

Part I: Chapters 0–3

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1 Chapter 0 — Motivation: A First RL Experiment

Vlad Prytula

1.1 0.0 Who Should Read This?

This chapter is an optional warm-up: it is deliberately light on mathematics and heavy on code. We build a tiny search world, train a small agent to learn context-adaptive boost weights, and observe the core RL loop in action. Chapters 1–3 provide the rigorous foundations that explain *why* the experiment works and *when* it fails.

Two reading paths work well:

- Practitioner track: begin here; the goal is a working end-to-end system in ~30 minutes, then return to theory as needed.
- Foundations track: skim this chapter for the concrete thread, then begin Chapter 1’s rigorous development; we return here whenever an example is useful.

Ethos: every theorem in this book compiles. Mathematics and code are in constant dialogue.

1.2 0.1 The Friday Deadline

We consider the following scenario. We have just joined the search team at zooplus, Europe’s leading pet supplies retailer. Our first task seems straightforward: improve the ranking for “cat food” searches.

The current system uses Elasticsearch’s BM25 relevance plus some manual boost multipliers—a `category_match` bonus, a `discount_boost` for promotions, a `margin_boost` for profitable products. Our manager hands us last week’s A/B test results and says:

“Revenue is flat, but profit dropped 8%. Can we fix the boosts by Friday?”

We dig into the data. The test increased `discount_boost` from 1.5 to 2.5, hoping to drive sales. It worked—clicks went up 12%. But the wrong people clicked. Price-sensitive shoppers loved the discounted bulk bags. Premium customers, who usually buy veterinary-grade specialty foods, saw cheap products ranked first and bounced. Click-through rate (CTR) rose, but conversion rate (CVR) plummeted for high-value segments.

The problem is clear: one set of boost weights cannot serve all users. Price hunters need `discount_boost = 2.5`. Premium shoppers need `discount_boost = 0.3`. Bulk buyers fall somewhere in between.

We need **context-adaptive weights** that adjust to user type. But testing all combinations manually would take months of A/B experiments.

This is where reinforcement learning enters the story.

1.3 0.2 The Core Insight: Boosts as Actions

We reframe the problem in RL language. If any terminology is unfamiliar, we treat it as a working placeholder: Chapters 1–3 make each object precise and state the assumptions under which it is well-defined.

Context (what we observe): User segment, query type, session history **Action** (what we choose): Boost weight template $\mathbf{w} = [w_{\text{discount}}, w_{\text{quality}}, w_{\text{margin}}, \dots]$ **Outcome** (what happens): User clicks, purchases, abandons **Reward** (what we optimize): GMV + profitability + engagement (we'll make this precise in a moment)

Traditional search tuning treats boosts as **fixed parameters** to optimize offline. RL treats them as **actions to learn online**, adapting to each context.

The Friday deadline problem becomes: *Can an algorithm learn which boost template to use for each user type, using only observed outcomes (clicks, purchases, revenue)?*

The answer is yes; we now build it.

1.4 0.3 A Tiny World: Toy Simulator and Reward

We start with a high-signal toy environment. Three user types, ten products, a small action space. The goal is intuition and a quick end-to-end run. Chapter 4 builds the realistic simulator (`zoosim`).

1.4.1 0.3.1 User Types

Real search systems have complex user segmentation (behavioral embeddings from clickstreams, transformer-based intent models, predicted LTV, real-time session signals). Our toy has three archetypes:

```
from typing import NamedTuple

class UserType(NamedTuple):
    """User preferences over product attributes.

    Fields:
        discount: Sensitivity to discounts (0 = indifferent, 1 = only buys discounts)
        quality: Sensitivity to brand quality (0 = indifferent, 1 = only buys premium)
    """
    discount: float
    quality: float

USER_TYPES = {
    "price_hunter": UserType(discount=0.9, quality=0.1),  # Budget-conscious
    "premium":      UserType(discount=0.1, quality=0.9),  # Quality-focused
    "bulk_buyer":   UserType(discount=0.5, quality=0.5),  # Balanced
}
```

These map to real patterns: - **Price hunters**: ALDI shoppers, coupon clippers, bulk buyers - **Premium**: Brand-loyal, willing to pay for specialty/veterinary products - **Bulk buyers**: Multi-pet households, mix of price and quality

1.4.2 0.3.2 Products (Sketch)

Ten products with simple features:

```
from dataclasses import dataclass

@dataclass
class Product:
    id: int
    base_relevance: float # BM25-like score for query "cat food"
    margin: float          # Profit margin (0.1 = 10%)
    quality: float         # Brand quality score (0-1)
    discount: float        # Discount flag (0 or 1)
    price: float           # EUR per item
```

Example: Product 3 is a premium veterinary diet (high quality, high margin, no discount, high price). Product 7 is a bulk discount bag (low quality, low margin, discounted, low price per kg).

We'll use deterministic generation with a fixed seed so results are reproducible.

1.4.3 0.3.3 Actions: Boost Weight Templates

The full action space is continuous: $\mathbf{a} = [w_{\text{discount}}, w_{\text{quality}}, w_{\text{margin}}] \in [-2, 2]^3$.

For this chapter, we **discretize** to a 5×5 grid (25 templates) to keep learning tabular and fast:

```
import numpy as np

# Discretize [-1, 1] x [-1, 1] into a 5x5 grid
discount_values = np.linspace(-1, 1, 5) # [-1.0, -0.5, 0.0, 0.5, 1.0]
quality_values = np.linspace(-1, 1, 5)

ACTIONS = [
    (w_disc, w_qual)
    for w_disc in discount_values
    for w_qual in quality_values
] # 25 total actions
```

Each action is a **template**: a pair $(w_{\text{discount}}, w_{\text{quality}})$ that modifies the base relevance scores.

Why do we discretize? Tabular Q-learning needs a finite action space. Chapter 7 handles continuous actions via regression and optimization. Here we use the simplest algorithm that works end-to-end.

1.4.4 0.3.4 Toy Reward Function

Real search systems balance multiple objectives (see Chapter 1, (1.2) for the full formulation). Our toy uses a simplified scalar:

$$R_{\text{toy}} = 0.6 \cdot \text{GMV} + 0.3 \cdot \text{CM2} + 0.1 \cdot \text{CLICKS}$$

Components:

- **GMV** (Gross Merchandise Value): Total EUR purchased (simulated based on user preferences + product attributes + boost-induced ranking)
- **CM2** (Contribution Margin 2): Profitability after variable costs
- **CLICKS**: Engagement signal (prevents pure GMV exploitation; see Chapter 1, Section 1.2.1 for why this matters)

Notes:

- No explicit STRAT (strategic exposure) term in the toy
- Chapter 1 presents the general, numbered formulation that this toy instantiates
- The weights (0.6, 0.3, 0.1) are business parameters, not learned

Pedagogical Simplification

The full R_{toy} formula requires simulating user interactions (clicks, purchases, cart dynamics). For Chapter 0's Q-learning demonstration, we use a **closed-form surrogate** (Section 0.4.3) that captures the essential preference-alignment structure without simulator complexity. The true GMV/CM2/click-based reward appears in Chapter 4+ with the full `zoosim` environment.

Key property: R_{toy} is stochastic. The same user type and boost weights can yield different outcomes due to user behavior noise (clicks are probabilistic, cart abandonment is random). This forces the agent to learn robust policies.

1.5 0.4 A First RL Agent: Tabular Q-Learning

We now arrive at the core idea: learn which boost template to use for each user type via ε -greedy tabular learning.

1.5.1 0.4.1 Problem Recap

- **Contexts \mathcal{X}** : Three user types `{price_hunter, premium, bulk_buyer}`
- **Actions \mathcal{A}** : 25 boost templates (5×5 grid)
- **Reward R** : Stochastic R_{toy} from Section 0.3.4
- **Goal**: Find a policy $\pi : \mathcal{X} \rightarrow \mathcal{A}$ that maximizes expected reward

This is a **contextual bandit** (Chapter 1 makes this formal). Each episode:

1. Sample user type $x \sim \rho$ (uniform over 3 types)
2. Choose action $a = \pi(x)$ (boost template)
3. Simulate user behavior under ranking induced by a
4. Observe reward $r \sim R(x, a)$
5. Update policy π

No sequential state transitions (yet). Single-step decision. Pure exploration-exploitation.

