Simulations in Statistical Physics

Course for MSc physics students

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Percolation model

Bond [site] percolation

- Let us have a lattice (network)
- Each bond [site] is occupied with probability p
- (unoccupied with probability $1 - p$)
- A cluster is a set of sites connected by occupied bonds
  [A cluster is a set of occupied sites]

Hoshen-Kopelman Algorithm

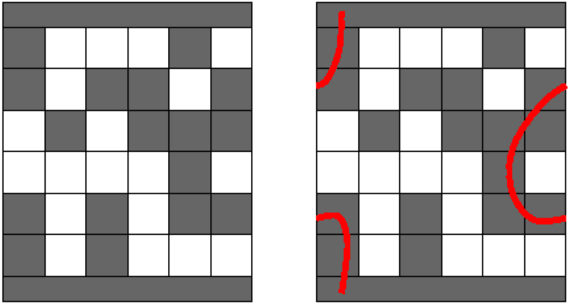
- Numerical task: find clusters
- Identify clusters
- Visit all sites
- Mark them with numbers

1	0	1	1	0	0	1	1	1	1	1	1	1	1	0
0	0	1	0	0	1	0	0	1	1	1	0	0	0	1
0	1	1	1	1	0	0	0	0	1	0	1	1	1	1
1	0	1	1	0	1	0	0	0	0	1	1	0	0	1
0	0	1	1	0	0	0	0	1	0	0	0	1	0	1
1	0	1	0	1	0	0	0	1	0	0	1	0	1	1
1	1	0	0	1	0	1	1	1	1	1	1	1	1	0
1	0	0	1	1	1	0	0	1	1	1	0	0	1	1
1	1	0	1	1	1	0	1	0	1	0	0	1	0	0
0	0	1	0	0	1	1	0	1	1	0	1	1	0	0

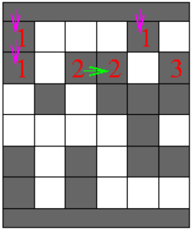
1	0	2	2	0	0	3	3	3	3	3	3	3	3	0
0	0	2	0	0	4	0	0	3	3	3	0	0	0	5
0	2	2	2	2	0	0	0	0	3	0	5	5	5	5
6	0	2	2	0	7	0	0	0	0	5	5	0	0	5
0	0	2	2	0	0	0	0	5	0	0	0	8	0	5
9	0	2	0	10	0	0	0	5	0	0	5	0	5	5
9	9	0	0	10	0	5	5	5	5	5	5	5	5	0
9	0	0	10	10	10	0	0	5	5	5	0	0	5	5
9	9	0	10	10	10	0	11	0	5	0	0	12	0	0
0	0	13	0	0	10	10	0	5	5	0	12	12	0	0

Hoshen-Kopelman Algorithm

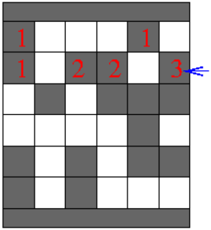
- Site percolation
- Helical boundary conditions
- Go through site in typewriter style
- Check left and above



Hoshen-Kopelman Algorithm, Helical BC



link[1]=1
link[2]=2
link[3]=3



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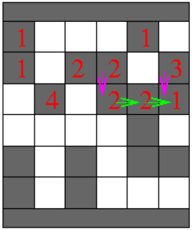
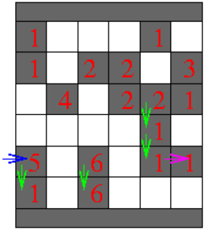
link[2]=2
link[3]=1



link[1]=1
link[2]=1
link[3]=1
link[4]=4



link[1]=1
link[2]=1
link[3]=1
link[4]=4
link[5]=1
link[6]=6

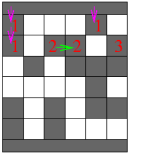
Hoshen-Kopelman Algorithm

```
largest_label = 0;
for (y = 0;y < n_rows;y++) {
  for (x = 0;x < n_columns;x++) {
    if (occupied[x][y]) {
      left = occupied[x-1][y];
      above = occupied[x][y-1];
      if (left == 0) && (above == 0) {
        largest_label ++;
        label[x][y] = largest_label;

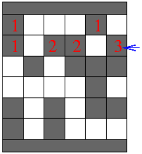
      } else if (left != 0) && (above == 0) {
        label[x,y] = find(left);

      } else if (left == 0) && (above != 0) {
        label[x,y] = find(above);

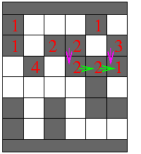
      } else {
        label[x,y] = union(left,above);
      }
    }
  }
  /* Helical boundary conditions */
  if (occupied[n_columns-1][y]) && (occupied[0][y]) {
    union(occupied[n_columns-1][y],occupied[0][y])
  }
}
```



