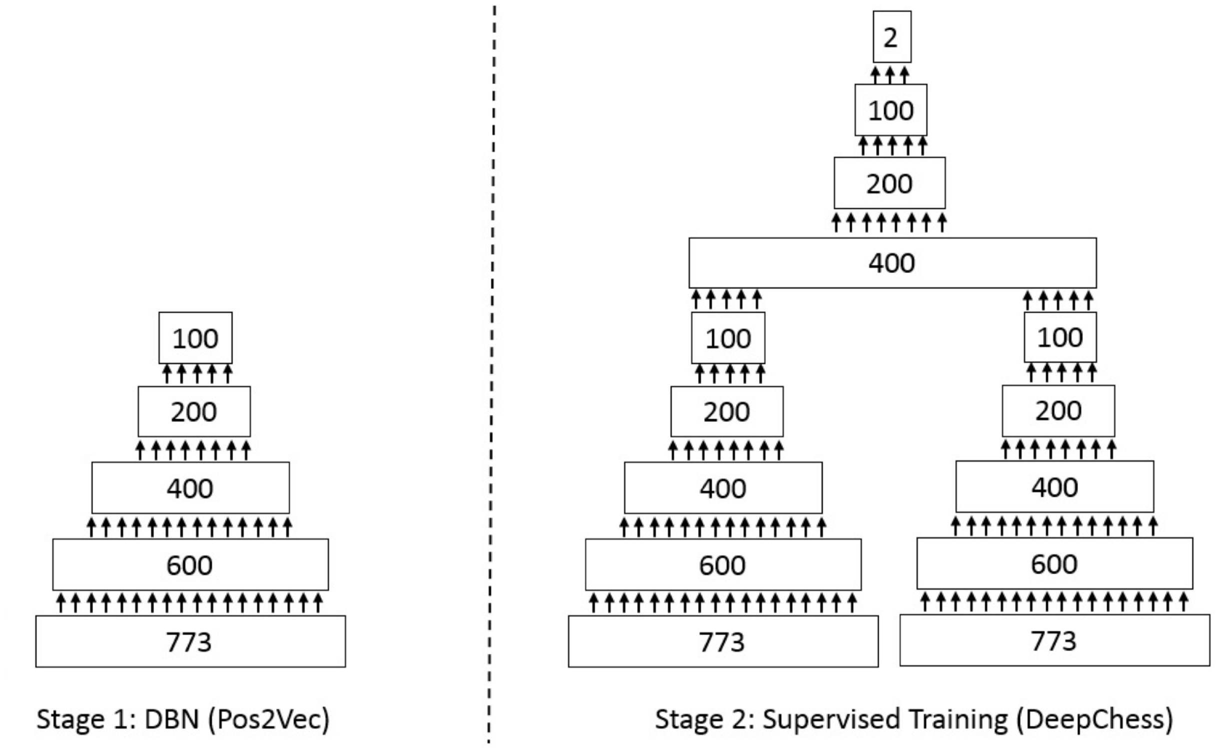
Methodlogy

1. Autoencoder + Siamese Network

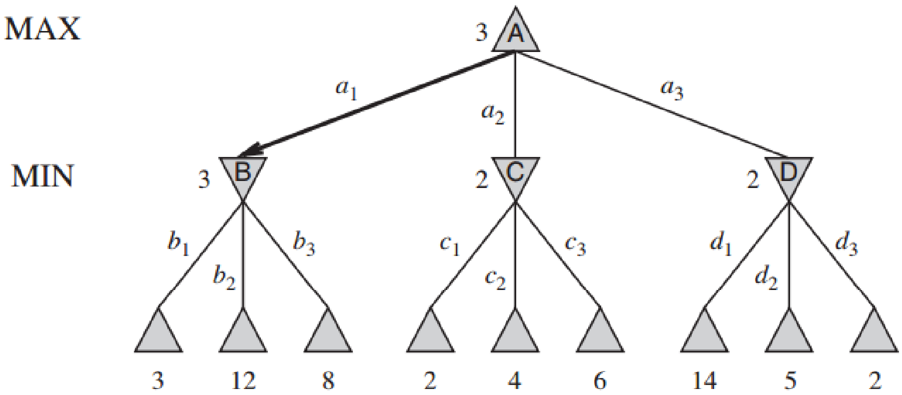


DeepChess Score Estimator

- Autoencoder: This embedding the state board into a lower-dimensional space.
  - Encoder: maps the input to a lower-dimensional latent space
  - Decoder: maps the latent space back to the original input space
- Siamese Network: This learned to compare two input mapping it to end score
  - The network takes two inputs: the current state and the next state
  - The network outputs a score

