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Finding a global minimum is hard!

We’ll settle for a local minimum (maybe with multiple restarts).
Consider a set of observations \( X = (x_1, \cdots, x_N) \).

Assume \( x_i \sim p(x_i|\theta) \)

Maximum likelihood:

\[
\theta_{MLE} = \arg\max p(X|\theta) = \arg\max \prod_{i=1}^{N} p(x_i|\theta)
\]

More convenient to maximize the log-likelihood:

\[
\theta_{MLE} = \arg\max \log p(X|\theta) = \arg\max \sum_{i=1}^{N} \log p(x_i|\theta)
\]
First-order conditions

The gradient $\nabla f = \left[ \frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_D} \right]^T$
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At a local minimum, Hessian $\nabla^2 f \succeq 0$ (positive semidefinite)

$$[\nabla^2 f]_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$
Find a bracket \((a, b)\) with a third point \(c \in (a, b)\), with

\[ f(a) > f(c) < f(b) \]

Implies a local minimum lies in \((a, b)\).
Finding an initial bracketing is not always easy. E.g.

- Pick two points $l$ and $r$, $l < r$
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- Pick two points \( l \) and \( r \), \( l < r \)
- If \( f(l) < f(r) \), \( c = l \) and \( b = r \), else \( a = l \) and \( c = r \).
Finding an initial bracketing is not always easy. E.g.

- Pick two points $l$ and $r$, $l < r$
- If $f(l) < f(r)$, $c = l$ and $b = r$, else $a = l$ and $c = r$.
- In the first case, choose $a < c$, and keep decreasing till $f(a) > f(c)$ (similarly with $b$ for second case)
Having done this, successively refine \((a, c)\) or \((c, b)\).

- Pick \(d\) in the longer interval \((a, c)\) or \((c, b)\).
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- Suppose it is \((c, b)\). Then either \((a, c, d)\) and \((c, d, b)\) forms a bracket.
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- Choose and repeat
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Doesn’t extend easily to higher dimensions.
The simplex algorithm (Nelder & Mead)

Find minimum of some function $f : \mathbb{R}^D \rightarrow \mathbb{R}$.

Requires only function evaluations. Very general purpose, but not very efficient.
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In 1-d we could bracket the minimum.
In higher dims, we must use other heuristics.
Start with an initial simplex.

Typically, pick an initial point \( \mathbf{P}_0 \).
Also set \((\mathbf{P}_1, \ldots, \mathbf{P}_{N+1})\) with \( \mathbf{P}_i = \mathbf{P}_0 + \lambda_i \mathbf{e}_i \).
Here \( \mathbf{e}_i \) is the \( i \)th coordinate direction, and \( \lambda_i \) is the length-scale in that direction.
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Assume $f(P_0) \leq f(P_1) \leq \cdots \leq f(P_{N+1})$. 
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Assume \( f(P_0) \leq f(P_1) \leq \cdots \leq f(P_{N+1}) \).

At each step, try to improve the worst point \( P_{N+1} \) using one of a sequence of moves.
Get initial simplex
Simplex algorithm

Find worst point, and find centroid of the remaining.
Reflect worst point.
This new point is now either worst, best or in the middle.
If this is the best point, extend.
and go back to step one.
If this is the worst point, contract.
If this is the worst point, contract.
Else shrink all points except the best.
Let $x_{old}$ be our current value

Update $x_{new}$ as 

\[ x_{new} = x_{old} - \eta \left. \frac{df}{dx} \right|_{x_{old}} \]

The steeper the slope, the bigger the move
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$\eta$: sometimes called the ‘learning rate’

(terminology from the neural network literature)
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Choosing $\eta$ is a dark art:
Gradient descent

Let $x_{old}$ be our current value

Update $x_{new}$ as  

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The steeper the slope, the bigger the move

$\eta$: sometimes called the ‘learning rate’
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Choosing $\eta$ is a dark art:

Better methods adapt step-size according to the curvature of $f$. 
Gradient descent in higher-dimensions

Gradient descent applies to higher dimensions too:

\[ x_{\text{new}} = x_{\text{old}} - \eta \nabla f\big|_{x_{\text{old}}} \]
Steepest descent

An any iteration, set $p$ to the direction of steepest descent.

$$p = \nabla f(x_i)$$

Minimize along that direction:  

$$\lambda_{min} = \arg\min_{\lambda} f(x_i + \lambda p)$$

Set $x_{i+1} = x_i + \lambda_{min} p$. 
Steepest descent

Can get trapped in long narrow valleys, where successive steps cancel each other.
Can get trapped in long narrow valleys, where successive steps cancel each other.
Conjugate gradient avoids moves along the same direction.
For a $D$-dim quadratic loss reaches minimum in $D$ steps
Common default method
NEWTON’S METHOD

Uses the second derivative (curvature) to decide the step-size $\eta$.

At current point $x_i$, evaluate $f(x_i), f'(x_i)$ and $f''(x_i)$. Fit a parabola having these values and set $x_{i+1}$ to its minimum.
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Easy to see that (show it!):

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$
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Easy to see that (show it!):

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$

If $f''$ is large, we’re uncertain about $f'$, so take a small step.
Update rule:

\[ x_{i+1} = x_i - [\nabla^2 f(x_i)]^{-1} \nabla f(x_i) \]
Newton’s method in higher dimensions

Update rule:

\[ x_{i+1} = x_i - \left[ \nabla^2 f(x_i) \right]^{-1} \nabla f(x_i) \]

Need to calculate the Hessian \( \nabla^2 f \): \( N^2 \) elements.

Need to invert the Hessian: \( N^3 \) operations.
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Each iteration can be expensive.
Quasi-Newton methods try to alleviate this issue.

We have to be wary about taking wild steps.
Set $p$ to the minimum of the local quadratic approximation.

$$p = [\nabla^2 f(x)]^{-1} \nabla f(x_i)$$

Reaches minimum of quadratic loss in 1 step
Quasi-Newton methods

Newton’s method: \( \mathbf{p} = [\nabla^2 f(\mathbf{x})]^{-1} \nabla f(\mathbf{x}_i) \)

Steepest’s descent: \( \mathbf{p} = I \nabla f(\mathbf{x}_i) \)
Newton’s method: \( p = \left[ \nabla^2 f(x) \right]^{-1} \nabla f(x_i) \)

Steepest’s descent: \( p = I \nabla f(x_i) \)

Quasi-Newton methods use other matrices \( B \):

\[ p = B \nabla f(x_i) \]
Quasi-Newton methods

Newton’s method: \( p = [\nabla^2 f(x)]^{-1} \nabla f(x_i) \)

Steepest’s descent: \( p = l \nabla f(x_i) \)

Quasi-Newton methods use other matrices \( B \):

\[ p = B \nabla f(x_i) \]

Usually, \( B \) is allowed to vary from iteration to iteration, with

\[ B_i \rightarrow [\nabla^2 f(x)]^{-1} \]

Get benefits of Newton’s method, without \( O(N^3) \) computations.
E.g. BFGS
Saw this last lecture

Simple, clean and inexpensive.
Often the 1-d problems can be solved exactly.
Convergence can be slow.
Exception: axis aligned ellipses need just $D$ steps.
Optimization in R

Use the `optim` function

Syntax:

```r
optim(par, fn, gr = NULL, ..., 
    method = c('Nelder-Mead', 'BFGS', 'CG', 'L-BFGS-B', 'SANN', 
               'Brent'),
    lower = -Inf, upper = Inf,
    control = list(), hessian = FALSE)
```

- `fn`: function to be optimized
- `gr`: gradient function (calculate numerically if `NULL`)
- `par`: initial value of parameter to be optimized (should be first argument of `fn`)