1.5.2 0.4.2 Algorithm: ε -Greedy Q-Learning

We'll maintain a **Q-table**: $Q(x, a) \approx \mathbb{E}[R | x, a]$ (expected reward for using boost template a in context x).

Policy: - With probability ε : explore (random action) - With probability $1-\varepsilon$: exploit ($a^* = \arg \max_a Q(x, a)$)

Update rule (after observing r):

$$Q(x, a) \leftarrow (1 - \alpha)Q(x, a) + \alpha \cdot r$$

This is **incremental mean estimation** (stochastic approximation), not Q-learning in the MDP sense. With constant learning rate α , this converges to a weighted average of recent rewards. With decaying $\alpha_t \propto 1/t$, it converges to $\mathbb{E}[R | x, a]$ by the Robbins-Monro theorem (Robbins and Monro 1951).

We call this "Q-learning" informally because we are learning a Q-table, but the standard Q-learning algorithm for MDPs includes a $\gamma \max_{a'} Q(s', a')$ term for bootstrapping future values. In bandits ($\gamma = 0$), this term vanishes, reducing to the update above. Chapter 3's Bellman contraction analysis applies to the general MDP case; for bandits, standard stochastic approximation suffices.

1.5.3 0.4.3 Minimal Implementation

Here's the complete agent in ~50 lines.

Pedagogical reward model. Rather than simulate full user interactions (GMV, CM2, clicks), we use a closed-form reward that encodes user preferences directly:

- Price hunters prefer high discount weight (w_{disc})
- Premium users prefer high quality weight (w_{qual})
- Bulk buyers prefer balanced, moderate weights

This surrogate enables rapid Q-learning iterations while preserving the essential optimization structure. The output rewards are **preference-alignment scores** (not EUR), with values typically in $[-2, 3]$.

Discretization note. We index the 5×5 grid of weight pairs for compactness: action (i, j) maps to weights via $w = -1 + 0.5 \cdot \text{index}$. Thus $(0, 0) \mapsto (-1, -1)$ and $(4, 4) \mapsto (1, 1)$.

```
import numpy as np
from typing import List, Tuple

# Setup
rng = np.random.default_rng(42)  # Reproducibility
X = ["price_hunter", "premium", "bulk_buyer"]  # Contexts
A = [(i, j) for i in range(5) for j in range(5)]  # 25 boost templates (indexed)

# Initialize Q-table: Q[context][action] = 0.0
Q = {x: {a: 0.0 for a in A} for x in X}

def choose_action(x: str, eps: float = 0.1) -> Tuple[int, int]:
    """Epsilon-greedy action selection.

    Args:
        x: User context (type)
        eps: Exploration probability

    Returns:
        Boost template (w_discount_idx, w_quality_idx)
    """
    if rng.random() < eps:
        return A[rng.integers(len(A))]  # Explore
    return max(A, key=lambda a: Q[x][a])  # Exploit

def reward(x: str, a: Tuple[int, int]) -> float:
    """Simulate reward for context x and action a.

    Toy model: preference alignment + noise.
    In reality, this would run the full simulator (rank products,
    simulate clicks/purchases, compute GMV+CM2+CLICKS).

    Args:
        x: User type
        a: Boost template indices (i, j) in [0, 4] x [0, 4]

    Returns:
        Scalar reward ~ R_toy from Section 0.3.4
    """

```

```

"""
i, j = a # i = discount index, j = quality index

# Map indices to [-1, 1] weights
# i=0 -> w_discount=-1.0, i=4 -> w_discount=1.0
w_discount = -1.0 + 0.5 * i
w_quality = -1.0 + 0.5 * j

# Simulate reward based on user preferences
if x == "price_hunter":
    # Prefer high discount boost (i=4), low quality boost (j=0)
    base = 2.0 * w_discount - 0.5 * w_quality
elif x == "premium":
    # Prefer high quality boost (j=4), low discount boost (i=0)
    base = 2.0 * w_quality - 0.5 * w_discount
else: # bulk_buyer
    # Balanced preferences: penalize extreme boosts, prefer moderate values
    base = 1.0 - abs(w_discount) - abs(w_quality)

# Add stochastic noise (user behavior variability)
noise = rng.normal(0.0, 0.5)

return float(base + noise)

```



```

def train(T: int = 3000, eps: float = 0.1, lr: float = 0.1) -> List[float]:
    """Train Q-learning agent for T episodes.

    Args:
        T: Number of training episodes
        eps: Exploration probability (epsilon-greedy)
        lr: Learning rate ($\alpha$ in update rule)

    Returns:
        List of rewards per episode (for plotting learning curves)
    """
    history = []

    for t in range(T):
        # Sample context (user type) uniformly
        x = X[rng.integers(len(X))]

        # Choose action (boost template) via epsilon-greedy
        a = choose_action(x, eps)

        # Simulate outcome and observe reward
        r = reward(x, a)

        # Q-learning update: Q(x,a) <- (1-alpha)Q(x,a) + alpha*r
        Q[x][a] = (1 - lr) * Q[x][a] + lr * r

        history.append(r)

    return history

```

```

# Train agent
hist = train(T=3000, eps=0.1, lr=0.1)

# Evaluate learned policy
print(f"Final average reward (last 100 episodes): {np.mean(hist[-100:]):.3f}")
print("\nLearned policy:")
for x in X:
    a_star = max(A, key=lambda a: Q[x][a])
    print(f" {x:15s} -> action {a_star} (Q = {Q[x][a_star]:.3f})")

```

With a fixed seed, we obtain representative output of the form (preference-alignment scores, not EUR):

```

Final average reward (last 100 episodes): 1.640 # preference-alignment scale
Learned policy:
  price_hunter      -> action (4, 1) (Q = 1.948)
  premium           -> action (1, 4) (Q = 2.289)
  bulk_buyer        -> action (2, 2) (Q = 0.942)

```

What just happened?

1. The agent explored $25 \text{ boost templates} \times 3 \text{ user types} = 75$ state-action pairs
2. After 3000 episodes, it learned:
 - **Price hunters:** Use $(4, 1)$ = high discount boost (+1.0), low quality boost (-0.5)
 - **Premium shoppers:** Use $(1, 4)$ = low discount boost (-0.5), high quality boost (+1.0)
 - **Bulk buyers:** Use $(2, 2)$ = balanced boosts (0.0, 0.0) — exactly optimal.
3. This matches our intuition from Section 0.3.1!

Stochastic convergence. Across random seeds, the learned actions might vary slightly (e.g., $(4, 0)$ vs $(4, 1)$ for price hunters), but the pattern holds: discount-heavy for price hunters, quality-heavy for premium shoppers, balanced for bulk buyers.

1.5.4 0.4.4 Learning Curves and Baselines

We visualize learning progress and compare to baselines.

```

import matplotlib.pyplot as plt

def plot_learning_curves(history: List[float], window: int = 50):
    """Plot smoothed learning curve with baselines."""
    # Compute rolling average
    smoothed = np.convolve(history, np.ones(window)/window, mode='valid')

    fig, ax = plt.subplots(figsize=(10, 6))

    # Learning curve
    ax.plot(smoothed, label='Q-learning (smoothed)', linewidth=2)

    # Baselines
    random_baseline = np.mean([reward(x, A[rng.integers(len(A))])
                               for _ in range(1000)
                               for x in X])
    ax.axhline(random_baseline, color='red', linestyle='--',
               label=f'Random policy ({random_baseline:.2f})')

    # Static best (tuned for average user)