Minimax Search

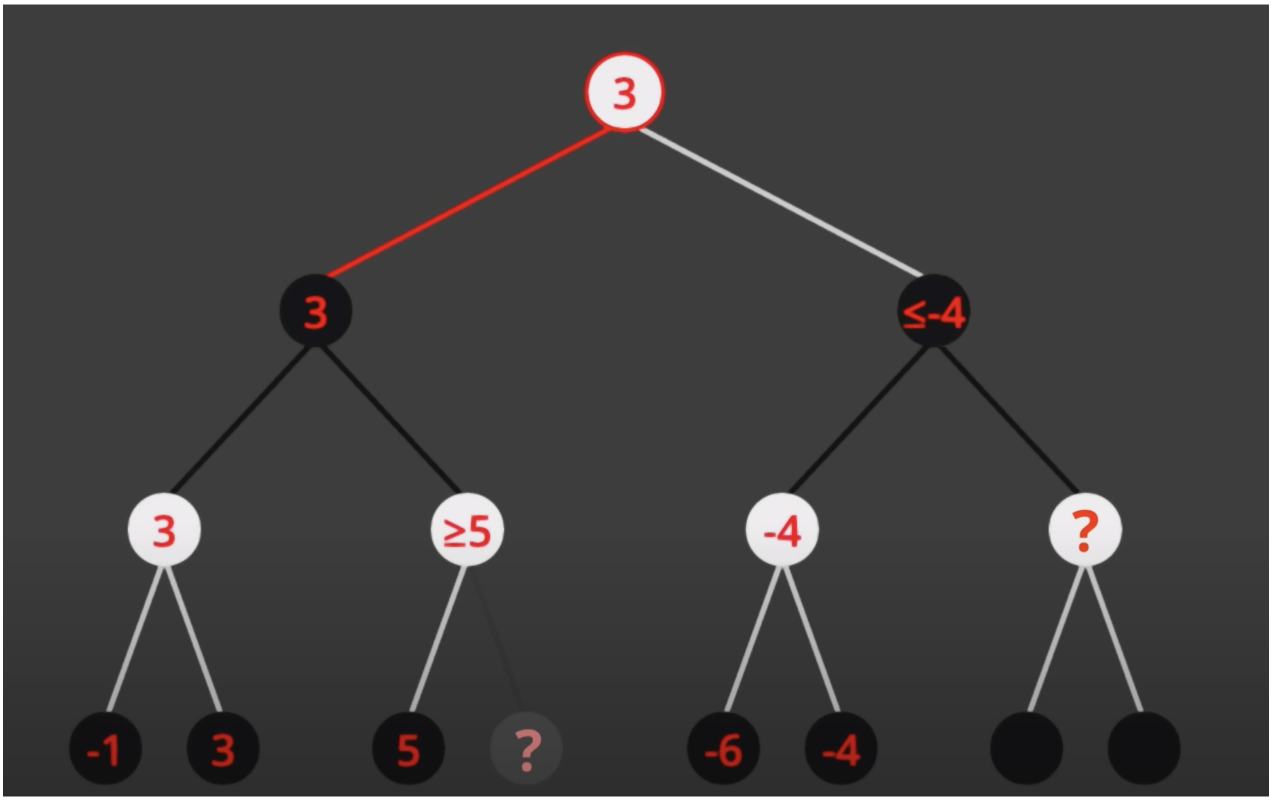
- Minimax Search: This is a search algorithm that is used to find the best move in a game.
  - The algorithm works by recursively exploring the game tree and evaluating the possible moves at each level.
  - The algorithm assumes that both players play optimally, and it tries to minimize the maximum loss for the player.
- We use the score which be outputted from the DeepChess Score Estimator as the evaluation function for the Minimax Search.




```
function minimax(position, depth, maximizingPlayer)
    if depth == 0 or game over in position
        return static evaluation of position

    if maximizingPlayer
        maxEval = -infinity
        for each child of position
            eval = minimax(child, depth - 1, false)
            maxEval = max(maxEval, eval)
        return maxEval

    else
        minEval = +infinity
        for each child of position
            eval = minimax(child, depth - 1, true)
            minEval = min(minEval, eval)
        return minEval

// initial call
minimax(currentPosition, 3, true)
```