link[1]=1
link[2]=2
link[3]=3



link[1]=1
link[2]=2
link[3]=1



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Hoshen-Kopelman Algorithm

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      } else if (left != 0) && (above == 0) {
        label[x,y] = find(left);

      } else if (left == 0) && (above != 0) {
        label[x,y] = find(above);

      } else {
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      }
    }
  }
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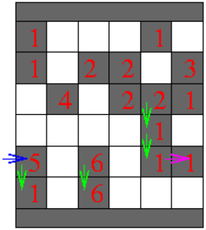
  if (occupied[n_columns-1][y]) && (occupied[0][y]) {
    union(occupied[n_columns-1][y],occupied[0][y])
  }
}
```



link[1]=1
link[2]=1
link[3]=1
link[4]=4
link[5]=1
link[6]=6

```
int link[N];

int find(int x) {
 while (link[x] != x)
   x = link[x];
 return x;
}
```

```
int union(int x, int y) {
  int fx = find(x);
  int fy = find(y);
  if (fx < fy) {
    link[fy] = fx;
    return (fx);
  } else {
    link[fx] = fy;
    return (fy);
  }
}
```

Hoshen-Kopelman Algorithm

- Go through lattice as typewriter
- Check neighbors
- Resolve conflicts by linking clusters together
- Original trick: use link[] array for cluster size measure
  - link[] positive: number of sites in the cluster
  - link[] negative: cluster is linked to on other cluster
  - Not necessary faster than a seperate arrey for size

Percolation on networks (graphs)

- Network is defined by nodes and links
- Two arrays:
  - node[] list of nodes
  - link[i][] list of links of node i
  - link[i][j] is a link between i and j
- Cluster: nodes connected with links
- Links can be directed link[i][j] is a link from i $\rightarrow$ j

Stack (Verem – Hole/Pitfall)

- Last in forst out (LIFO)
- Code:

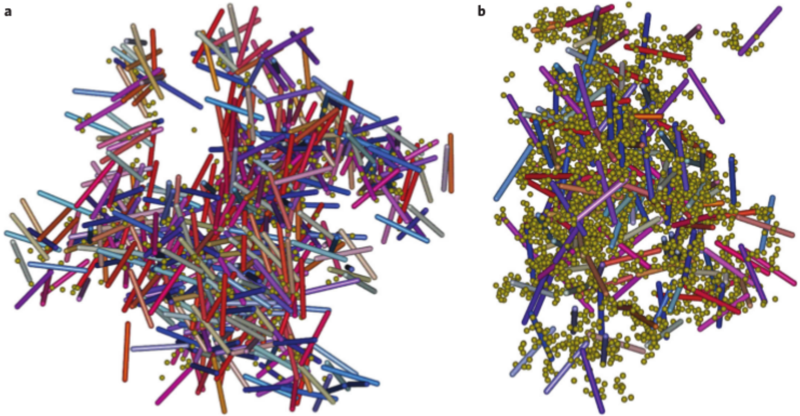
```
int Stack_size = Hopefully_large_enough_number;
int stack[Stack_size];
int sp=0;

void push(int item) {
  stack[sp++] = item;
  if (sp == Stack_size) enlarge_array(stack);
}