```

Learning Curves

Figure 1: Learning Curves

```
static_best = np.mean([reward(x, (2, 2)) for _ in range(300) for x in X])
ax.axhline(static_best, color='orange', linestyle='--',
           label=f'Static best ({static_best:.2f})')

# Oracle (knows user type, chooses optimally)
# Optimal actions: price_hunter->(4,0), premium->(0,4), bulk_buyer->(2,2)
oracle_rewards = {
    "price_hunter": np.mean([reward("price_hunter", (4, 0)) for _ in range(50)]),
    "premium": np.mean([reward("premium", (0, 4)) for _ in range(50)]),
    "bulk_buyer": np.mean([reward("bulk_buyer", (2, 2)) for _ in range(50)])
}
oracle = np.mean(list(oracle_rewards.values()))
ax.axhline(oracle, color='green', linestyle='--',
           label=f'Oracle ({oracle:.2f})')

ax.set_xlabel('Episode')
ax.set_ylabel('Reward (smoothed)')
ax.set_title('Learning Curve: Contextual Bandit for Boost Optimization')
ax.legend()
ax.grid(alpha=0.3)

plt.tight_layout()
return fig

# Generate and save plot
fig = plot_learning_curves(hist)
fig.savefig('docs/book/ch00/learning_curves.png', dpi=150)
print("Saved learning curve to docs/book/ch00/learning_curves.png")
```

Expected output:

- **Random policy** (red dashed): ~0.0 average reward (baseline—random actions average out)
- **Static best** (orange dashed): ~0.3 (one-size-fits-all (2,2) helps bulk buyers but hurts price hunters and premium)
- **Q-learning** (blue solid): Starts near 0, converges to ~1.6 by episode 1500
- **Oracle** (green dashed): ~2.0 (theoretical maximum with perfect knowledge of optimal actions per user)

Key insight: Q-learning reaches about 82% of oracle performance by learning from experience alone. No manual tuning and no A/B tests are required. In this run, the bulk buyer segment recovers the optimal action (2, 2).

1.6 0.5 Reading the Experiment: What We Learned

1.6.1 Convergence Pattern

The learning curve has three phases:

1. **Pure exploration** (episodes 0–500): High variance, ε -greedy tries random actions, Q-values are noisy
2. **Exploitation begins** (episodes 500–1500): Agent identifies good actions per context, reward climbs steadily

3. **Convergence** (episodes 1500–3000): Q-values stabilize, reward plateaus at ~82% of oracle

This is **regret minimization** in action. Chapter 1 formalizes this; Chapter 6 analyzes convergence rates.

1.6.2 Per-Segment Performance

If we track rewards separately by user type:

```
# Track per-segment performance
segment_rewards = {x: [] for x in X}

for _ in range(100): # 100 test episodes
    for x in X:
        a = max(A, key=lambda a: Q[x][a]) # Greedy policy (no exploration)
        r = reward(x, a)
        segment_rewards[x].append(r)

for x in X:
    print(f'{x}: mean reward = {np.mean(segment_rewards[x]):.3f}'")
```

Output:

```
price_hunter : mean reward = 2.309
premium      : mean reward = 2.163
bulk_buyer   : mean reward = 0.917
```

Analysis:

- **Price hunters** get the highest rewards (~2.3)—the agent found a near-optimal action (4, 1) with high discount boost
- **Premium shoppers** get high rewards (~2.2)—high quality boost (1, 4) closely matches their preferences
- **Bulk buyers** get lower rewards (~0.9) because their **balanced preferences** have inherently lower optimal reward (base=1.0 at (2,2)) compared to polarized users (base=2.5). But the agent finds the **exact optimal!**
- All three segments dramatically beat the static baseline (~0.3 average) through personalization

This is **personalization** at work: different users get different rankings, each optimized for their revealed preferences.

1.6.3 What We (Hand-Wavily) Assumed

This toy experiment “just worked,” but we made implicit assumptions:

1. **Rewards are well-defined expectations** over stochastic outcomes (Chapter 2 makes this measure-theoretically rigorous)
2. **Exploration is safe** (in production, bad rankings lose users; Chapter 9 introduces off-policy evaluation for safer testing)
3. **The logging policy and new policy have sufficient overlap** to compare fairly (importance weights finite; Chapter 9)
4. **ϵ -greedy tabular Q converges** (for bandits, this follows from stochastic approximation theory; Chapter 3’s Bellman contraction analysis applies to the full MDP case with $\gamma > 0$)
5. **Actions are discrete and state space is tiny** (Chapter 7 handles continuous actions; Chapter 4 builds realistic state)

None of these are free. The rest of the book makes them precise and shows when they hold (or how to proceed when they don’t).

1.6.4 Theory-Practice Gap: ε -Greedy Exploration

Our toy used ε -greedy exploration with constant $\varepsilon = 0.1$. This deserves scrutiny.

What theory says: In a stochastic K -armed bandit, a constant exploration rate ε forces perpetual uniform exploration and yields linear regret. If $\varepsilon_t \rightarrow 0$ with a suitable schedule, ε -greedy can achieve sublinear regret, but its exploration remains uniform over non-greedy arms. By contrast, UCB-type algorithms direct exploration through confidence bounds and achieve logarithmic (gap-dependent) regret and worst-case $\tilde{O}(\sqrt{KT})$ regret (Auer et al. 2002; Lattimore and Szepesvári 2020).

What practice shows: ε -greedy with constant $\varepsilon \in [0.05, 0.2]$ is often competitive because:

1. **Trivial to implement:** No confidence bounds, no posterior sampling, just a random number generator
2. **Handles non-stationarity gracefully:** Continues exploring even after “convergence” (useful when user preferences drift)
3. **The regret difference matters only at scale:** For the short horizons in this chapter, the gap between ε -greedy and UCB is typically negligible

When ε -greedy fails: High-dimensional action spaces where uniform exploration wastes samples. For our 25-action toy problem, it is adequate. For Chapter 7’s continuous actions (10^{100} effective arms), we need structured exploration (UCB, Thompson Sampling).

Modern context: Google’s 2010 display ads paper (Li et al. 2010) used ε -greedy successfully at scale. In many contemporary bandit systems, Thompson Sampling is a strong default due to its uncertainty-driven exploration and empirical performance (Russo et al. 2018; Lattimore and Szepesvári 2020).

Why UCB and Thompson Sampling? (Preview for Chapter 6)

ε -greedy explores **uniformly**—it wastes samples on arms it already knows are bad. UCB explores **optimistically**—it tries arms whose rewards *might* be high given uncertainty:

- **UCB:** Choose $a_t = \arg \max_a [Q(x, a) + \beta\sigma(x, a)]$ where σ is a confidence width. Explores arms with high uncertainty, not randomly.
- **Thompson Sampling:** Maintain posterior $P(Q^* \mid \text{data})$, sample $\tilde{Q} \sim P$, act greedily on sample. Naturally balances exploration (high posterior variance \rightarrow diverse samples) with exploitation.

Both achieve $\tilde{O}(d\sqrt{T})$ regret for d -dimensional linear bandits—matching the lower bound up to logarithms (Chu et al. 2011; Lattimore and Szepesvári 2020). In this structured setting, naive uniform exploration can be provably suboptimal, and the gap widens in high dimensions.

1.7 0.6 Limitations: Why We Need the Rest of the Book

Our toy is **pedagogical**, not production-ready. Here’s what breaks at scale:

1.7.1 1. Discrete Action Space

We used 25 templates. Real search has continuous boosts: $\mathbf{w} \in [-5, 5]^{10}$ (ten features, unbounded). Discretizing to a grid would require $100^{10} = 10^{20}$ actions—intractable.

Solution: Chapter 7 introduces **continuous action bandits** via $Q(x, a)$ regression and cross-entropy method (CEM) optimization.

1.7.2 2. Tabular State Representation

We had 3 user types. Real search has thousands of user segments (RFM bins, geographic regions, device types, time-of-day). Plus query features (length, specificity, category). A realistic context space is **high-dimensional and continuous**.

Solution: Chapter 6 (neural linear bandits), Chapter 7 (deep Q-networks with continuous state/action).

1.7.3 3. No Constraints

Our agent optimized R_{toy} without guardrails. Real systems must enforce:

- Profitability floors (CM2 \geq threshold)
- Exposure targets (strategic products get visibility)
- Rank stability (limit reordering volatility)

Solution: Chapter 10 introduces production **guardrails** (CM2 floors, $\Delta \text{Rank}@k$ stability), with Chapter 3 (Section 3.5) providing the formal CMDP theory and Lagrangian methods.

1.7.4 4. Simplified Position Bias

We didn't model how clicks depend on rank. Real users exhibit **position bias** (top-3 slots get 80% of clicks) and **abandonment** (quit after 5 results if nothing relevant).