Minimax Search with Alpha-Beta Pruning

- Speed up the Minimax Search by eliminating branches that do not need to be explored.




```
function minimax(position, depth, alpha, beta, maximizingPlayer)
    if depth == 0 or game over in position
        return static evaluation of position

    if maximizingPlayer
        maxEval = −infinity
        for each child of position
            eval = minimax(child, depth − 1, alpha, beta, false)
            maxEval = max(maxEval, eval)
            alpha = max(alpha, eval)
            if beta <= alpha
                break    // beta cutoff
        return maxEval

    else
        minEval = +infinity
        for each child of position
            eval = minimax(child, depth − 1, alpha, beta, true)
            minEval = min(minEval, eval)
            beta = min(beta, eval)
            if beta <= alpha
                break    // alpha cutoff
        return minEval
```

2. Heuristic Search

Component	Description	Purpose
1. Material Score	Fixed value per piece (e.g., pawn = 100, knight = 320)	Measure of piece count advantage
2. Piece-Square Table (PST)	Bonus/penalty per piece depending on its square location	Encourage good piece positioning
3. Game Phase Score	Interpolation factor (0 to 1) based on remaining material	Adjust importance of features between opening and endgame
4. Pawn Structure Score	Includes:	
- Isolated Pawn Penalty	- Penalty if no adjacent same-color pawns	Penalize weak, undefended pawns
- Passed Pawn Bonus	- Bonus for pawns with no enemy pawn in front or adjacent	Encourage promotion potential
5. Bishop Pair Bonus	Bonus if player owns both bishops	Recognize strength in open positions
6. Rook on Open File	Bonus if rook is on a file with no pawns	Encourage control of open files
7. Mobility Score	Difference in number of legal moves between players	Favor active positions, punish cramped setups
8. Interpolation Score	Weighted average of opening/endgame scores using game phase factor	Make the evaluation responsive to game stage

$\Longrightarrow$ Also use Minimax Search with Alpha-Beta Pruning to choose the best move for board state.

3. Deep Q-Learning

Core Components

a) ChessQNetwork

- **What**: A convolutional neural network (CNN) with 3 convolutional blocks and a dense head.
- **Key Features**:
    - **Input**: 903 features (8x8 board encoding + game state metadata + action features).
    - **Architecture**:
        - `Conv2d(14,128) → BatchNorm → ReLU` (×3 conv layers)
        - `Linear(512*8*8+9 → 1024 → 1)` (dense layers)
    - **Purpose**: Predicts Q-values for (board state, move) pairs.

b) PrioritizedReplayBuffer

- **What**: Experience replay with priority sampling.
- **Key Mechanics**:
    - **Priority**: Samples transitions with TD-error-based importance.
    - **Annealing**: Uses `alpha=0.6` (priority exponent), `beta=0.4` (importance sampling).
    - **Stability**: Clips priorities to avoid extremes (`np.clip(priorities, 1e-5, None)`).

c) Board Encoding

- **What**: Converts chess boards to 903D vectors.
- **Structure**:
    - **Piece channels**: 14-layer 8x8 tensor (6 piece types × 2 colors + 2 empty).
    - **Metadata**: Castling rights, turn, check, move count.

d) Reward Function

- **Components**:
    - Material gain/loss
    - Center control
    - King safety
    - Mobility penalty
    - Repetition penalty
- **Design Choice**: Combines handcrafted heuristics with learned values.