int pop() {
  return(stack[--sp]);
}
```

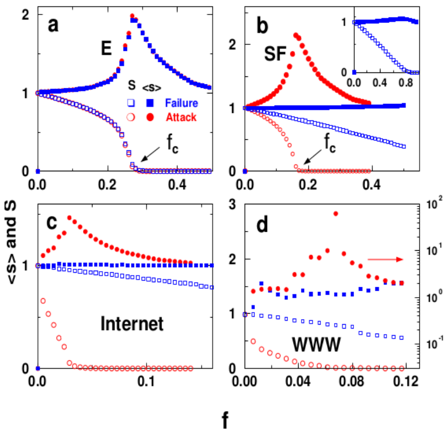
- Error handling?
- Size of the stack?

Percolation on networks (graphs)



Percolation on networks (graphs)

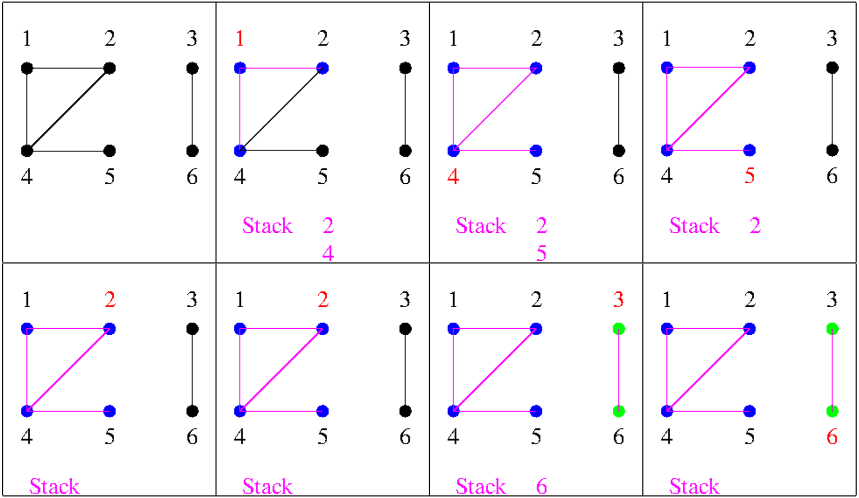
- Connected components
- Theory: p_c for random graph: number of links L is half of the number of nodes N: $L = N/2$
- Robustness:



Algorithm percolation on networks (graphs)

1. Go through each node
2. Put node in the stack
3. Get a node from the stack
4. Go through each unmarked link of the node
5. Put other end of links in the stack if it is not marked
6. Mark nodes
7. If the stack not empty Go to 3.
8. If the stack empty Go to 1.

Algorithm percolation on networks (graphs)



Algorithm percolation on networks (graphs)

```c
int node[N];
int nlink[N];
int link[N][N];
int stack[N]
int sp;

void percol() {
  int a,b,i;
  int cluster;