Solution: Chapter 2 develops PBM/DBN click models; Chapter 5 implements them in `zoosim`.

1.7.5 5. Online Exploration Risk

We trained by interacting with users directly (episodes = real searches). In production, bad rankings **cost real money** and **lose real users**. We need safer evaluation.

Solution: Chapter 9 introduces **off-policy evaluation (OPE)**: estimate new policy performance using logged data from old policy, without deploying.

1.7.6 6. Single-Episode Horizon

We treated each search as independent. Real users return across sessions. Today's ranking affects tomorrow's retention.

Solution: Chapter 11 extends to **multi-episode MDPs** with inter-session dynamics (retention, satisfaction state).

1.8 0.7 Map to the Book

Here's how our toy connects to the rigorous treatment ahead:

Toy Concept	Formal Treatment	Chapter
User types	Context space \mathcal{X} , distribution ρ	1
Boost templates	Action space \mathcal{A} , policy π	1, 6, 7
R_{toy}	Reward function $R : \mathcal{X} \times \mathcal{A} \times \Omega \rightarrow \mathbb{R}$, constraints	1
ε -greedy Q-learning	Bellman operator, contraction mappings	3
Stochastic outcomes	Probability spaces, click models (PBM/DBN)	2
Learning curves	Regret bounds, sample complexity	6
Static best vs oracle	Importance sampling, off-policy evaluation	9
Guardrails (missing)	CMDP (Section 3.5), production guardrails	3, 10
Engagement proxy	Multi-episode MDP, retention modeling	11

Chapters 1–3 provide foundations: contextual bandits, measure theory, Bellman operators. Chapters 4–8 build the simulator and core algorithms. Chapters 9–11 handle evaluation, robustness, and production deployment. Chapters 12–15 cover frontier methods (slate ranking, offline RL, multi-objective optimization).

1.9 0.8 How to Use This Book

1.9.1 For Practitioners

We recommend working through Chapter 0 in full: we run the code, modify the reward function (Exercise 0.1), and compare exploration strategies (Exercise 0.2).

We then skim Chapters 1–3 on a first read. We focus on: - The reward formulation (#EQ-1.2 in Chapter 1) - Why engagement matters (Section 1.2.1) - The Bellman contraction intuition (Chapter 3, skip proof details initially)

We then dive into Chapters 4–11 (simulator, algorithms, evaluation). This provides the implementation roadmap.

We return to theory as needed. When something fails (e.g., divergence in a Q-network), we revisit Chapter 3’s convergence analysis.

1.9.2 For Researchers / Mathematically Inclined

We skim Chapter 0 to see the concrete thread.

We start at Chapter 1. We work through definitions, theorems, and proofs, and we verify that the code validates the mathematics.

We do the exercises: a mix of proofs (30%), implementations (40%), experiments (20%), and conceptual questions (10%).

We use Chapter 0 as a touchstone. When abstractions feel heavy, we return to the toy: “How does this theorem explain why the tabular method stabilized in Section 0.4?”

1.9.3 For Everyone

Ethos: mathematics and code are inseparable. Every theorem compiles. Every algorithm is proven rigorous, then implemented in production-quality code. Theory and practice in constant dialogue.

If a proof appears without code or code appears without theory, something is missing.

1.10 Exercises (Chapter 0)

Exercise 0.1 (Reward Sensitivity) [15 minutes]

Modify `reward()` to use different weights in R_{toy} : - (a) Pure GMV: (1.0, 0.0, 0.0) (no profitability or engagement terms) - (b) Profit-focused: (0.4, 0.5, 0.1) (prioritize CM2 over GMV) - (c) Engagement-heavy: (0.5, 0.2, 0.3) (high click weight)

For each, train Q-learning and report: - Final average reward - Learned actions per user type - Does the policy change? Why?

Hint: Case (c) risks “clickbait” strategies (see Chapter 1, Section 1.2.1). Monitor conversion quality.

Exercise 0.2 (Action Geometry) [30 minutes]

Compare two exploration strategies:

Strategy A (current): ε -greedy with uniform random action sampling

Strategy B (neighborhood): ε -greedy with **local perturbation**: when exploring, sample action near current best $a^* = \arg \max_a Q(x, a)$:

```

def explore_local(x, sigma=1.0):
    a_star = max(A, key=lambda a: Q[x][a])
    i_star, j_star = a_star
    i_new = np.clip(i_star + rng.integers(-1, 2), 0, 4)
    j_new = np.clip(j_star + rng.integers(-1, 2), 0, 4)
    return (i_new, j_new)

```

Implement both, train for 1000 episodes, and plot learning curves. Which converges faster? Why?

Reflection: This is **structured exploration**. Chapter 6 introduces UCB and Thompson Sampling, which balance exploration and exploitation more principled than ε -greedy.

Exercise 0.3 (Regret Shape) [45 minutes, extended]

Define **cumulative regret** as the gap between oracle and agent:

$$\text{Regret}(T) = \sum_{t=1}^T (R_t^* - R_t)$$

where R_t^* is the oracle reward (best action for context x_t) and R_t is the agent's reward.

(a) Implement regret tracking:

```

def compute_regret(history, contexts, oracle_Q):
    regret = []
    cumulative = 0.0
    for t, (x, r) in enumerate(zip(contexts, history)):
        r_star = oracle_Q[x]
        cumulative += (r_star - r)
        regret.append(cumulative)
    return regret

```

(b) Plot cumulative regret vs episode count. Is it sublinear (i.e., does $\text{Regret}(T)/T \rightarrow 0$)?

(c) Fit a curve: $\text{Regret}(T) \approx C\sqrt{T}$. Does this match theory? (Chapter 6 derives $O(\sqrt{T})$ regret for UCB.)

Exercise 0.4 (Advanced: Constraints) [60 minutes, extended]

Add a simple CM2 floor constraint: reject actions that violate profitability.

Setup: Modify `reward()` to return `(r, cm2)`. Define a floor $\tau = 0.3$ (30% margin minimum).

Constrained Q-learning:

```

def choose_action_constrained(x, eps, tau_cm2):
    # Filter feasible actions
    feasible = [a for a in A if expected_cm2(x, a) >= tau_cm2]
    if not feasible:
        return A[rng.integers(len(A))] # Fallback to unconstrained

    if rng.random() < eps:
        return feasible[rng.integers(len(feasible))]

    return max(feasible, key=lambda a: Q[x][a])

```

(a) Implement `expected_cm2(x, a)` (running average like Q).

(b) Train with $\tau = 0.3$. How does performance change vs unconstrained?

(c) Plot the Pareto frontier: GMV vs CM2 as τ varies over [0.0, 0.5].

Connection: This is a **Constrained MDP (CMDP)**. Chapter 3 (Section 3.5) develops the Lagrangian theory, and Chapter 10 implements production guardrails for multi-constraint optimization.

Exercise 0.5 (Bandit-Bellman Bridge) [20 minutes, conceptual]

Our toy is a **contextual bandit**: single-step decisions, no sequential states.

The **Bellman equation** (Chapter 3) for an MDP is:

$$V^*(s) = \max_a \left\{ R(s, a) + \gamma \sum_{s'} P(s' | s, a) V^*(s') \right\}$$

where $\gamma \in [0, 1]$ is a discount factor.

Question: Show that our Q-learning update is the $\gamma = 0$ special case of Bellman.

Hint: - Set $\gamma = 0$ in Bellman equation - Note that with no future states, $V^*(s) = \max_a R(s, a)$ - Our Q-table is $Q(x, a) \approx \mathbb{E}[R | x, a]$, so $V^*(x) = \max_a Q(x, a)$ - This is **one-step value iteration**

Reflection: Contextual bandits are MDPs with horizon 1. Multi-episode search (Chapter 11) requires the full Bellman machinery.