Training Pipeline

a) Self-Play Generation

- **Process**:
    i. Uses ε-greedy exploration (`EPSILON_START=1.0 → EPSILON_END=0.1`).
    ii. Augments data with board rotations/flips.
    iii. Applies final reward based on game outcome.

b) Network Update

- **Key Steps**:
    i. Samples prioritized transitions from buffer.
    ii. Computes Q-values using **online network**.
    iii. Computes target Q-values using **target network** (synced every `SYNC_INTERVAL=200`).
    iv. Updates priorities based on TD errors.

c) Loss & Optimization

- **Loss**: Prioritized MSE loss (`(weights * (Q - target_Q)^2`).
- **Optimizer**: AdamW with learning rate `LR=1e-5`, gradient clipping (`clip_grad_norm=1.0`).

Hyperparameters

Parameter	Value	Purpose
`BATCH_SIZE`	512	Batch size for training
`BUFFER_SIZE`	100,000	Experience replay capacity
`GAMMA`	0.999	Discount factor for future rewards
`SYNC_INTERVAL`	200	Target network sync frequency
`EPSILON_DECAY`	0.99999	Exploration rate decay (per episode)

Key Interactions

a) QNet ⇔ Environment

- **Flow**: `Board → encode_board() → QNet → Q-values → ε-greedy action → New state`

b) Experience Replay ⇔ Training

- **Loop**:
  i. Self-play games → Buffer (with priorities).
  ii. Sample batch → Compute loss → Update QNet.
  iii. Adjust priorities → Repeat.

c) Target Network Stabilization

- **Why**: Avoids "chasing moving targets" in Q-value estimation.
- **How**: Delayed sync (`SYNC_INTERVAL`) of target network weights.

Evaluation Challenge

Stockfish Integration Issue

- **Symptoms**: Fails to load Stockfish engine (path/library issues).
- **Impact**: Cannot benchmark AI against a strong baseline.
- **Workaround**:
  - Temporarily uses self-play win rates (`evaluate_model()` fallback).
  - Requires fixing engine path/OS compatibility for proper evaluation.

Architecture Diagram

```
[Self-Play]
   │
   ▼
[Prioritized Buffer] → Sampled Batch → [QNet] ←→ [Target Net]
   ▲                        │                │
   └──Priority Update───────┘                │
                                      [Optimizer (AdamW)]
```

Notable Design Choices

1. **Action Encoding**: Normalizes move squares (`from_square/63` , `to_square/63`).
2. **Board Augmentation**: Random rotations/flips for data diversity.
3. **Delayed Rewards**: Adds game outcome reward to all transitions in an episode.

4. Discrete Diffusion Model + ASA

Problem Settings

- We describe Chess game as a Markov Process (Which is a type of Markov Decision Process - Given the current state, the next state is independent of the previous states)
  - State Space (S): The state of the board
  - Action Space (A): The set of all possible moves
  - State transition function ($f(s, a)$): The function that takes a state and an action and returns the next state
  - Action Probability Distribution ($p(a|s)$): The probability of taking action a in state s
  - $o_i = 1 || -1$: terminal reward at time i (win/loss)
  - Value function ($v^p(s)$): The expected return when both player play with the same strategy p

$$v^p(s) = \mathrm{E}\left[o_i | s_i = s, a_{i...I} \sim p\right]$$

$\implies$ Our target is maximize the value function $v^p(s)$ for my engine. Then to do that we need to find the best action a^* in state s.
In other words, we need to find the best policy π^* that maximizes the value function $v^p(s)$. $\implies$ Learning the best probability distribution $\pi^*(a|s)$ for each state s.