  sp = 0;
  cluster = 1;
  for (a = 0; a < N; a++) node[N]=0;
  for (a = 0; a < N; a++) {
    if (node[a] == 0) {
      stack[sp++] = a;
      node[a] = cluster++;
    }
    while (sp > 0) {
      i = stack[--sp];
      for (b = 0; b < nlink[i]; b++) {
        if (node[b] == 0) {
          stack[sp++] = b;
          node[b] = node[a];
        }
      }
    }
  }
}
```

1. Go through each node
2. Put node in the stack
3. Get a node from the stack
4. Go through each unmarked link of the node
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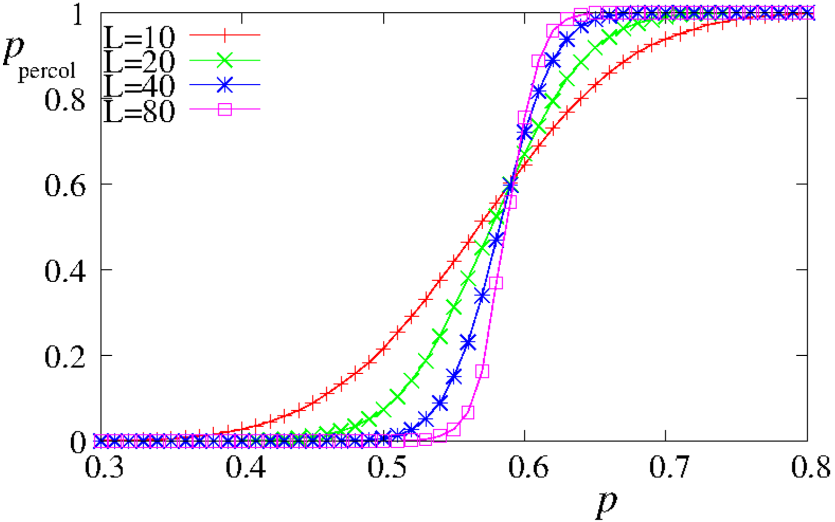
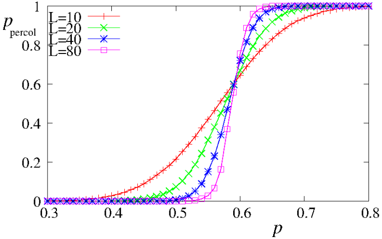
Result

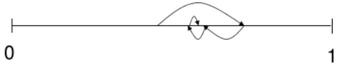


Determine p_c

- From order parameter:

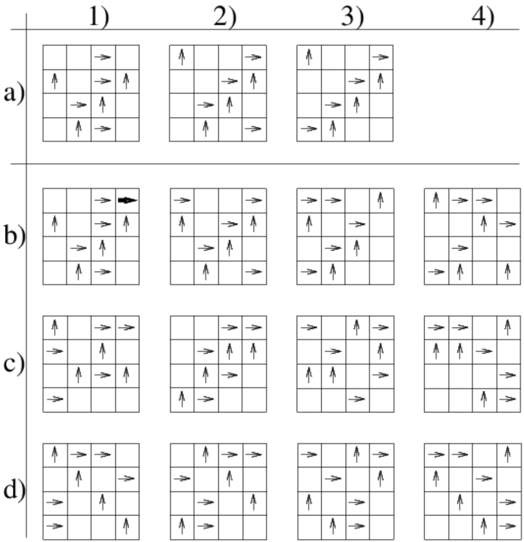


- Increase and decrease p by $p/2$ to converge to p_c
- Use the monotonity of the percolation
- Same random number sequence can be generated!



Monotonity

Not always true!



9. ábra: Az a/1 helyen található konfigurációból kiindulva blokkolt határciklushoz jutunk (a/3). A b/1 helyen az a/1 konfigurációhoz hozzávettük még a vastagon kihúzott nyilat, így a b/1-ben a sűrűség nagyobb lett, mint az a/1-ben. Innét indítva a modellt Szabadon mozgó fázishoz jut (d/4).

Ising-model

- Spins
  - Interact with extrenal field h_i
  - Interact with neighbors with coeff. J_{ij}
- The Hamiltonian:

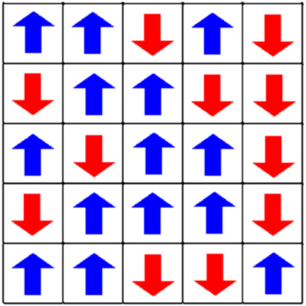
$$H(\sigma) = -\sum_{\langle i\ j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_i h_i\sigma_i$$

- Order parameter magnetization

$$M = \sum_i \sigma_i$$

2D Ising-model

- 2 dimensions
- Homogeneous interaction: $J_{ij} = J$
- No external field (for the time being) $h = 0$



Importance sampling

- Given a Hamiltonian $H(\mathbf{q}, \mathbf{p})$
- We ask for the time average of a dynamics quantity at temperature T

$$\bar{A} = \int A(\mathbf{q}, \mathbf{p}) P^{eq}(\mathbf{q}, \mathbf{p}, T) d\mathbf{q} d\mathbf{p}$$

- In the canonical ensemble

$$P^{eq}(\mathbf{q}, \mathbf{p}, T) = \frac{1}{Z} e^{-\beta H(\mathbf{q}, \mathbf{p})}$$

- If A depends only on the energy (often the case):

