have a tendency to make many parameters zero)

HW2

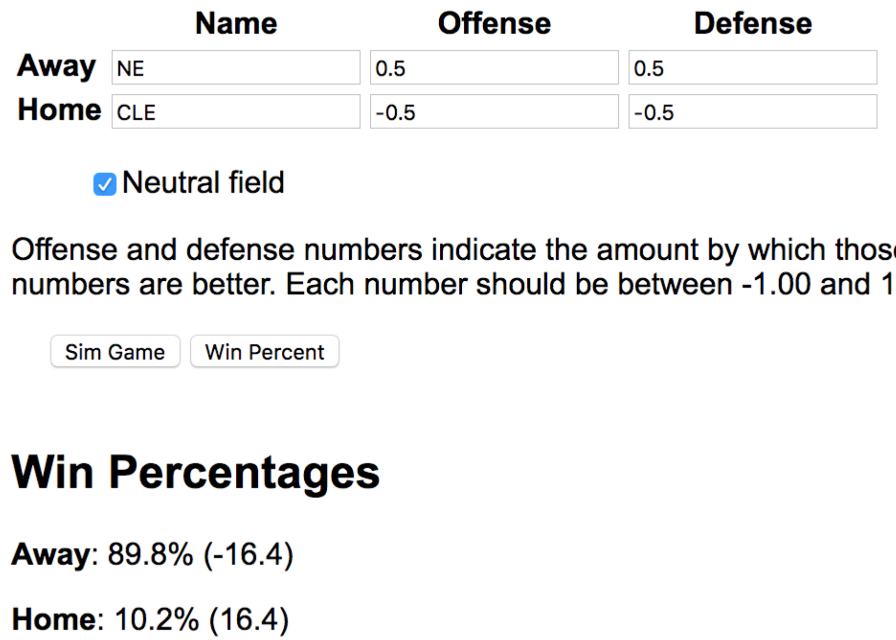
- Fit a model to describe NFL teams
- Each NFL game as a sequence of “drives”
  - drive is a series of consecutive plays with one team’s offense against the other team’s defense
  - drive starts somewhere on the field and ends somewhere else
    - the team on offense wants it to end in the end zone (6 points)
    - team on defense wants it to end on the other side (-2 points)
  - consider expected points for drives start & end points
    - average points scored by teams starting (ending) at that position

HW2

- More drives than games. More data = more predictive
- Fit a model to explain change in expected points on each drive
- Two parameters per team t: A_t for offense, B_t for defense
  - also a constant term C

$$\sum_{\text{drive } i} (y_i - (\mathrm{A}_{\text{offense } i} - \mathrm{B}_{\text{defense } i} + \mathrm{C}))^2 + \sum_{\text{team } t} |A_t| + |B_t|$$

HW2



> Web page to test out the model (if you want):
  - http://homes.cs.washington.edu/~kevinz/football-sim/
  - simulate a game OR
  - compute win probability (⇔ point spread)