The No Free Lunch Theorem of Optimization and Sampling

Blind Search

Definition
If we have no closed-form mathematical expression for the forward function

$$\mathbf{d} = g(\mathbf{m})$$

but only an algorithm that allows pointwise evaluation of g, then

We are performing a **blind search** for the solution

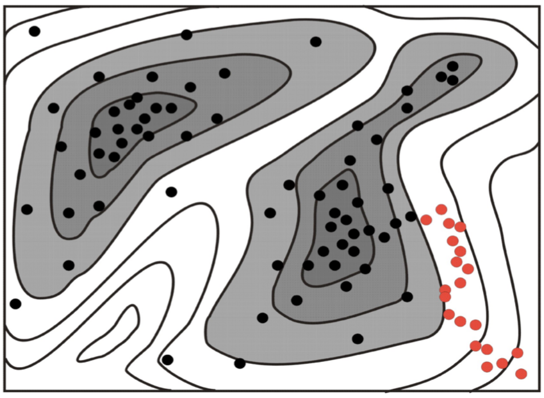
The No-Free-Lunch Theorem for optimization

The performance of all "blind" optimization algorithms is exactly the same, when averaged over all concievable problems.

Wolpert, D.H., Macready, W.G. (1997), No Free Lunch Theorems for Optimization, IEEE Transactions on Evolutionary Computation 1, 67

This statement is true for any performance measure

Why is the No-Free-Lunch Theorem relevant for sampling problems?



The initial phase of any random-walk-based sampling is essentially an optimization!

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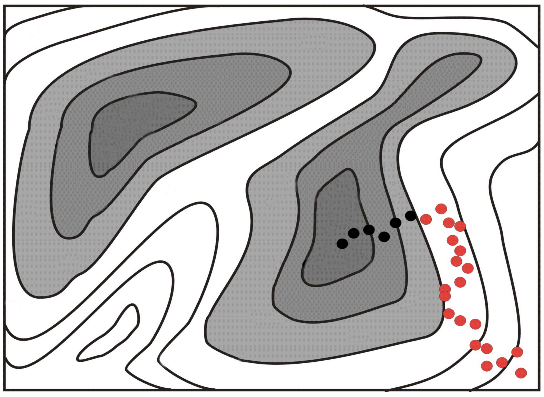

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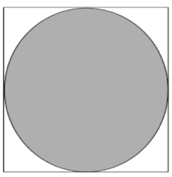
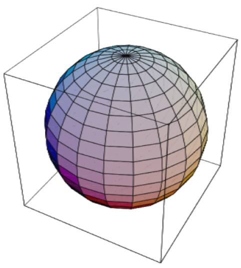
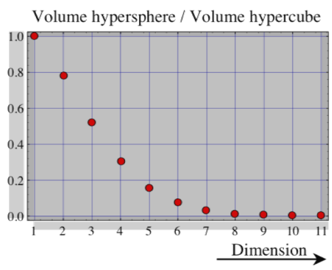
The size of high-probability areas shrinks as the dimension of the space goes up

The “curse of dimensionality”:

$2R$	πR^2	$\frac{4}{3}\pi R^3$	$(...)$	$\frac{\pi^n}{n!} R^{2n}$	$\frac{2^{n+1}\pi^n}{(2n+1)!!} R^{2n+1}$
$2R$	$(2R)^2$	$(2R)^3$	$(...)$	$(2R)^{2n}$	$(2R)^{2n+1}$



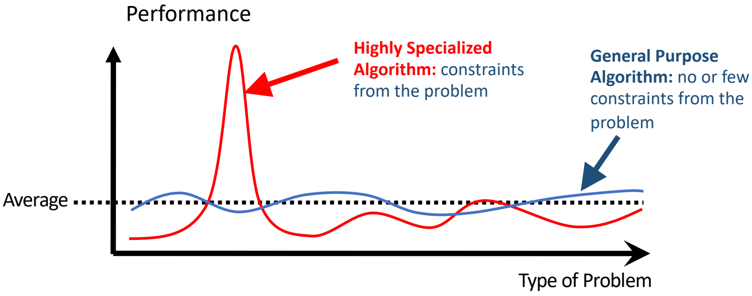




"Blind" Algoritms for Inversion

- Steepest Descend
- Conjugate Gradient
- Markov Chain Monte Carlo (MCMC)
- Neighbourhood Algorithms
- Transdimensional Sampling
- Genetic Algorithms
- Machine Learning Strategies
- Simulated Annealing
- Rejection Sampling
- Plain Metropolis
- Taboo Search
- ...

The main legacy of the "No-Free-Lunch Theorem"



- Generally, multi-purpose algorithms perform modestly
- Efficient algorithms are tuned to the problem