$$\bar{A} = \int A(E) \omega(E) P^{eq}(E, T) dE$$

Importance sampling is needed!

Importance sampling

- $\omega(E)P^{eq}(E,T)$ has a very sharp peak (for large N)
- System spends most of its time *in equilibrium*
- Importance sampling:

Generate configurations with the equilibrium probability

- if configurations are chosen accordingly, the for K measurements:

$$\bar{A} \simeq \frac{1}{K}\sum_{i=1}^{K} A_i$$

How togenerate equilibrium configurations?

Metropolis algorithm

(Metropoli-Rosenbluth-Rosenbluth-Teller-Teller=MR^{2}T^2 algorithm)

- Sequence of configurations using a Markov chain
- Configuration is generated from the previous one
- Transition probability: equilibrium probability
- Detailed balance:

$$P(x)P(x \to x') = P(x')P(x' \to x)$$

- Rewritten:

$$\frac{P(x \to x')}{P(x' \to x)} = \frac{P(x')}{P(x)} = e^{-\beta \Delta E}$$

- Only the ration of transition probabilities are fixed

Metropolis algorithm

(Metropoli-Rosenbluth-Rosenbluth-Teller-Teller=MR^2T^2 algorithm)

$$\frac{P(x \to x')}{P(x' \to x)} = \frac{P(x')}{P(x)} = e^{-\beta \Delta E}$$

- Metropolis:

$$P(x \to x') = \begin{cases} e^{-\beta \Delta E} & \text{if}\, \Delta E > 0 \\ 1 & \text{otherwise} \end{cases}$$

- Symmetric:

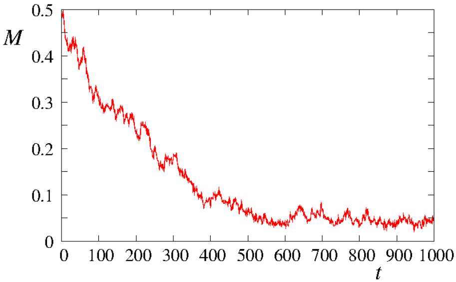
$$P(x \to x') = \frac{e^{-\beta \Delta E}}{1 + e^{-\beta \Delta E}}$$

Characteristic time

- Equilibrium: system is stationary.
- We can measure after relaxation time
- New measurement after correlation time

$$\phi_{EE}(t) = \frac{\langle E(t')E(t'+t)\rangle - \langle E\rangle^2}{\langle E^2\rangle - \langle E\rangle^2}, \quad \tau = \int_0^\infty \phi_{EE}(t)dt$$

- Sample with intervals $\Delta t > \tau$



Metropolis algorithm

Recipes:

- Choose an elementary step $x \to x'$
- Calculate ΔE
- Calculate $P(x \to x')$
- Generate random number $r \in [0, 1]$
- If $r < P(x \to x')$ then new state is x'; otherwise it remains x
- Increase time
- Measure what you want
- Restart

:-)

Metropolis algorithm, proposal probability

Transition probability:

$$P(x \to x') = g(x \to x')A(x \to x')$$

