Lecture 9

Information Theory and Simulated Annealing

Last Time:

- BackPropagation
- Neural Nets and Universal Approximation
- KL-Divergence

TODAY

- KL divergence
- entropy and cross-entropy
- maximum entropy distributions

Model Comparison

- deviance and a simulation to understand it
- AIC as a in-sample correction for overfitting

MORE TODAY

- Baseball example and AIC for linear Regression
- AIC and variable (feature) selection
- local search with random starts
- simulated annealing

What did we learn about learning?

- x-validation: minimizes loss on training, fits hyperparams on validation
- test risk approximates out-of-sample risk
- regularization or complexity selection helps avoid overfitting
- we have seen the context of supervised learning $p(y|x)$

In unsupervised learning, want $p(x)$. Also need to learn these params using MLE or similar.

KL-Divergence

$$D_{KL}(p, q) = E_p[log(p) - log(q)] = E_p[log(p/q)]$$
$$= \sum_i p_i log(\frac{p_i}{q_i}) \ or \int dPlog(\frac{p}{q})$$

$$D_{KL}(p, p) = 0$$

KL divergence measures distance/dissimilarity of the two distributions p(x) and q(x).

KL-Divergence is always non-negative

Jensen's inequality: given a convex function $f(x)$:

$$E[f(X)] \geq f(E[X])$$

$$\implies D_{KL}(p,q) \geq 0 \text{ (0 iff } q = p \, \forall x\text{).}$$

$$D_{KL}(p,q) = E_p[log(p/q)] = E_p[-log(q/p)] \geq -\log(E_p[q/p]) = -\log(\int dQ) = 0$$

PROBLEM: we dont know distribution p. If we did, why do inference?

SOLUTION: Use the empirical distribution

That is, approximate population expectations by sample averages.

Maximum Likelihood justification

$$D_{KL}(p, q) = E_p[log(p/q)] = \frac{1}{N}\sum_i (log(p_i) - log(q_i))$$

Minimizing KL-divergence $\implies$ maximizing $\sum_i log(q_i)$

Which is exactly the log likelihood! MLE!

Information and Uncertainty

- coin at 50% odds has maximal uncertainty
- reflects my lack of knowledge of the physics
- many ways for 50% heads.
- an election with $p = 0.99$ has a lot of Information

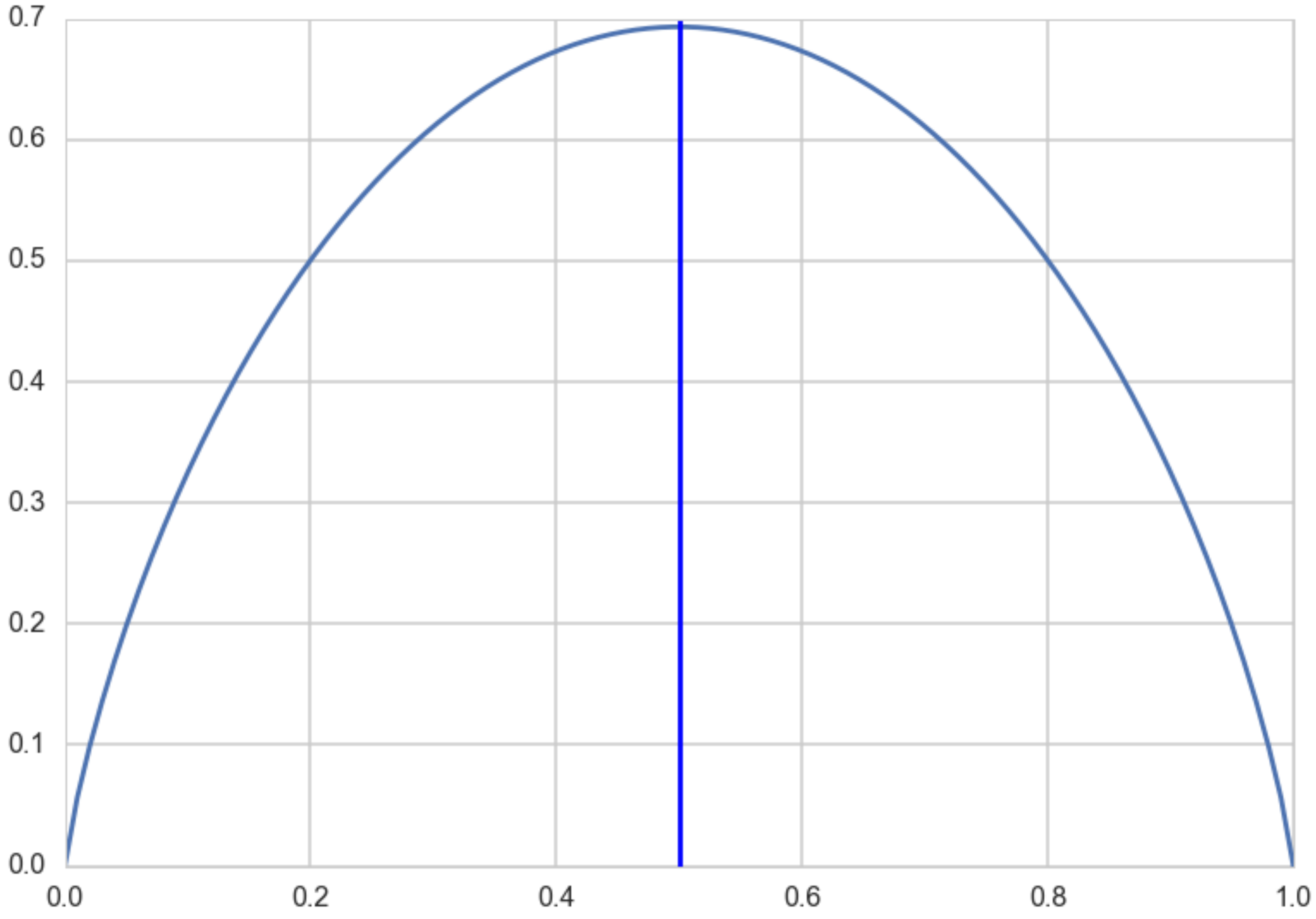
information is the reduction in uncertainty from learning an outcome