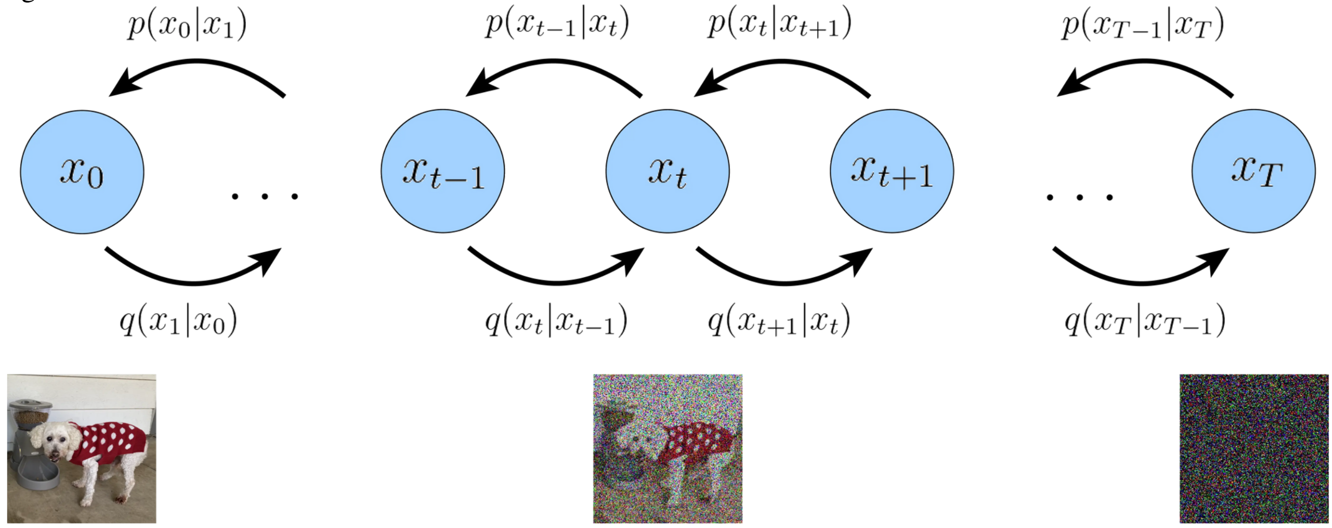
Discrete Diffusion Model

- Diffusion Models are a class of generative model which consist 2 processes: forward and reverse processes. Both processes are Markov chains.
  - The forward process is a Markov chain that gradually adds noise to the data,
  - The reverse process is a Markov chain that gradually removes noise from the data.
- Suppose we want to learn a target sample $x_0 \sim q(x_0)$, x_0 is a discrete random variable with K possible values. Defining the forward and backward processes as follows:
  - **Forward process**: gradually adds noise to the data

$$q(x_{1:T} | x_0) = \prod_{t=1}^{T} q(x_t | x_{t-1})$$

  - **Reverse process**: gradually removes noise from the data

$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} | x_t)$$



- We propose the target function for conditioning the forward process on the action a:

$$K(q_\psi(\cdot|x), p_\theta(\cdot, x)) = \int_{-\infty}^{\infty} q_\psi(z|x)\log(\frac{q_\psi(z|x)}{p_\theta(z|x)})$$

$$\mathrm{L} = \mathrm{E}_{q_\psi(\cdot|x)}[\log(\frac{p_\theta(x,Z)}{q_\psi(Z|x)})]$$

$$\begin{aligned} \log p_\theta(x) &= \int_{-\infty}^{\infty} q(\cdot|x)\log(p_\theta(x))dz \\ \Longrightarrow \quad &= \int_{-\infty}^{\infty} q_\psi(\cdot|x)\log(\frac{p_\theta(x,Z)}{q_\psi(z|x)})dz + \int_{-\infty}^{\infty} q_\psi(z|x)\log(\frac{q_\psi(z|x)}{p_\theta(z|x)})dz \\ &= \mathrm{L} + K(q_\psi(\cdot|x), p_\theta(\cdot, x)) \\ &\geq \mathrm{L} \\ \Longrightarrow \quad & \mathrm{L} \geq -\log p_\theta(x) \end{aligned}$$

