Introduction of emulator

The advantabge of eigenvector countinuation

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2023 年 9 月 19 日

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Simulator and Emulator

Simulator and Emulator

Simulator: a simulator is used to create a detailed model of a specific system or process. This model can be used to predict the behaviour or response of the system.

Emulator: an emulator is typically used to approximate or replicate the behaviour of a complex system, but without needing to simulate all the details. It is a fast surrogate model capable of reliably approximating high-fidelity models. And it can be regarded as a kind of supervise learning.

The advantabge of emulator: Emulator can be used to predict the behaviour of a system or process much faster than a simulator. This is because the emulator is a simplified model of the system, and so it is much faster to run. However, the high speed does not demand the loss of accuracy. That means emulator can be trained to be as accurate as the simulator.

An example

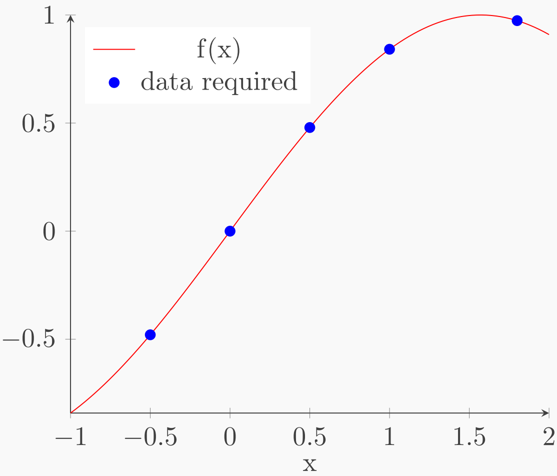


图: Simulator

If we use simulators to specify the curve we need, we may need lots of data points to get a smooth curve.

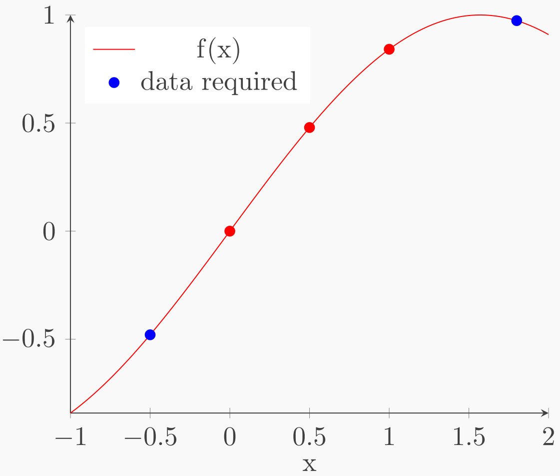


图: Emulator

If we use simulators to specify the curve we need, we may need lots of data points to get a smooth curve.

But If we use emulator, we may need only a few data points (Blue Points) to get a smooth curve. And we can get the red points after some calculation from the blue points which take quite a short time.

Eigenvector continuation

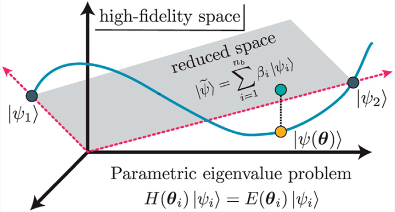
EC(Eigenvalue continuation)

Eigenvalue continuation is a kind of emulator and it is a numerical method for computing the eigenvalues of a matrix depending on a parameter.

$$\mathrm{H}\left(\boldsymbol{\theta}_{\mathrm{i}}\right)\left|\psi_{\mathrm{i}}\right\rangle = \mathrm{E}\left(\boldsymbol{\theta}_{\mathrm{i}}\right)\left|\psi_{\mathrm{i}}\right\rangle \tag{1}$$

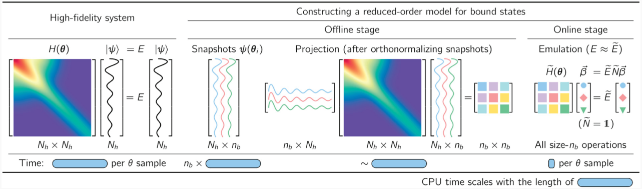
instead of calculating all the eigenvalues and eigenvectors of $\mathrm{H}\left(\boldsymbol{\theta}_{\mathrm{i}}\right)$, we randomly choose several $\{\boldsymbol{\theta}_{\mathrm{i}}\}_{1\leq \mathrm{i}\leq \mathrm{n_b}}$ and we precisely calculate $\{|\psi_{\mathrm{i}}\rangle\}_{1\leq \mathrm{i}\leq \mathrm{n_b}}$ which corresponds to the BLUE POINT. The we use a linear combinition of $\{|\psi_{\mathrm{i}}\rangle\}_{1\leq \mathrm{i}\leq \mathrm{n_b}}$ to get the remaining $|\psi\rangle$ which corresponds to the RED POINT

Accuracy of EC



This picture can explain why EC can produce the correct answer with quite astonishing accuracy. The reason lies in continuation which means: when $\boldsymbol{\theta}_{\mathrm{i}}$ goes from $\boldsymbol{\theta}_{\mathrm{initial}}$ to $\boldsymbol{\theta}_{\mathrm{final}}$, the eigenvector transfer countiously from $|\psi_1\rangle$ to $|\psi_2\rangle$, thus the trajectory must pass through the plane spanned by $|\psi_1\rangle$ and $|\psi_2\rangle$. This means, to some extent, the real eigenvector must stay quite close to this plane, so the projection of the real eigenvector on this plane, which is the linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ is quite a good approximation.

Effiency of EC



This is picture can explain why EC can solve the problem efficiently. We know it takes a long time to solve the eigenvalue problem with H a $\mathrm{N_b} \times \mathrm{N_b}$ mateix, and it takes even a much longer time to solve the eigenvalue problem for each $\boldsymbol{\theta}$. But if we take several snapshots (for example $\mathrm{n_b}$ snapshots with $\mathrm{n_b} << \mathrm{N_b}$), and project H to these snapshots, we can transfer $\mathrm{N_b} \times \mathrm{N_b}$ H to $\mathrm{n_b} \times \mathrm{n_b}$ $\tilde{\mathrm{H}}$. Since $\mathrm{n_b} << \mathrm{N_b}$, it takes much less time to solve the eigenvalue problem for $\tilde{\mathrm{H}}$ with each $\boldsymbol{\theta}$.

Thanks!