Information Entropy, a measure of uncertainty

Desiderata:
- must be continuous so that there are no jumps
- must be additive across events or states, and must increase as the number of events/states increases

$$H(p) = -E_p[log(p)] = -\int p(x)log(p(x))dx \;\; OR \; -\sum_i p_i log(p_i)$$

Entropy for coin fairness



$$H(p) = -E_p[log(p)] = -p * log(p) - (1-p) * log(1-p)$$

```
def h(p):
    if p==1.:
        ent = 0
    elif p==0.:
        ent = 0
    else:
        ent = - (p*math.log(p) + (1-p)* math.log(1-p))
```

Maximum Entropy (MAXENT)

- finding distributions consistent with constraints and the current state of our information
- what would be the least surprising distribution?
- The one with the least additional assumptions?

The distribution that can happen in the most ways is the one with the highest entropy

For a gaussian

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$

$$H(p) = E_p[log(p)] = E_p[-\frac{1}{2}log(2\pi\sigma^2) - (x-\mu)^2/2\sigma^2]$$

$$= -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2\sigma^2}E_p[(x-\mu)^2] = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2} = \frac{1}{2}log(2\pi e\sigma^2)$$

Cross Entropy

$$H(p, q) = -E_p[log(q)]$$

Then one can write:

$$D_{KL}(p, q) = H(p, q) - H(p)$$

KL-Divergence is additional entropy introduced by using q instead of p.

We saw this for Logistic regression

- $H(p, q)$ and $D_{KL}(p, q)$ are not symmetric.
- if you use a unusual , low entropy distribution to approximate a usual one, you will be more surprised than if you used a high entropy, many choices one to approximate an unusual one.

Corollary: if we use a high entropy distribution to approximate the true one, we will incur lesser error.

Gaussian is MAXENT for fixed mean and variance

Consider $D_{KL}(q,p) = E_q[log(q/p)] = H(q,p) - H(q) >= 0$

$$H(q,p) = E_q[log(p)] = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2\sigma^2}E_q[(x-\mu)^2]$$

$E_q[(x-\mu)^2]$ is CONSTRAINED to be σ^2.

$$H(q,p) = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2} = -\frac{1}{2}log(2\pi e\sigma^2) = H(p) >= H(q)!!!$$

Importance of MAXENT

- most common distributions used as likelihoods (and priors) are in the exponential family, MAXENT subject to different constraints.
- gamma: MAXENT all distributions with the same mean and same average logarithm.
- exponential: MAXENT all non-negative continuous distributions with the same average inter-event displacement

Importance of MAXENT

- Information entropy enumerates the number of ways a distribution can arise, after having fixed some assumptions.
- choosing a maxent distribution as a likelihood means that once the constraints has been met, no additional assumptions.

The most conservative distribution we could choose consistent with our constraints!

MODEL COMPARISON

Likelihood Ratio

$H(p)$ cancels out!!

$$D_{KL}(p,q) - D_{KL}(p,r) = H(p,q) - H(p,r) = E_p[log(r) - log(q)] = E_p[log(\frac{r}{q})]$$

In the sample approximation we have:

$$D_{KL}(p,q) - D_{KL}(p,r) = \frac{1}{N}\sum_i log(\frac{r_i}{q_i}) = \frac{1}{N}log(\frac{\prod_i r_i}{\prod_i q_i}) = \frac{1}{N}log(\frac{\mathcal{L}_r}{\mathcal{L}_q})$$

Model Comparison: Deviance

You only need the sample averages of the logarithm of r and q:

$$D_{KL}(p,q) - D_{KL}(p,r) = \langle log(r) \rangle - \langle log(q) \rangle$$

Define the deviance: $D(q) = -2 \sum_i log(q_i)$, a risk (e.g., -2 $\times$ ℓ, although the distribution need not be a likelihood)...

$$D_{KL}(p,q) - D_{KL}(p,r) = \frac{2}{N}(D(q) - D(r))$$

Example

Generate data from:

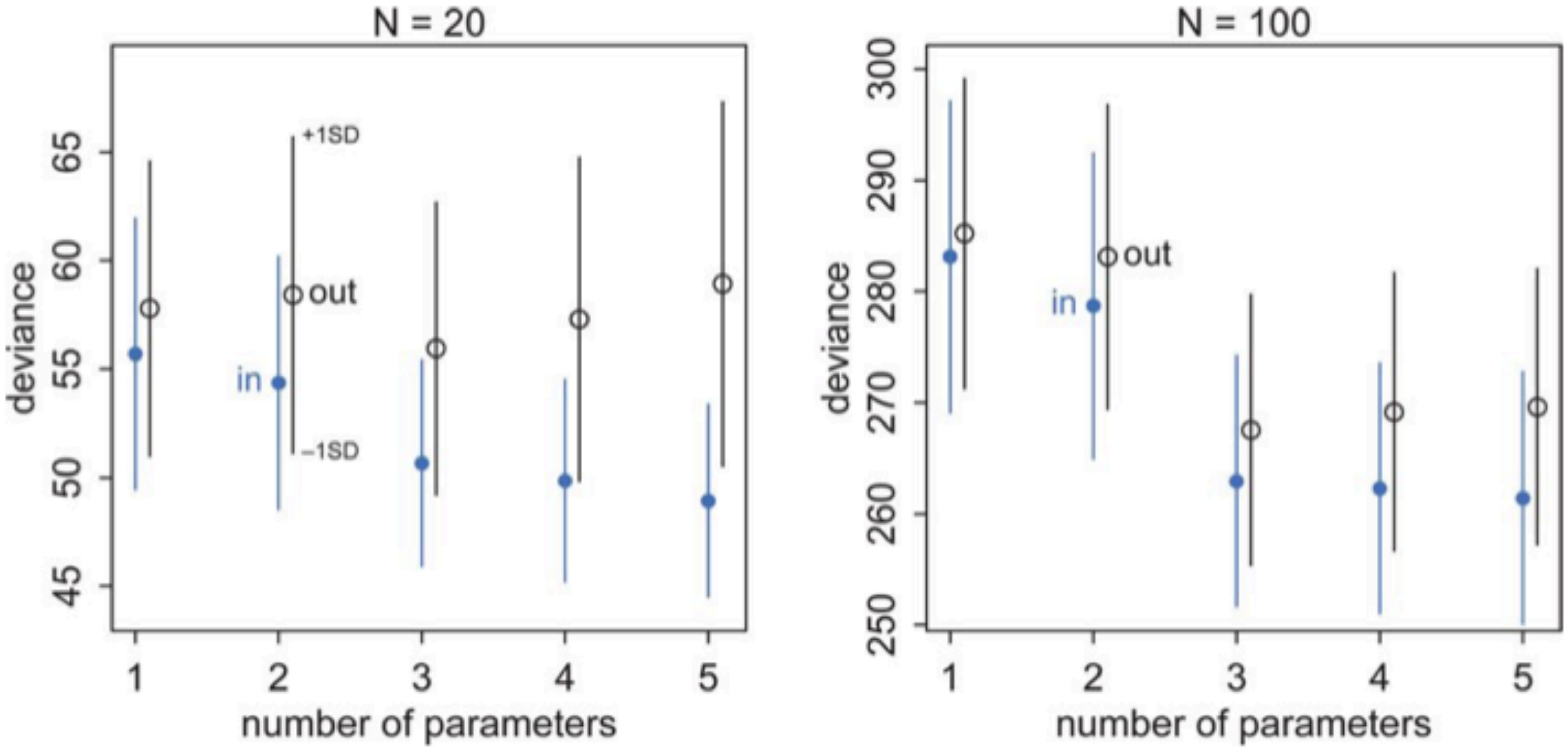
$$\mu_i = 0.15x_{1,i} - 0.4x_{2,i}\,,\;\; y \sim N(\mu, 1)$$

2 parameter model.

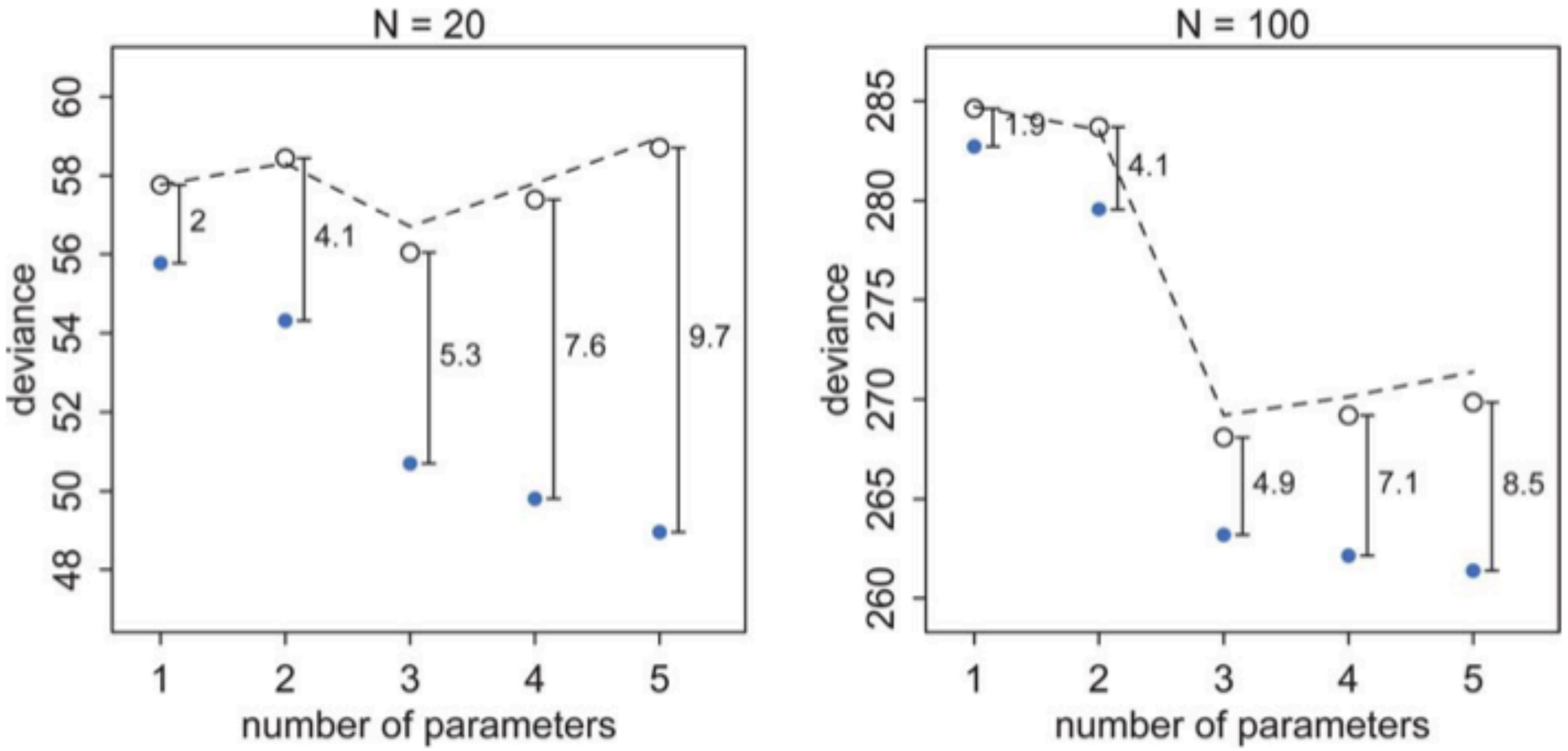
Generate 10,000 realizations, for 1-5 parameters, 20 data points and 100 data points.