$\Longrightarrow$ We call L as ELBO (Evidence Lower Bound)
When $q(\cdot|x)$ close $p_\theta(\cdot|x)$, then ELBO simiar to \log p_\theta(x) $\Longrightarrow$ L is an upper bound on the negative log-likelihood
$\Longrightarrow$ Minimizing this upper bound L brings us closer to minimizing the true negative log-likelihood.
$\Longrightarrow$ We got the general type of loss function

$$\mathrm{L}_{vb} = -\log p_\theta(x) + K(q_\psi(\cdot|x), p_\theta(\cdot, x))$$

$\Longrightarrow$ We can use above loss for muiltiple steps:

$$\mathrm{L} = \mathrm{E}_{q(x_0)}[\underbrace{D_{\mathrm{KL}}[q(x_T|x_0) \| p(x_T)]}_{L_T} + \underbrace{\sum_{t=2}^{T} \mathrm{E}_{q(x_t|x_0)}[D_{\mathrm{KL}}[q(x_{t-1}|x_t, x_0) \| p_\theta(x_{t-1}|x_t)]]}_{L_{t-1}} - \underbrace{\mathrm{E}_{q(x_1|x_0)}[\log p_\theta(x_0|x_1)]}_{L_0}]$$

- We could simplified the above loss function by using the following equation:

$$K(q(x_{t-1}|x_t, x_0) \| p_\theta(x_{t-1}|x_t)) = -\lambda_t 1_{x_t = x_o} x_0^T \log f(x_t, \theta)$$

$$\Longrightarrow L_{vb} = -\mathrm{E}_{q(x_0)}[\sum_{t=1}^{T} \lambda_t \mathrm{E}_{q(x_t|x_0)} 1_{x_t = x_o} x_0^T \log f(x_t, \theta)]$$

- $\lambda_t = \frac{\alpha_{t-1} - \alpha_t}{1 - \alpha_t}$: time-dependent reweighting term that assigns lower weight for noisier x_t
- $\alpha_t \in [0, 1]$: predefined noise scheduler

ASA - Action/State/Action

- Our probability distribution is a function of the state and action.

$$p_\theta(a_i, s_{i+1}, a_{i+1}, ..., s_{i+h-1} . a_{i+h-1} | s_i)$$

Training

- Data: use the output of the stockfish engine as the training data.

$$\mathrm{D} = \{(s_i, (a_i^{SF}, s_{i+1}, ..., a_{i+h-1}^{SF}))\}$$

Inference

$$\arg\max p_\theta(a_i, s_{i+1}, a_{i+1}, ..., s_{i+h-1}, a_{i+h-1} | s_i)$$

Algorithm 1 DiffuSearch Training

Input: dataset $\mathcal{D} = \{(s, (a, z))\}$, neural network $f(\cdot; \boldsymbol{\theta})$, timesteps T.
Output: model parameters $\boldsymbol{\theta}$.
Denote state length $l = |s|$;
repeat
  Draw $(s, (a, z)) \sim \mathcal{D}$ and obtain $\mathbf{x}_{0,1:N} = s \,||\, a \,||\, z$ ($||$: concat);
  Draw $t \in \mathrm{Uniform}(\{1, \ldots, T\})$;
  Draw $\mathbf{x}_{t,n} \sim q(\mathbf{x}_{t,n} | \mathbf{x}_{0,n})$ for $n \in \{l+1, \ldots, N\}$;
  $L(\boldsymbol{\theta}) = -\lambda_t \sum_{n=l+1}^{N} 1_{\mathbf{x}_{t,n} \neq \mathbf{x}_{0,n}} \mathbf{x}_{0,n}^{\top} \log f(\mathbf{x}_{t,n}; \boldsymbol{\theta})$;
  Minimize $L(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$;
until converged

Algorithm 2 DiffuSearch Inference

Input: board state s, trained network $f(\cdot; \boldsymbol{\theta})$, timesteps T.
Output: next action a.
Denote state length $l = |s|$;
Initialize $\mathbf{x}_{T,1:l} = s$ and $\mathbf{x}_{T,l+1:N} \sim q_{\text{noise}}$;
for $t = T, \ldots, 1$ **do**
  for $n = l+1, \ldots, N$ **do**
    Draw $\widetilde{\mathbf{x}}_{0,n} \sim \mathrm{Cat}\left(f(\mathbf{x}_{t,n}; \boldsymbol{\theta})\right)$;
    Draw $\mathbf{x}_{t-1,n} \sim q(\mathbf{x}_{t-1,n} \mid \mathbf{x}_{t,n}, \widetilde{\mathbf{x}}_{0,n})$;
  end for
end for
Return $a = \mathbf{x}_{0,l+1}$.