1.11 0.9 Code Artifacts

All code from this chapter is available in the repository:

Code-Artifact Mapping

- **Run script:** `scripts/ch00/toy_problem_solution.py:1` (use `--chapter0` to reproduce this chapter's output) - **Sanity tests:** `tests/ch00/test_toy_example.py:1` (deterministic regression for Chapter 0 output) - **Learning curve plot:** `docs/book/ch00/learning_curves.png:1` (generated artifact)

To reproduce:

```
uv run python scripts/ch00/toy_problem_solution.py --chapter0  
uv run pytest -q tests/ch00
```

Expected output:

```
Final average reward (last 100 episodes): 1.640
```

Learned policy:

```
price_hunter    -> action (4, 1) (Q = 1.948)  
premium        -> action (1, 4) (Q = 2.289)  
bulk_buyer     -> action (2, 2) (Q = 0.942)
```

```
Saved learning curve to docs/book/ch00/learning_curves.png
```

1.12 0.10 What's Next?

We have now trained a first RL agent for search ranking. It learned context-adaptive boost weights from scratch, achieving near-oracle performance without manual tuning.

But we cheated. We used a tiny discrete action space, three user types, and online exploration without safety guarantees. Real systems need:

1. **Rigorous foundations** (Chapters 1–3): Formalize contextual bandits, measure-theoretic probability, Bellman operators
2. **Realistic simulation** (Chapters 4–5): Scalable catalog generation, position bias models, rich user dynamics
3. **Continuous actions** (Chapter 7): Regression-based Q-learning, CEM optimization, trust regions
4. **Constraints and guardrails** (Chapter 10): CM2 floors, Δ Rank@k stability, safe fallback policies
5. **Safe evaluation** (Chapter 9): Off-policy evaluation (IPS, DR, FQE) for production deployment
6. **Multi-episode dynamics** (Chapter 11): Retention modeling, long-term value, engagement as state

The journey from toy to production is the journey of this book.

In **Chapter 1**, we formalize everything we hand-waved here: What exactly is a contextual bandit? Why is the reward function (1.2) mathematically sound? How do constraints become a CMDP? Why does engagement matter, and when should it be implicit vs explicit?

Let us make it rigorous.

End of Chapter 0

2 Chapter 1 — Search Ranking as Optimization: From Business Goals to RL

Vlad Prytula

2.1 1.1 The Problem: Balancing Multiple Objectives in Search

A concrete dilemma. A pet supplies retailer faces a challenge. User A searches for “cat food”—a price-sensitive buyer who abandons carts if shipping costs are high. User B issues the same query—a premium shopper loyal to specific brands, willing to pay more for quality. The current search system shows them **identical rankings** because boost weights are static, tuned once for the “average” user. User A sees expensive premium products and abandons. User B sees discount items and questions the retailer’s quality. Both users are poorly served by a one-size-fits-all approach.

The business tension. Every e-commerce search system must balance competing objectives:

- **Revenue (GMV)**: Show products users will buy, at good prices
- **Profitability (CM2)**: Prioritize items with healthy margins
- **Strategic goals (STRAT)**: Promote strategic products (new launches, house brands, clearance)—tracked as **purchases** in the reward and **exposure** in guardrails
- **User experience**: Maintain relevance, diversity, and satisfaction

Traditional search systems rely on **manually tuned boost parameters**: category multipliers, price/discount bonuses, profit margins, strategic product flags. Before writing the scoring function, we fix our spaces.

Spaces (Working Definitions).

- \mathcal{P} : **Product catalog**, a finite set of M products. Each $p \in \mathcal{P}$ carries attributes (price, category, margin, embedding).
- \mathcal{Q} : **Query space**, the set of possible search queries. In practice, a finite vocabulary or embedding space $\mathcal{Q} \subset \mathbb{R}^{d_q}$.
- \mathcal{U} : **User space**, characterizing users by segment, purchase history, and preferences. Finite segments or embedding space $\mathcal{U} \subset \mathbb{R}^{d_u}$.
- \mathcal{X} : **Context space**, typically $\mathcal{X} \subseteq \mathcal{U} \times \mathcal{Q} \times \mathcal{H} \times \mathcal{T}$ where \mathcal{H} is session history and \mathcal{T} is time features. We assume \mathcal{X} is a compact subset of \mathbb{R}^{d_x} for some d_x (verified in Chapter 4).
- $\mathcal{A} = [-a_{\max}, +a_{\max}]^K$: **Action space**, a compact subset of \mathbb{R}^K (boost weights bounded by $a_{\max} > 0$).

- Ω : **Outcome space**, the sample space for stochastic user behavior (clicks, purchases, abandonment). Equipped with probability measure \mathbb{P} (formalized in Chapter 2).

Measure-theoretic structure (σ -algebras, probability kernels, conditional distributions) is developed in Chapter 2. For this chapter, we work with these as sets supporting the functions and expectations below.

A typical scoring function looks like:

$$s : \mathcal{P} \times \mathcal{Q} \times \mathcal{U} \rightarrow \mathbb{R}, \quad s(p, q, u) = r_{\text{ES}}(q, p) + \sum_{k=1}^K w_k \phi_k(p, u, q) \quad (1.1)$$

where: - $r_{\text{ES}} : \mathcal{Q} \times \mathcal{P} \rightarrow \mathbb{R}_+$ is a **base relevance score** (e.g., BM25 or neural embeddings) - $\phi_k : \mathcal{P} \times \mathcal{U} \times \mathcal{Q} \rightarrow \mathbb{R}$ are **engineered features** (margin, discount, bestseller status, category match) - $w_k \in \mathbb{R}$ are **manually tuned weights**, collected as $\mathbf{w} = (w_1, \dots, w_K) \in \mathbb{R}^K$

Note that we've made the user dependence explicit: $s(p, q, u)$ depends on product $p \in \mathcal{P}$, query $q \in \mathcal{Q}$, and user $u \in \mathcal{U}$ through the feature functions ϕ_k .

Why manual tuning fails. The core problem: w_k cannot adapt to context. The “price hunter” (User A) cares about bulk pricing and discounts. The “premium shopper” (User B) values quality over price. A generic query (“cat food”) tolerates exploration; a specific query (“Royal Canin Veterinary Diet Renal Support”) demands precision.

Numerical evidence of the problem. Suppose we tune $w_{\text{discount}} = 2.0$ to maximize average GMV across all users. For price hunters, this works well—they click frequently on discounted items. But for premium shoppers, this destroys relevance—they see cheap products ranked above their preferred brands, leading to zero purchases and session abandonment. Conversely, if we tune $w_{\text{discount}} = 0.3$ for premium shoppers, price hunters see full-price items and also abandon.

Manual weights are **static, context-free, and suboptimal** by design. We need weights that adapt.

Our thesis: Treat $\mathbf{w} = (w_1, \dots, w_K) \in \mathbb{R}^K$ as **actions to be learned**, adapting to user and query context via reinforcement learning.

In Chapter 0 (Motivation: A First RL Experiment), we built a tiny, code-first prototype of this idea: three synthetic user types, a small action grid of boost templates, and a tabular Q-learning agent that learned context-adaptive boosts. In this chapter, we strip away implementation details and **formalize and generalize** that experiment as a contextual bandit with constraints.

Notation

Throughout this chapter: - **Spaces**: \mathcal{X} (contexts), \mathcal{A} (actions), Ω (outcomes), \mathcal{Q} (queries), \mathcal{P} (products), \mathcal{U} (users) - **Distributions**: ρ (context distribution over \mathcal{X}), $P(\omega | x, a)$ (outcome distribution) - **Probability**: \mathbb{P} (probability measure), \mathbb{E} (expectation) - **Real/natural numbers**: $\mathbb{R}, \mathbb{N}, \mathbb{R}_+$ (non-negative reals) - **Norms**: $\|\cdot\|_2$ (Euclidean), $\|\cdot\|_\infty$ (supremum) - **Operators**: \mathcal{T} (Bellman operator, introduced in Chapter 3)

We index equations as EQ-X.Y, theorems as THM-X.Y, definitions as DEF-X.Y, remarks as REM-X.Y, and assumptions as ASM-X.Y for cross-reference. Anchors like {#THM-1.7.2} enable internal linking.

On Mathematical Rigor

This chapter provides **working definitions** and builds intuition for the RL formulation. We specify function signatures (domains, codomains, types) but defer **measure-theoretic foundations**— σ -algebras on \mathcal{X} and Ω , measurability conditions, integrability requirements—to **Chapters 2–3**. Key results (existence of optimal policies and the regret lower-bound preview in §1.7.6) state their assumptions explicitly; verification that our search setting satisfies these assumptions appears in later chapters. Readers seeking Bourbaki-level rigor should treat this chapter as motivation and roadmap; the rigorous development begins in Chapter 2.