Split into train and test, and do OLS.

Train to Test



AIC



The test set deviances are $2 * p$ above the training set ones.

Akake **Information Criterion**:

AIC **estimates out-of-sample deviance**

$$AIC = D_{train} + 2p$$

- Assumption: likelihood is approximately multivariate gaussian.
- penalized log-likelihood or risk if we choose to identify our distribution with the likelihood: REGULARIZATION
- high p increases the out-of-sample deviance, less desirable.

Baseball data set

Description: Salaries in 1992 and 27 performance statistics for 337 baseball players (no pitchers) in 1991.

```
baseball = pd.read_table("data/baseball.dat", sep='\s+')
baseball.head()
```

	salary	average	obp	runs	hits	doubles	triples	homeruns	rbis	walks	sos	sbs	errors	freeagent	arbitration	ru
0	3300	0.272	0.302	69	153	21	4	31	104	22	80	4	4	1	0	0.
1	2600	0.269	0.335	58	111	17	2	18	66	39	69	0	4	1	0	0.
2	2500	0.249	0.337	54	115	15	1	17	73	63	116	6	6	1	0	0.
3	2475	0.260	0.292	59	128	22	7	12	50	23	64	21	22	0	1	0.
4	2313	0.273	0.346	87	169	28	5	8	58	70	53	3	9	0	1	1.

(from http://www.amstat.org/publications/jse/v6n2/datasets.watnik.html)

AIC for Linear Regression

$AIC = D_{train} + 2p$ where $D(q) = -2\sum_i log(q_i) = -2\ell$

$$\sigma^2_{MLE} = \frac{1}{N}SSE$$

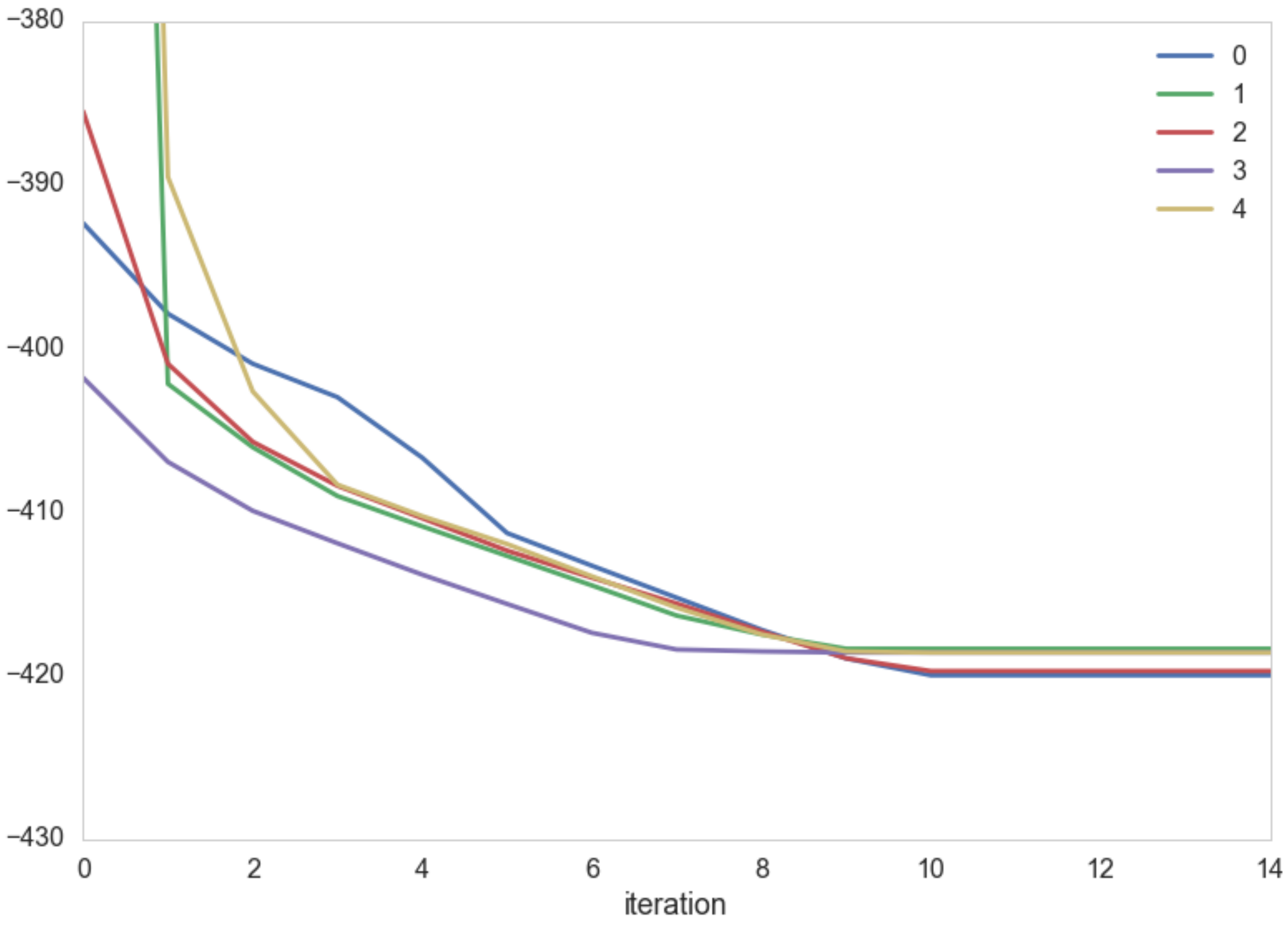
$$AIC = -2(-\frac{N}{2}(log(2\pi) + log(\sigma^2)) - 2(-\frac{1}{2\sigma^2_{MLE}} \times SSE) + 2p$$