- $g(x \to x')$: proposal probability
  - Generally uniform
  - If different interactions are present then it must be incorporated
- $A(x \to x')$: acceptance probability
  - Metropolis
  - Symmetric

Metropolis, *proof*

State flow
Let $E > E'$:

- $x \to x'$

$$P(x)g(x \to x')A(x \to x') = P(x)$$

- $x' \to x$

$$P(x')g(x' \to x)A(x' \to x) = P(x')e^{-\beta \Delta E}$$

- In equilibrium they are equal:

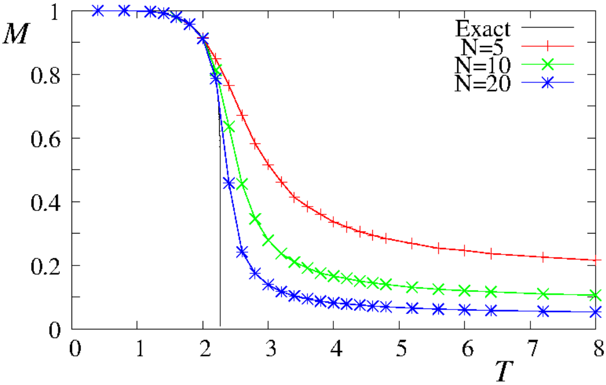
$$\frac{P(x)}{P(x')} = e^{\beta \Delta E}$$

- What we wanted.

Finite size effects

Magnetization 2d lattice Ising model

- Determine critical temperature
- Determine critical exponents
- System size dependence???



Finite size scaling

- Correlation length

$$\xi \propto |T - T_c|^{-\nu}$$

- Cannot be infinite!
- There will be a critical point for the finite system
- If L is finite ξ cannot be larger than L

$$L \propto |T(L) - T_c|^{-\nu}$$

- The position and the width of the transition

$$|T(L) - T_c| \propto L^{-1/\nu}$$

- 3 parameters to fit ν, $T(L)$, and a constant

Finite size scaling

- Binder Cumulant method (find something which does not scale with L)
- Find something which scales with ν
  - The standard deviation of the order parameter:

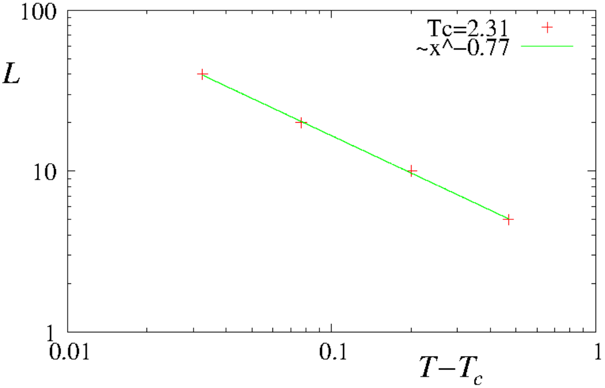
$$\sigma(L) \propto L^{-1/\nu}$$

  - Two steps, both with two parameter fits:

$$\sigma(L) \propto L^{-1/\nu}$$
$$|T(L) - T_c| \propto L^{-1/\nu}$$

Three parameter fit: Ising model

- Theory: $\nu = 1$, $T_c \simeq 2.27$



Finite size scaling: Ising model

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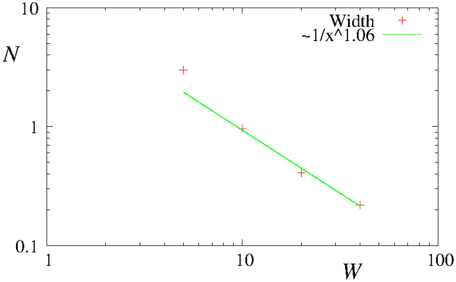
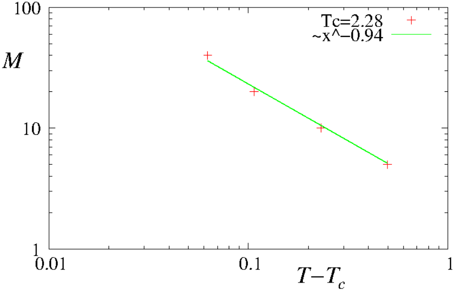




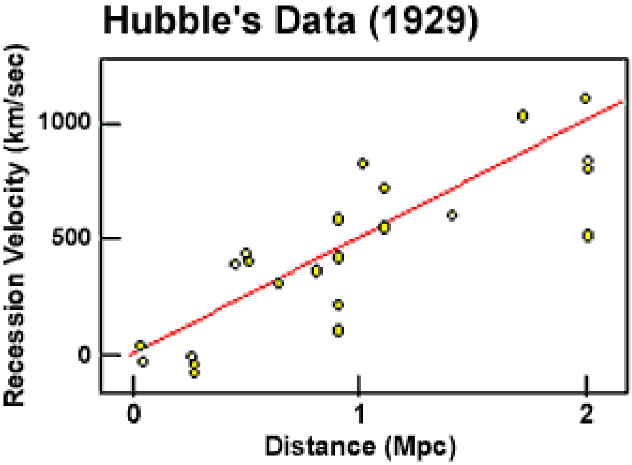
Fitting

Linear regression

$$
\begin{aligned}
y &= \alpha + \beta x \\
\hat{\beta} &= \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2} \\
\hat{\alpha} &= \bar{y} - \hat{\beta}\bar{x} \\
\rho &= \frac{\overline{xy}}{\sqrt{\bar{x}\bar{y}}} \qquad (1)
\end{aligned}
$$

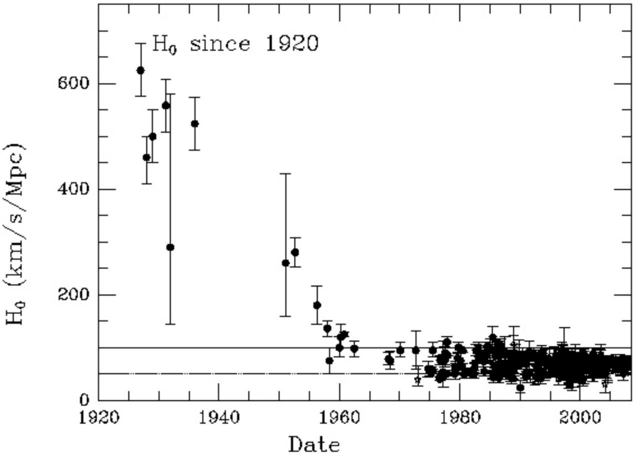
Fitting

Houbble original fit:



Fitting

Houbble change in time:



Fitting

Houbble change in time: