Multi-Grid-Monte-Carlo

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Monte Carlo Methods

2015

- Local Monte Carlo methods generate a new value $\phi_x^{'}$ at x of the lattice Λ assuming a fixed $\phi_{y \neq x}$

$$\mathcal{H}^{'}(\phi_x^{'}, \{\phi_y\}_{y \neq x}) \leftarrow \mathcal{H}(\phi_x, \{\phi_y\}_{y \neq x})$$

- We have encountered the Metropolis, Glauber and the Heat-Bath Monte Carlo Method as examples.
- In contrast to the global methods like the cluster algorithms they only introduce changes on a small length scale.
- If there is an inherent large length scale in the problem one encounters the problem of *critical slowing down*.

- A similar problem arises solving algebraic equations:

$$A\phi = f$$

- Let us try an iterative method

$$\phi^{(n+1)} = M\phi^{(n)} + g$$

- We want $A\phi = f$ to be a fix point of the iteration

$$\begin{aligned} \phi &= M\phi + g \\ \leftrightarrow A^{-1}f &= MA^{-1}f + g \\ \leftrightarrow g &= (I - M)A^{-1}f \end{aligned}$$

- Partition $A = N - P$, then with $M = N^{-1}P$

$$g = (1 - N^{-1}P)A^{-1}f = N^{-1}(N - P)A^{-1}f = N^{-1}f$$

- With this we find

$$\phi^{(n+1)} = M\phi^{(n)} + N^{-1}f$$

- the properties of the method are determined by the matrix M.
- Let us look at the standard decomposition

$$A = L + D + U$$

  (L =left lower, U = right upper triangular matrix, D = diagonal matrix).
- Choose $N + D + L$, $P = -U$, then

$$\phi^{(n+1)} = \underbrace{-(D+L)^{-1}U}_{=:M}\phi^{(n)} + (D+L)^{-1}f$$

- The above is know as the **Gauss-Seidel method**.
- component wise:

$$\phi_i^{(n+1)} = \frac{1}{Q_{ii}} \left(f_i - \sum_{j=1}^{i-1} a_{ij} \phi_j^{(n+1)} - \sum_{j=i+1}^{n} a_{ij} \phi_j^{(n)} \right)$$

- The Gauss-Seidel method is a **single step method**.
- This corresponds to a local update Monte Carlo method.
- To strengthen the point, let us look at

$$-\Delta\phi = f \qquad x \in \mathbf{R}^d \quad \text{on the lattice} \quad \Lambda \subset \mathbf{Z}^d$$

with Dirichlet boundary conditions $\phi_x \equiv 0 \; x \notin \Omega$

$$(-\Delta\phi)_x := 2d\phi_x - \sum_{x':|x-x'|=1} \phi_{x'} = f_x \Leftrightarrow A\phi = f \qquad |\Lambda| = n$$

- This is equivalent to

$$\begin{aligned} \text{min!} &= \mathcal{H}(\phi) := \frac{1}{2}\sum_{\langle xy \rangle}(\phi_x - \phi_y)^2 - \sum_x f_x \phi_x \qquad \phi_x \in \mathbf{R} \\ \Leftrightarrow &\quad \frac{1}{2}(\phi, A\phi) - (f, \phi) = \text{min!} \end{aligned}$$

- The matrix is block diagonal and positive devfinite

$$\phi A \phi \geq 0 \qquad \forall \phi \neq 0$$

and symmetric
- We claim that
  i. $\mathcal{H}(\phi)$ has an absolute minimum, i.e.,

$$\exists \phi_0 \in \mathbf{R}^n \quad \forall \phi \in \mathbf{R}^n : \quad \mathcal{H}(\phi_0) \leq \mathcal{H}(\phi)$$

  ii. ϕ_0 is the unique solution to $A\phi = f$

- Proof:
  Since A is positive definite $A\phi = f$ is the unique solution. Let ϕ_0 be the solution and $\phi = \psi - \phi_0 \in \mathbf{R}^n$. Then

$$
\begin{aligned}
\mathcal{H}(\psi) &= \mathcal{H}(\phi + \phi_0) \\
&= \frac{1}{2}(\phi + \phi_0, A(\phi + \phi_0)) - (f, \phi + \phi_0) \\
&= \frac{1}{2}(\phi, A(\phi + \phi_0)) + \frac{1}{2}(\phi_0, A(\phi + \phi_0)) - (f, \phi) - (f, \phi_0) \\
&= \frac{1}{2}(\phi, A\phi) + \frac{1}{2}(\phi, A\phi_0) + \frac{1}{2}(\phi, A\phi_0) + \frac{1}{2}(\phi_0, A\phi_0) - (f, \phi) - \\
&= \mathcal{H}(\phi_0) + \underbrace{\frac{1}{2}(\phi, A\phi)}_{\geq 0}
\end{aligned}
$$

  since A is symmetric, hence $(A\phi, \psi) = (\phi, A\psi)$.
- The solution of the Poisson equation is equivalent to the minimization of a Hamiltonian.

- Back to the properties of M! Consider the error

$$e^{(n)} := \phi^{(n)} - \phi \,.$$

- We have

$$\begin{aligned} e^{(n+1)} &= \phi^{(n+1)} - \phi = M\phi^{(n)} + N^{-1}f - A^{-1}f \\ &= M\left(e^{(n)} + \phi\right) + N^{-1}f - A^{-1}f \\ &= Me^{(n)} + \underbrace{M\phi + N^{-1}f - A^{-1}f}_{=0} \end{aligned}$$

- from which follows that $e^{(n)} = M^n e^{(0)}$
- Let $\rho(M) := \lim_{n\to\infty} ||M^n||^{1/n}$ be the spectral radius

$$\text{EW} < 1 \leftrightarrow \rho(M) < 1$$

- And further

$$||\Phi^{(n)} - \Phi|| \leq Kn^P \rho(M)^n$$

- **Problem:** How near is $\rho(M)$ to 1?
- Let us loo at a generalization of the Gauss-Seidel method

$$N = L + \frac{1}{\omega}D, \;\; P = \frac{1}{\omega}(1-\omega)D - U \qquad \omega \in (0,2)$$

- note that $\omega = 1$ is the Gauss-Seidel-method.

$$\Phi^{(n+1)} = (L + \frac{1}{\omega}D)^{-1}(\frac{1}{\omega}(1-\omega)D - U)\Phi^{(n)} + (L + \frac{1}{\omega}D)^{-1}f$$

- this method is know as the **damped Jacobi-method** or **SOR** (successive overrelaxation).

- One can show that

$$\omega_{\text{opti}} = \frac{2}{1+\sin\frac{\pi}{L+1}}, \lambda_{ij} = \frac{1}{2}\left(\cos\frac{i\pi}{L+1} + \cos j\pi L + 1\right)$$

$$\rho(M\omega_{\text{opti}}) = \frac{\cos^2\frac{\pi}{L+1}}{\left(1+\sin\frac{\pi}{L+1}\right)^2}$$

- if one restricts the integration to a square lattice $\mathbb{Z}^2$
- If one expands sin und cos to first order and traces L then

$$\rho(M\omega_{\text{opti}}) = \frac{\cos^2\frac{\pi}{L+1}}{\left(1+\sin\frac{\pi}{L+1}\right)^2} \sim O\left(\frac{\left(1-\frac{1}{L^2}\right)^2}{\left(1+\frac{1}{L^2}\right)^2}\right) \sim 1 - O\left(\frac{1}{L^2}\right)$$

- A critical slowing down arises as happens at the critical point

$$(-\Delta\phi)_x := 2d\phi_x - \sum_{x':|x-x'|=1} \phi_{x'} = f_x$$

  - Poisson equation, $\Omega \subset \mathbf{Z}^d, \quad x \notin \Omega : \quad \phi_x \equiv 0$
  - linear system of equations $A\phi = f$
  - $\phi^{(n+1)} = M\phi^{(n)} + Nf$

$$\phi_x^{(n+1)} = (1-\omega)\phi_x^{(n)} + \frac{\omega}{2d}\left[\sum_{x':|x-x'|=1} \phi_{x'} + f_x\right]$$

- In general: $A\phi = f$, A regular, $A : U \to V$, where $U, V \in \mathbf{VR}(n)$
  - Let $U_M := U$, U_{M-1}, ..., U_0
    and $V_M := V$, V_{M-1}, ..., V_0 two sequences of Spaces,
    where $\dim U_l = \dim V_l =: N_l$, $\forall 0 \leq l \leq M$,
    $n = N_M > N_{M-1} > \ldots > N_0$.
  - Let $r_{l-1,l}$: $V_l \to V_{l-1}$, $1 \leq l \leq M$ be restriction operators
  - Let $p_{l,l-1}$: $U_{l-1} \to U_l$, $1 \leq l \leq M$ be prolongation operators
  - Let $A_l : U_l \to V_l$, $0 \leq l \leq M-1$
  - Smothers $S_l : U_l \times V_l \to U_l$, $0 \leq l \leq M$,
    $S_l(\phi'_0, f_l) = \phi''_l$ approximate solution

procedure mym(l, ϕ, f)
$\phi \leftarrow S_l^{pre}(\phi, f)$
if $(l > 0)$ **then**
  $d \leftarrow -r_{l-1,l} \overbrace{(A_l\psi - f)}^{\text{Residual}}$
  $\phi \leftarrow 0$ starting value
  for $j = 1$ until γ_l **do**
    $\mathrm{mym}(l-1, \psi, d)$
  end for
  $\phi \rightarrow \phi + P_{l,l-1}\psi$
  $\phi \rightarrow S_l^{post}(\phi, f)$
end if
end procedure

γ_l number of iterations, $A_{l-1}\psi = d$

- Example
  - Trivial restriction $(r_{l-1,l}\phi_l)_x \equiv (\phi_l)_x, \; \forall x \in \Omega_{l-1} \subset \Omega_l$
  - Averaging
    $$(r_{l-1,l}\phi_l)_x = \frac{1}{4}\left[(\phi_l)_{x_1+1/2,x_2+1/2} + \ldots\right]$$
    or nine point averaging
    $$\begin{bmatrix} \frac{1}{16}\frac{1}{8}\frac{1}{16} \\ \frac{1}{8}\frac{1}{4}\frac{1}{8} \\ \frac{1}{16}\frac{1}{8}\frac{1}{16} \end{bmatrix}$$
  - piecewise constant insertion
    $$(p_{l,l-1}\phi_{l-1})_{x_1\pm 1/2,x_2\pm 1/2} = (\phi_l)_{x_1,x_2} \quad \forall x \in \Omega_{l-1}$$
  - piecewise linear insertion
    $$\begin{bmatrix} \frac{1}{4}\frac{1}{2}\frac{1}{4} \\ \frac{1}{2}1\frac{1}{2} \\ \frac{1}{4}\frac{1}{2}\frac{1}{4} \end{bmatrix}$$
  - $A_{l-1} = r_{l-1,l}A_l p_{l,l-1}$ Galerkin definition
  - i.a. $\gamma_l = \gamma \geq 1 \quad \forall 1 \leq l \leq M$

- Non-linear case
  $U \in V\mathbb{R}(n)$, $\mathcal{H} : U \to \mathbb{R}$ Hamilton function.
  Assume, $\exists!\ \mathbf{x} \in U :\ \mathcal{H} = \min$
  $U_M := U, U_{M-1}, \ldots, U_0$
  $\dim\ U_l =: N_l$
  $N = N_M > N_{M-1} > \ldots > N_0$
  Prolongation operators $P_{l,l-1} : U_{l-1} \to U_l$
  Smothers $S_l : U_l \times \mathcal{H}_l \to U_l \qquad 0 \leq l \leq M$
  Cycle control parameter $\gamma_l \geq 1, \qquad 1 \leq l \leq M$

procedure ulmym(l, ϕ, H_l)
$\phi \rightarrow S^{pre}(\phi, H_l)$
if $l > 0$ **then**
    `Compute` $H_{l-1}(.) := H_l(\phi + p_{l,l-1}.)$
    $\psi \rightarrow 0$
    `for j=1 until` γ_l `do ulmym`$(l-1, \psi, H_{l-1})$
    $\phi \rightarrow \phi + p_{l,l-1}\psi$
end if
$\phi \rightarrow S_l^{post}(\phi, H_l)$
end procedure

"Compute H_{l-1}":

$$H_l(\phi) = \frac{\alpha}{2} \sum_{|x-x'|=1} (\phi_x - \phi_{x'})^2 + \sum_x V_x(\phi_x)$$

$$V_x(\phi_x) = \lambda \phi_x^4 + u_x \phi_x^3 + A_x \phi_x^2 + h_x \phi_x$$

Assume: $p_{l,l-1}$ piecewise constant, need to compute

$$H_{l-1}(\psi) := H_l(\phi + p_{l,l-1}\psi)$$

$$
\begin{aligned}
\rightarrow \quad H_{l-1}(\psi) &= \frac{\alpha'}{2} \sum_{|y-y'|=1} (\psi_y - \psi_{y'})^2 + \sum_y V'_y(\psi_y) + \text{const} \\
V'_y(\psi_y) &= \lambda' \psi_y^4 + k'_y \psi_y^3 + A'_y \psi_y^2 + h'_y \psi_y \\
\alpha' &:= 2^{d-1}\alpha \\
\lambda' &:= 2^d \lambda \\
k'_y &:= \sum_{x \in B_y} (4\lambda\phi_x + K_x) \qquad |B_y| = 2^d \\
A'_y &:= \sum_{x \in B_y} (6\lambda\phi_x^2 + 3k_x\phi_x + A_x) \\
h'_y &:= \sum_{x \in B_y} (4\lambda\phi_x^3 + 3k_x\phi_x^2 + 2A_x\phi_x + h_x)
\end{aligned}
$$

Construct $\mathcal{H}_l$ such that

$$H_l \in \mathcal{H}_l \text{ und } \phi \in U_l \rightarrow H_{l-1} \in \mathcal{H}_{l-1}$$

Let U_α, $U = \bigcup_\alpha U_\alpha$, $\alpha, \beta \in O$, $\alpha \neq \beta$ $U_\alpha \cap U_\beta = \emptyset$

$$d\mu(\phi) = \int d\nu(\phi|\alpha) d\rho(\alpha)$$

$\rho(.)$ probability measure of $\mathcal{I}$
$d\nu(.|\alpha)$ probability measure of U_α, conditioned probability distribution of $d\mu(\phi)$ at fixed ϕ in U_α
Let $P(\phi \to \phi^{'})$ be a transition probability

$$\int d\nu(\phi|\alpha) P(\phi \to \phi^{'}) = d\nu(\phi^{'}|\alpha)$$

$$\Rightarrow \int d\mu(\phi) P(\phi \to \phi^{'}) = d\mu(\phi^{'})$$

Multi-Grid Monte Carlo is a special form of the partial resampling.

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