$$AIC = Nlog(SSE/N) + 2p + constant$$

Local Search with Random starts

- wish to find best set of features for prediction
- want parsimonious model, no overfitting
- Combinatoric search is hard
- 2^{27} sized search space for baseball problem
- make local perturbations

```python
from sklearn.linear_model import LinearRegression

runs_aic = np.empty((nstarts, iterations))

for i in range(nstarts):

    run_current = runs[i]

    for j in range(iterations):

        # Extract current set of predictors
        run_vars = predictors[predictors.columns[run_current]]
        g = LinearRegression().fit(X=run_vars, y=logsalary)
        run_aic = aic(g, run_vars, logsalary)
        run_next = run_current

        # Test all models in 1-neighborhood and select lowest AIC
        for k in range(ncols):
            run_step = run_current.copy()
            run_step[k] = not run_current[k]
            run_vars = predictors[predictors.columns[run_step]]
            g = LinearRegression().fit(X=run_vars, y=logsalary)
            step_aic = aic(g, run_vars, logsalary)
            if step_aic < run_aic:
                run_next = run_step.copy()
                run_aic = step_aic

        run_current = run_next.copy()
        runs_aic[i,j] = run_aic

    runs[i] = run_current
```

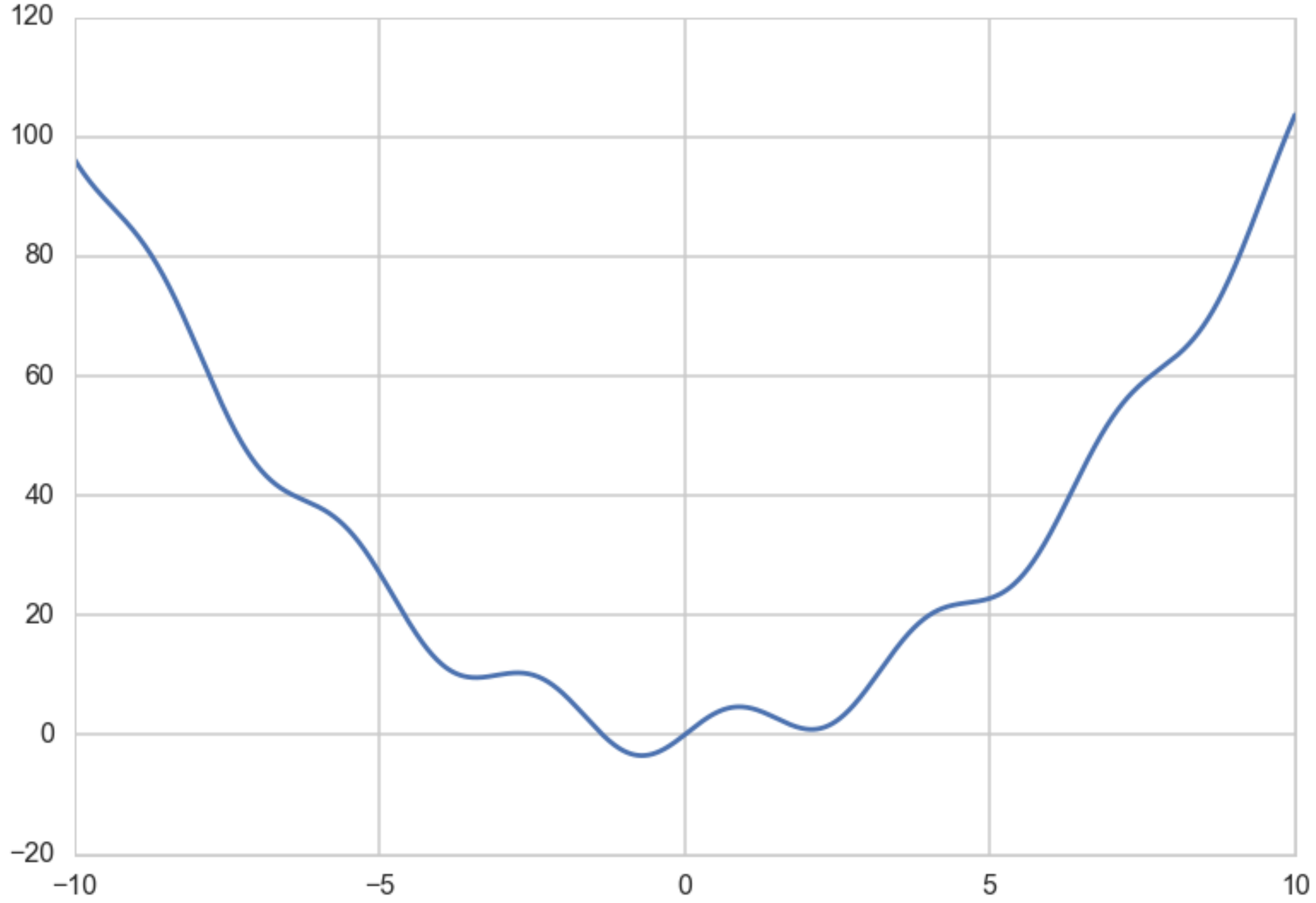


```
FEATURES

arbitration     5   BEST SOLUTION: (array([ 1,  2,  5,  7,  9, 11, 12, 13, 14, 15, 24, 25]),)
rbis            5
freeagent       5
obppererror     4       0 -420.000042669
sos             4       1 -418.380197435
hitsperso       3       2 -419.743167044
sbshits         3       3 -418.611888647
hitspererror    3       4 -418.611888647
sbsobp          3       AICs
soserrors       2
runs            2
hrsperso        2
```

Features present in most starts, left, best solution, right top, AICs, right

NEED GLOBAL OPTIM

Example: $x^2 + 4sin(2x)$

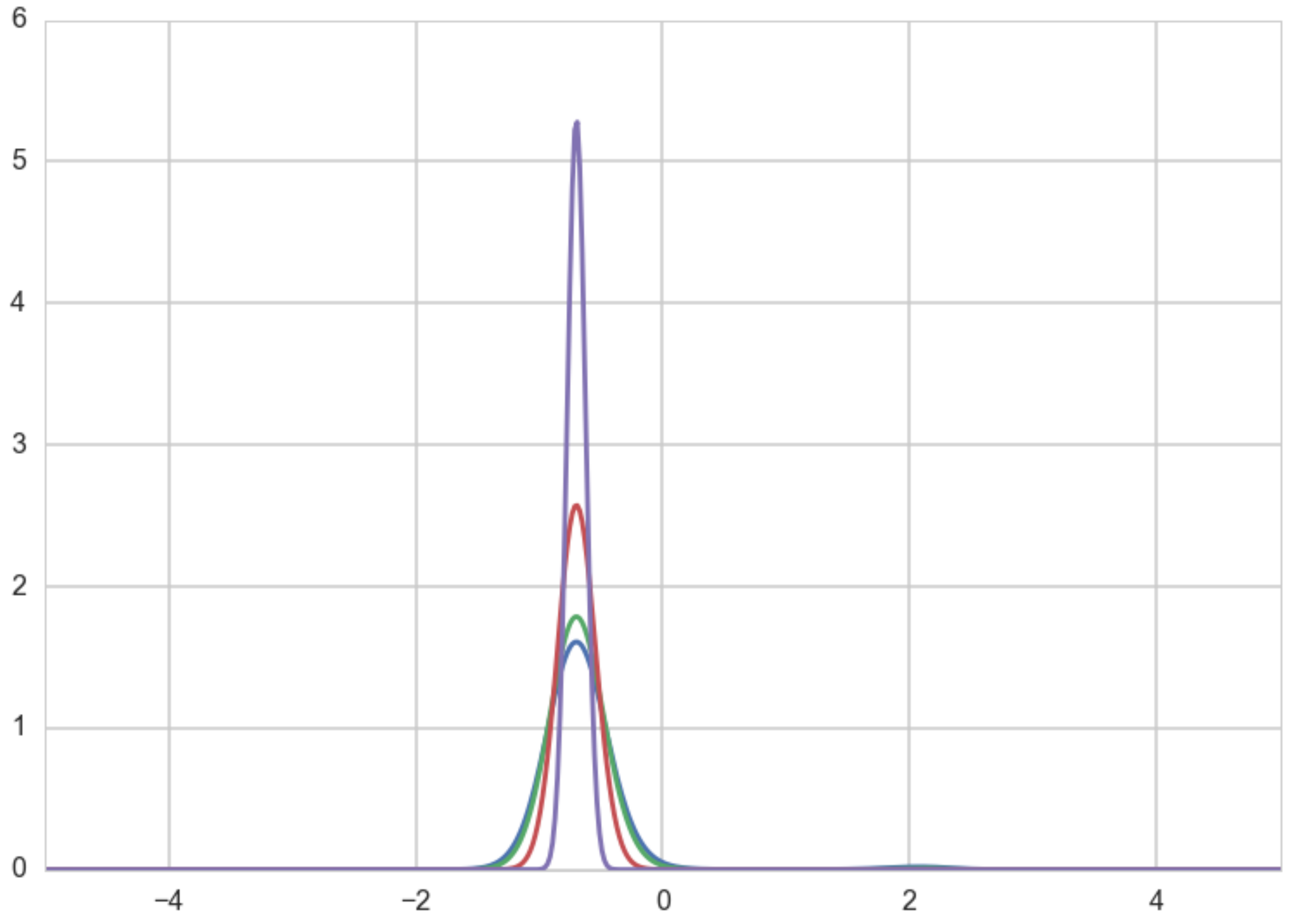


Observations:

If you identify a distribution $p(x) = e^{-f(x)}$ one may define a secondary distribution:

$$p_T(x) = e^{-f(x)/T} = P(x)^{1/T}$$

- [O1]: the exponentiation ensures that the peak from global minimum is favored over the rest in f
- [O2]: you get a peakier distribution as $T \to 0$ around the global minimum: distribution $\to$ optimum!



Physical Annealing

A system is first heated to a melting state and then cooled down slowly.

- when solid is heated, its molecules start moving randomly, and its energy increases
- [O3]: if subsequent process of cooling is slow, the energy decreases slowly, with some random increases governed by the Boltzmann distribution
- if cooling slow and deep enough, system will eventually settle down to the lowest energy state with minimal potential energy

Simulated Annealing

Minimize f by identifying with the energy of an imaginary physical system undergoing an annealing process.

Move from x_i to x_j via a **proposal**.

If the new state has lower energy, accept x_j.

[O3]: If the new state has higher energy, accept with probability

$$A = \exp\left(-\Delta f / kT\right)$$

- stochastic acceptance of higher energy states, allows our process to escape local minima.
- When T is high, the acceptance of these uphill moves is higher, and local minima are discouraged.
- As T is lowered, more concentrated search near current local minimum, since only few uphill moves will be allowed.
- Thus, if we get our temperature decrease schedule right, we can hope that we will converge to a global minimum.

If the lowering of the temperature is sufficiently slow, the system reaches "thermal equilibrium" at each temperature. Then Boltzmann's distribution applies:

$$p(X = i) = \frac{1}{Z(T)} \exp\left(\frac{-E_i}{kT}\right)$$

where

$$Z(T) = \sum_j \exp\left(\frac{-E_j}{kT}\right)$$

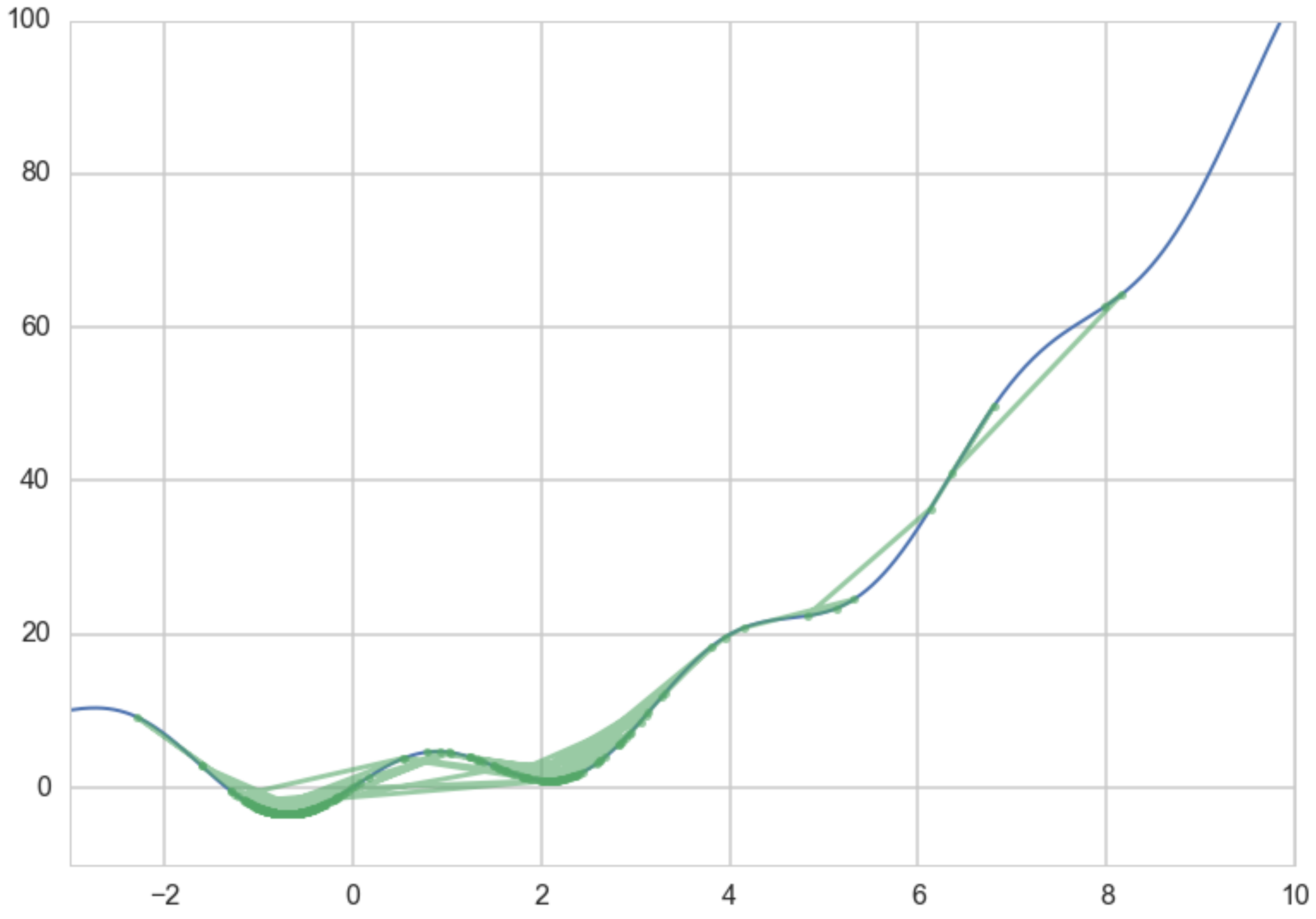
Proposal

- it proposes a new position x from a **neighborhood** $\mathcal{N}$ at which to evaluate the function.
- all the positions x in the domain we wish to minimize a function f over ought to be able to communicate.
- detailed balance: proposal is symmetric
- ensures $\{x_t\}$ generated by simulated annealing is a stationary markov chain with target boltzmann distribution: equilibrium

The Simulated Annealing Algorithm

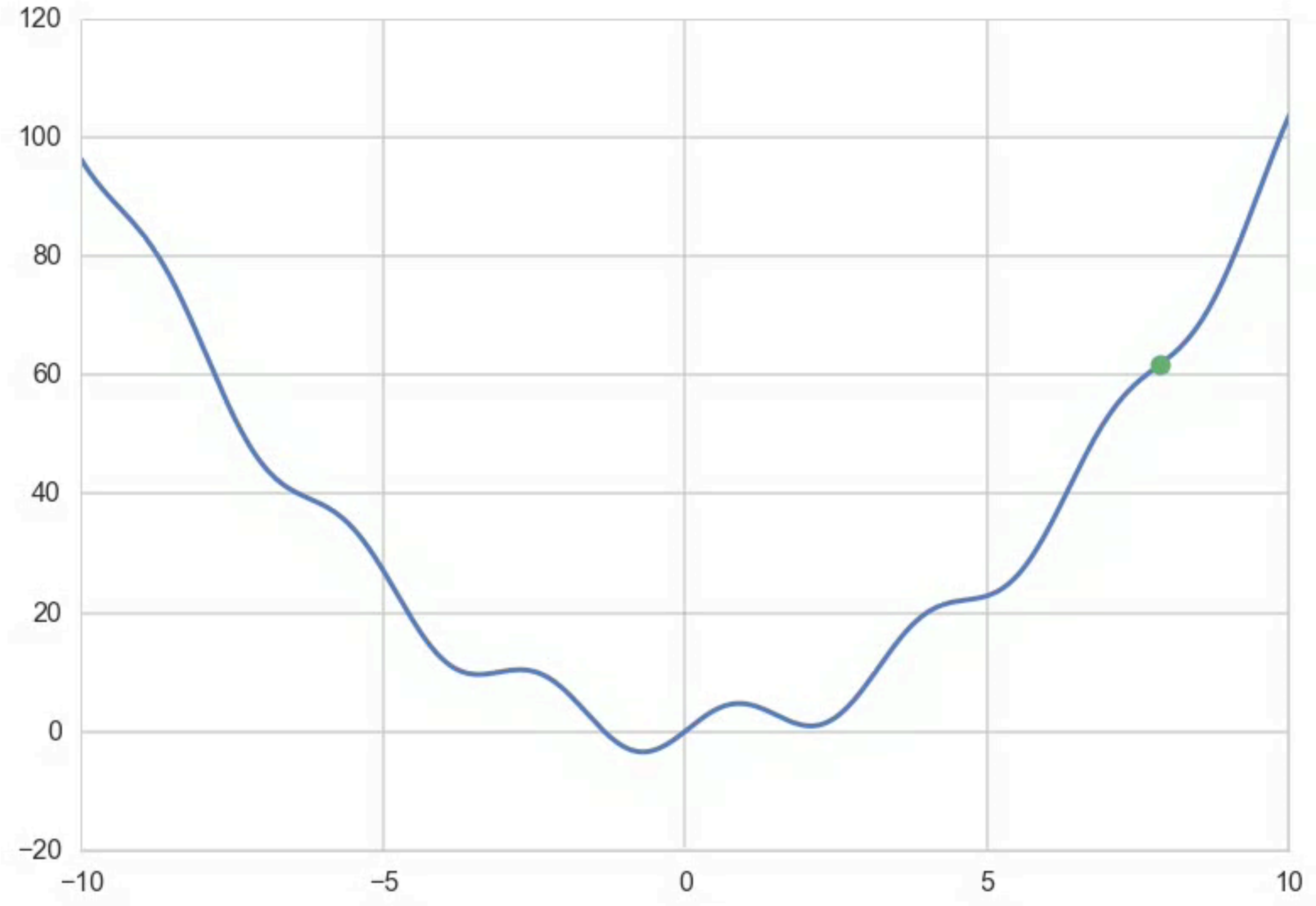
1. Initialize $x_i, T, L(T)$ where L = iterations at a particular temperature.
2. Perform L transitions:
   (a) propose x_j (b) If x_j is accepted (according to probability $P = e^{(-\Delta E/T)}$), set $x_{i+1} = x_j$, else set $x_{i+1} = x_i$
3. Update T and L, go to 2

```python
def sa(energyfunc, initials, epochs, tempfunc, iterfunc, proposalfunc):
    accumulator=[]
    best_solution = old_solution = initials['solution']
    T=initials['T']
    length=initials['length']
    best_energy = old_energy = energyfunc(old_solution)
    accepted=0
    total=0
    for index in range(epochs):
        print("Epoch", index)
        if index > 0:
            T = tempfunc(T)
            length=iterfunc(length)
        print("Temperature", T, "Length", length)
        for it in range(length):
            total+=1
            new_solution = proposalfunc(old_solution)
            new_energy = energyfunc(new_solution)
            # Use a min here as you could get a "probability" > 1
            alpha = min(1, np.exp((old_energy - new_energy)/T))
            if ((new_energy < old_energy) or (np.random.uniform() < alpha)):
                # Accept proposed solution
                accepted+=1
                accumulator.append((T, new_solution, new_energy))
                if new_energy < best_energy:
                    # Replace previous best with this one
                    best_energy = new_energy
                    best_solution = new_solution
                    best_index=total
                    best_temp=T
                old_energy = new_energy
                old_solution = new_solution
            else:
                # Keep the old stuff
                accumulator.append((T, old_solution, old_energy))

    best_meta=dict(index=best_index, temp=best_temp)
    print("frac accepted", accepted/total, "total iterations", total, 'bmeta', best_meta)
    return best_meta, best_solution, best_energy, accumulator
```



```python
tf = lambda t: 0.8*t #temperature function
itf = lambda length: math.ceil(1.2*length) #iteration function
inits=dict(solution=8, length=100, T=100)
bmeta, bs, be, out = sa(f, inits, 30, tf, itf, pf)
```

```
Epoch 0
Temperature 100 Length 100
Epoch 1
Temperature 80.0 Length 120
Epoch 2
Temperature 64.0 Length 144
Epoch 3
Temperature 51.2 Length 173
Epoch 4
Temperature 40.96000000000001 Length 208
Epoch 5
Temperature 32.76800000000001 Length 250
Epoch 6
Temperature 26.21440000000001 Length 300
Epoch 7
Temperature 20.97152000000001 Length 360
...
Epoch 27
Temperature 0.24178516392292618 Length 13863
Epoch 28
Temperature 0.19342813113834095 Length 16636
Epoch 29
Temperature 0.15474250491067276 Length 19964
frac accepted 0.7921531132581857 total iterations 119232 bmeta {'index': 112695, 'temp': 0.15474250491067276}
```



120
100
80
60
40
20
0
−20
−10
−5
0
5
10