This chapter establishes the mathematical foundation: we formulate search ranking as a **constrained optimization problem**, then show why it requires **contextual decision-making** (bandits), and finally preview the RL framework we'll develop.

2.2 1.2 From Clicks to Outcomes: The Reward Function

Let's make the business objectives precise. Consider a single search session:

1. User u with segment $\sigma \in \{\text{price_hunter}, \text{pl_lover}, \text{premium}, \text{litter_heavy}\}$ issues **query** q
2. System scores products $\{p_1, \dots, p_M\}$ using boost weights \mathbf{w} , producing ranking π
3. User examines results with **position bias** (top slots get more attention), clicks on subset $C \subseteq \{1, \dots, M\}$, purchases subset $B \subseteq C$
4. Session generates **outcomes**: GMV, CM2 (contribution margin 2), clicks, strategic purchases

We aggregate these into a **scalar reward**:

$$R(\mathbf{w}, u, q, \omega) = \alpha \cdot \text{GMV}(\mathbf{w}, u, q, \omega) + \beta \cdot \text{CM2}(\mathbf{w}, u, q, \omega) + \gamma \cdot \text{STRAT}(\mathbf{w}, u, q, \omega) + \delta \cdot \text{CLICKS}(\mathbf{w}, u, q, \omega) \quad (1.2)$$

where $\omega \in \Omega$ represents the stochastic user behavior conditioned on the ranking $\pi_{\mathbf{w}}(u, q)$ induced by boost weights \mathbf{w} , and $(\alpha, \beta, \gamma, \delta) \in \mathbb{R}_+^4$ are **business weight parameters** reflecting strategic priorities. The outcome components (GMV, CM2, STRAT, CLICKS) depend on the full context (\mathbf{w}, u, q) through the ranking, though we often abbreviate this dependence when clear from context.

Two strategic quantities: reward vs. constraints

In the reward (1.2), $\text{STRAT}(\omega)$ counts **strategic purchases** in the session (purchased items whose **strategic_flag** is true). In guardrails like (2.2.1), we instead track **strategic exposure**—how many strategic items were shown in the ranking, regardless of whether they were bought.

We keep both on purpose: reward incentivizes realized strategic outcomes, while exposure floors enforce minimum visibility even before conversion. In code, the reward-side quantity appears as `RewardBreakdown.strat` in `zoosim/dynamics/reward.py:34-39`.

Standing assumption (Integrability). Throughout this chapter, we assume $R : \mathcal{A} \times \mathcal{U} \times \mathcal{Q} \times \Omega \rightarrow \mathbb{R}$ is measurable in ω and $\mathbb{E}[|R(\mathbf{w}, u, q, \omega)|] < \infty$ for all (\mathbf{w}, u, q) . This ensures expectations like $\mathbb{E}[R | \mathbf{w}]$ are well-defined. The formal regularity conditions appear as **Assumption 2.6.1 (OPE Probability Conditions)** in Chapter 2, §2.6; verification for our bounded-reward setting is in Chapter 2.

Remark (connection to Chapter 0). The Chapter 0 toy used a simplified instance of this reward with $(\alpha, \beta, \gamma, \delta) \approx (0.6, 0.3, 0, 0.1)$ and no explicit STRAT term. All analysis in this chapter applies to that setting.

Key insight: R depends on \mathbf{w} indirectly through the ranking π induced by scores from (1.1). A product ranked higher gets more exposure, more clicks, and influences downstream purchases. This is **not a simple function**—it's stochastic, nonlinear, and noisy.

2.2.1 Constraints: Not All Rewards Are Acceptable

High GMV alone is insufficient. A retailer must enforce **guardrails**:

$$\mathbb{E}[\text{CM2} | \mathbf{w}] \geq \tau_{\text{margin}} \quad (1.3a)$$

$$\mathbb{E}[\text{Exposure}_{\text{strategic}} | \mathbf{w}] \geq \tau_{\text{STRAT}} \quad (1.3b)$$

$$\mathbb{E}[\Delta\text{rank}@k \mid \mathbf{w}] \leq \tau_{\text{stability}} \quad (1.3c)$$

where the notation $\mathbb{E}[\cdot \mid \mathbf{w}]$ denotes expectation over stochastic user behavior ω and context distribution $\rho(x)$ when action (boost weights) \mathbf{w} is applied, i.e., $\mathbb{E}[\text{CM2} \mid \mathbf{w}] := \mathbb{E}_{x \sim \rho, \omega \sim P(\cdot|x, \mathbf{w})}[\text{CM2}(\mathbf{w}, x, \omega)]$.

Definition ($\Delta\text{rank}@k$). Let $\pi_{\mathbf{w}}(q) = (p_1, \dots, p_M)$ be the ranking induced by boost weights \mathbf{w} for query q , and let $\pi_{\text{base}}(q)$ be a reference ranking (e.g., the production baseline). Let $\text{TopK}_{\mathbf{w}}(q)$ and $\text{TopK}_{\text{base}}(q)$ denote the *sets* of top- k items under these rankings. Define:

$$\Delta\text{rank}@k(\mathbf{w}, q) := 1 - \frac{|\text{TopK}_{\mathbf{w}}(q) \cap \text{TopK}_{\text{base}}(q)|}{k}$$

the fraction of top- k items that changed (set churn). Values range in $[0, 1]$; $\Delta\text{rank}@k = 0$ means identical top- k set (reordering within the top- k does not count), and $\Delta\text{rank}@k = 1$ means the two top- k sets are disjoint.

This is the set-based stability metric used in Chapter 10 DEF-10.4 and implemented in `zoosim/monitoring/metrics.py:89-1`. A position-wise mismatch rate is a different metric; if we use it, we will name it explicitly and not call it “Delta-Rank@k”.

- **CM2 floor** (1.3a): Prevent sacrificing profitability for revenue
- **Exposure floor** (1.3b): Ensure strategic products (new launches, house brands) get visibility
- **Rank stability** (1.3c): Limit reordering volatility (users expect consistency); $\tau_{\text{stability}} \approx 0.2$ is typical

Taken together, the scalar objective (1.2) and constraints (1.3a–c) define a **constrained stochastic optimization** problem over the boost weights \mathbf{w} . Formally, we would like to choose \mathbf{w} to solve

$$\max_{\mathbf{w} \in \mathbb{R}^K} \mathbb{E}_{x \sim \rho, \omega \sim P(\cdot|x, \mathbf{w})}[R(\mathbf{w}, x, \omega)] \quad \text{subject to (1.3a–c).}$$

From the perspective of a single query, there is no internal state evolution: each query arrives with a context x , we apply fixed boost weights \mathbf{w} , observe a random outcome, and then move on to the next independent query. This “context + one action + one noisy payoff” structure is exactly the **contextual bandit** template.

In §1.3 we move from a single global choice of \mathbf{w} to an explicit **policy** π that maps each context x to boost weights $\pi(x)$. In **Chapter 11**, when we introduce multi-step user/session dynamics with states and transitions, the resulting model becomes a **constrained Markov decision process (CMDP)**. Contextual bandits are the $\gamma = 0$ special case of an MDP.

Now we understand the complete optimization problem: maximize the scalar reward (1.2) subject to constraints (2.2.1). This establishes what we’re optimizing. Next, we’ll dive deep into one critical component—the engagement term—before implementing the reward function.

Code \$\leftarrow\$ Config (constraints)

Constraint-related knobs (`MOD-zoosim.config`) live in configuration so experiments remain reproducible and auditable. These reserve the knobs for (2.2.1) constraint definitions:

- Rank stability multiplier (soft constraint): `lambda_rank` in `zoosim/core/config.py:230` (reserved for primal–dual constrained RL in Chapter 14; not wired in current simulator)
- Profitability floor (CM2) threshold: `cm2_floor` in `zoosim/core/config.py:232` (hard feasibility-filter pattern in Chapter 10, Exercise 10.3)
- Exposure floors (strategic products): `exposure_floors` in `zoosim/core/config.py:233` (reserved; enforcement deferred to Chapter 10 hard filters and Chapter 14 soft constraints)

Implementation status: These config fields exist for forward compatibility; constraint enforcement logic appears in later chapters:

- `cm2_floor`: Active enforcement in Chapter 10 (feasibility filter)
- `exposure_floors`: Reserved; enforcement in Chapter 10
- `lambda_rank`: Reserved; primal-dual optimization in Chapter 14

2.2.2 1.2.1 The Role of Engagement in Reward Design

In practice, search objectives are **hierarchically structured**, not flat:

1. **Viability constraints** (must satisfy or system is unusable): $\text{CTR} > 0$, latency $< 500\text{ms}$, uptime $> 99.9\%$
2. **Business outcomes** (what we optimize): GMV, profitability (CM2), strategic positioning
3. **Strategic nudges** (tiebreakers for long-term value): exploration, new product exposure, brand building

Engagement (clicks, dwell time, add-to-cart actions) **straddles this hierarchy**: it is partly viability (zero clicks \Rightarrow dead search, users abandon platform), partly outcome (clicks signal incomplete attribution—mobile browse, desktop purchase), and partly strategic (exploration value—today's clicks reveal preferences for tomorrow's sessions).

Why include $\delta \cdot \text{CLICKS}$ in the reward?

We include $\delta \cdot \text{CLICKS}$ as a **soft viability term** in the reward function (1.2). This serves three purposes:

1. **Incomplete attribution**: E-commerce has imperfect conversion tracking. A user clicks product p on mobile, adds to cart, completes purchase on desktop 3 days later. We observe the click, but GMV attribution goes to a different session (or is lost entirely in cross-device gaps). The click is a **leading indicator** of future GMV not captured in ω .
2. **Exploration value**: Clicks reveal user preferences even without immediate purchase. If user u clicks on premium brand products but doesn't convert, we learn u is exploring that segment—valuable for future sessions. This is **information acquisition**: clicks are samples from the user's latent utility function.
3. **Platform health**: A search system with high GMV but near-zero CTR is **brittle**—one price shock or inventory gap causes catastrophic user abandonment. Engagement is a **leading indicator of retention**: users who click regularly have higher lifetime value (LTV) than those who occasionally convert high-value purchases but otherwise ignore search results.

The clickbait risk. However, δ **must be carefully bounded**. If δ/α is too large, the agent learns “clickbait” strategies: optimize CTR at the expense of conversion rate ($\text{CVR} = \text{purchases}/\text{clicks}$). The pathological case: show irrelevant but visually attractive products (e.g., cute cat toys for dog owners), achieve high clicks but zero sales, and still get rewarded due to $\delta \cdot \text{CLICKS} \gg 0$.

Practical guideline: Set $\delta/\alpha \in [0.01, 0.10]$ —engagement is a *tiebreaker*, not the primary objective. We want clicks to be a **soft regularizer** that prevents GMV-maximizing policies from collapsing engagement, not a dominant term that drives the optimization.

Diagnostic metric: Monitor **revenue per click (RPC)**

$$\text{RPC}_t = \frac{\sum_{i=1}^t \text{GMV}_i}{\sum_{i=1}^t \text{CLICKS}_i}$$

(cumulative GMV per click up to episode t). If RPC_t drops $> 10\%$ below baseline while CTR rises during training, the agent is learning clickbait—reduce δ immediately.

Control-theoretic analogy: This is similar to LQR with **state and control penalties**: $c(x, u) = x^\top Qx + u^\top Ru$. We penalize both deviation from target state (GMV, CM2) and control effort (engagement as “cost” of achieving GMV). The relative weights Q, R encode the tradeoff. In our case, $\alpha, \beta, \gamma, \delta$ play the role of Q ,

and we're learning the optimal policy $\pi^*(x)$ under this cost structure. See Appendix B (and Section 1.10) for deeper connections to classical control.

Multi-episode perspective (Chapter 11 preview): In a **Markov Decision Process (MDP)** with inter-session dynamics, engagement enters *implicitly* through its effect on retention and lifetime value:

$$V^\pi(s_0) = \mathbb{E}_\pi \left[\sum_{t=0}^{\infty} \gamma^t \text{GMV}_t \mid s_0 \right] \quad (1.2')$$

If today's clicks increase the probability that user u returns tomorrow (state transition $s_{t+1} = f(s_t, \text{clicks}_t, \dots)$), then maximizing (1.2')e automatically incentivizes engagement. We wouldn't need $\delta \cdot \text{CLICKS}$ in the single-step reward—it would be *derived* from optimal long-term value.

However, the **single-step contextual bandit** (our MVP formulation) cannot model inter-session dynamics. Each search is treated as independent: user arrives, we rank, user interacts, episode terminates. No s_{t+1} , no retention modeling. Including $\delta \cdot \text{CLICKS}$ is a **heuristic proxy** for the missing LTV component—mathematically imperfect, but empirically essential for search systems.

The honest assessment: This is a **theory-practice tradeoff**. The “correct” formulation is (1.2')e (multi-episode MDP), but it requires modeling complex user dynamics (churn, seasonality, cross-session preferences) that are expensive to simulate and hard to learn from. The single-step approximation (1.2) with $\delta \cdot \text{CLICKS}$ is **pragmatic**: it captures 80% of the value with 20% of the complexity. For the MVP, this is the right tradeoff. Chapter 11 extends to multi-episode settings where engagement is properly modeled as state dynamics.

Cross-reference — Chapter 11

The full multi-episode treatment and implementation live in [Chapter 11 - Multi-Episode Inter-Session MDP](#) (see `docs/book/syllabus.md`). There we add `zoosim/multi_episode/session_env.py` and `zoosim/multi_episode/retention.py` to operationalize (1.2')e with a retention/hazard state and validate that engagement raises long-term value without needing an explicit $\delta \cdot \text{CLICKS}$ term.

Code \Rightarrow Config (reward weights)

Business weights in `RewardConfig` (`MOD-zoosim.config`) implement (1.2) parameters and must satisfy engagement bounds from this section:

- α (GMV): Primary objective, normalized to 1.0 by convention
- β/α (CM2 weight): Profit sensitivity, typically $\in [0.3, 0.8]$ (higher \Rightarrow prioritize margin over revenue)
- γ/α (STRAT weight): Strategic priority (reward units per strategic purchase; see `RewardConfig.gamma_strat`, default $\gamma = 2.0$ in this repo)
- δ/α (**CLICKS weight**): **Bounded** $\in [0.01, 0.10]$ **to prevent clickbait strategies**

Validation (enforced in code): see `zoosim/dynamics/reward.py:56` for an assertion on δ/α in the production reward path. The numerical range $[0.01, 0.10]$ is an engineering guardrail motivated by clickbait failure modes; Appendix C provides the duality background for constrained optimization, not a derivation of this specific bound.

Diagnostic: Compute $\text{RPC}_t = \sum \text{GMV}_i / \sum \text{CLICKS}_i$ after each policy update. If RPC drops > 10% while CTR rises, reduce δ by 30–50%.

Code \Rightarrow Simulator Layout

- `zoosim/core/config.py` (`MOD-zoosim.config`): `SimulatorConfig/RewardConfig` with seeds, guardrails, and reward weights
- `zoosim/world/{catalog,users,queries}.py`: deterministic catalog + segment + query gen-

- eration (Chapter 4)
- `zoosim/ranking/{relevance,features}.py`: base relevance and boost feature engineering (Chapter 5)
 - `zoosim/dynamics/{behavior,reward}.py` (`MOD-zoosim.behavior`, `MOD-zoosim.reward`): click/abandonment dynamics + reward aggregation for (1.2)
 - `zoosim/envs/{search_env.py,gym_env.py}` (`MOD-zoosim.env`): single-step environment and Gym wrapper wiring the simulator together
 - `zoosim/multi_episode/{session_env.py,retention.py}`: Chapter 11's retention-aware MDP implementing (1.2)'e

2.2.3 Verifying the Reward Function

Before diving into theory, let's implement (1.2) and see what it does:

```
# Minimal implementation of #EQ-1.2 (full version: Lab 1.3 in exercises_labs.md)
def compute_reward(gmv, cm2, strat, clicks, alpha=1.0, beta=0.5, gamma=0.2, delta=0.1):
    """R = alpha*GMV + beta*CM2 + gamma*STRAT + delta*CLICKS"""
    return alpha * gmv + beta * cm2 + gamma * strat + delta * clicks

# Strategy A (GMV-focused): gmv=120, cm2=15, strat=1, clicks=3
# Strategy B (Balanced):      gmv=100, cm2=35, strat=3, clicks=4
R_A = compute_reward(120, 15, 1, 3) # = 128.00
R_B = compute_reward(100, 35, 3, 4) # = 118.50
```

Strategy	GMV	CM2	STRAT	CLICKS	Reward
A (GMV-focused)	120	15	1	3	128.00
B (Balanced)	100	35	3	4	118.50

Wait—Strategy A won? With profitability-focused weights ($\alpha = 0.5, \beta = 1.0, \gamma = 0.5, \delta = 0.1$), the result flips: Strategy A scores 75.80, Strategy B scores **86.90**. The optimal strategy depends on business weights—this is a multi-objective tradeoff, not a fixed optimization. See **Lab 1.3–1.4** for full implementations and weight sensitivity analysis.

Revenue-per-click diagnostic (clickbait detection): Strategy A gets fewer clicks (3 vs 4) but 60% higher GMV per click (EUR 40 vs EUR 25)—*quality over quantity*. The metric $RPC = GMV/CLICKS$ monitors for clickbait: if RPC drops while CTR rises, reduce δ immediately. See **Lab 1.5** for the full implementation with alerting thresholds.

The bound $\delta/\alpha = 0.10$ is at the upper limit. We recommend starting with $\delta/\alpha = 0.05$ and monitoring RPC over time. If RPC degrades, the agent has learned to exploit the engagement term.

Code \$\leftarrow\$ Simulator

The minimal example above mirrors the simulator's reward path. In production, `RewardConfig` (`MOD-zoosim.config`) in `zoosim/core/config.py` holds the business weights, and `compute_reward` (`MOD-zoosim.reward`) in `zoosim/dynamics/reward.py` implements (1.2) aggregation with a detailed breakdown. Keeping these constants in configuration avoids magic numbers in code and guarantees reproducibility across experiments.

RPC monitoring (for production deployment): Log $RPC_t = \sum_{i=1}^t GMV_i / \sum_{i=1}^t CLICKS_i$ as a running average per Section 1.2.1. Alert if RPC drops $> 10\%$ below baseline. See Chapter 10 (Robustness) for drift detection and automatic δ adjustment.

Key observation: The **optimal strategy depends on business weights** $(\alpha, \beta, \gamma, \delta)$. This is not a fixed optimization problem—it's a **multi-objective tradeoff** that requires careful calibration. In practice, these weights are set by business stakeholders, and the RL system must respect them.

2.3 1.3 The Context Problem: Why Static Boosts Fail

Current production systems use **fixed boost weights** $\mathbf{w}_{\text{static}}$ for all queries. Let's see why this fails.

2.3.1 Experiment: User Segment Heterogeneity

Simulate two user types with different preferences. See `zoosim/dynamics/behavior.py` for the production click/abandonment model; the toy model in **Lab 1.6** is simplified for exposition.

Code \$\leftarrow\$ Behavior (production click model)

Production (`MOD-zoosim.behavior`, concept CN-ClickModel) implements an examination–click–purchase process with position bias:

- Click probability: `click_prob = sigmoid(utility)` in `zoosim/dynamics/behavior.py`
- Position bias: `_position_bias()` using `BehaviorConfig.pos_bias` in `zoosim/core/config.py`
- Purchase: `sigmoid(buy_logit)` in `zoosim/dynamics/behavior.py`

Chapter 2 formalizes click models and position bias; Chapter 5 connects these to off-policy evaluation.

Experiment results (full implementation: **Lab 1.6** in `exercises_labs.md`):

With static discount boost $w = 2.0$, user segments respond dramatically differently:

User Type	Expected Clicks	Relative Performance
Price hunter	0.997	Baseline
Premium shopper	0.428	57% fewer clicks

Analysis: The static weight is **over-optimized for price hunters** and **under-performs for premium shoppers**. Ideally, we'd adapt per segment: price hunters get $w_{\text{discount}} \approx 2.0$, premium shoppers get $w_{\text{discount}} \approx 0.5$. But production systems use **one global \mathbf{w}** —this is wasteful.

Note (Toy vs. Production Models): The toy model uses linear utility and multiplicative position bias. Production uses sigmoid probabilities, calibrated position bias from `BehaviorConfig`, and an examination–click–purchase cascade. The toy suffices to show **user heterogeneity**; Chapter 2 develops the full PBM/DBN click model with measure-theoretic foundations.

2.3.2 The Context Space

Define **context** x as the information available at ranking time:

$$x = (u, q, h, t) \in \mathcal{X} \quad (1.4)$$

where: - u : User features (segment, past purchases, location) - q : Query features (tokens, category, specificity) - h : Session history (coarse, not full trajectory—this is a bandit) - t : Time features (seasonality, day-of-week)

Key insight: The optimal boost weights $\mathbf{w}^*(x)$ should be a **function of context**. This transforms our problem from:

$$\text{Static optimization: } \max_{\mathbf{w} \in \mathbb{R}^K} \mathbb{E}_{x \sim \rho, \omega \sim P(\cdot|x, \mathbf{w})} [R(\mathbf{w}, x, \omega)] \quad (1.5)$$

to:

$$\text{Contextual optimization: } \max_{\pi: \mathcal{X} \rightarrow \mathbb{R}^K} \mathbb{E}_{x \sim \rho, \omega \sim P(\cdot | x, \pi(x))} [R(\pi(x), x, \omega)] \quad (1.6)$$

where we've made the conditioning explicit: ω is drawn **after** observing context x and choosing action $a = \pi(x)$, consistent with the causal graph $x \rightarrow a \rightarrow \omega \rightarrow R$.

This is **no longer a static optimization problem**—it's a **function learning problem**. We must learn a **policy** π that maps contexts to actions. Welcome to reinforcement learning.

2.4 1.4 Contextual Bandits: The RL Formulation

Let's formalize the RL setup. We'll start with the **single-step (contextual bandit)** framing, then preview the full MDP extension.

2.4.1 Building Intuition: Why “Bandit” Not “MDP”?

In traditional RL, an agent interacts with an environment over multiple timesteps, and actions affect future states (e.g., a robot's position determines what it can reach next). In search ranking, each query is **independent**—showing User A a certain ranking doesn't change what User B sees when they search later. There's no “state” that evolves over time within a single session. This simplification is called a **contextual bandit**: one-shot decisions conditioned on context, with no sequential dependencies.

Let's build up the components incrementally:

Context \mathcal{X} : “What do we observe before choosing boosts?” - User features: segment (price_hunter, premium, litter_heavy, pl_lover), purchase history, location - Query features: tokens, category match, query specificity - Session context: time of day, device type, recent browsing - In our pet supplies example: ($u = \text{premium}$, $q = \text{"cat food"}$, $h = \text{empty cart}$, $t = \text{evening}$)

Action \mathcal{A} : “What do we control?” - Boost weights $\mathbf{w} \in [-a_{\max}, +a_{\max}]^K$ for K features (discount, margin, private label, bestseller, recency) - Bounded to prevent catastrophic behavior: $|w_k| \leq a_{\max}$ (typically $a_{\max} \in [0.3, 1.0]$) - Continuous space—not discrete arms like classic bandits

Reward R : “What do we optimize?” - Scalar combination from (1.2): $R = \alpha \cdot \text{GMV} + \beta \cdot \text{CM2} + \gamma \cdot \text{STRAT} + \delta \cdot \text{CLICKS}$ - Stochastic—depends on user behavior ω (clicks, purchases) - Observable after each search session

Distribution ρ : “How are contexts sampled?” - Real-world query stream from users - We don't control this—contexts arrive from the environment - Must generalize across the distribution of contexts

Now we can formalize this as a mathematical object.

2.4.2 Problem Setup

Working Definition 1.4.1 (Contextual Bandit for Search Ranking).

A contextual bandit is a tuple $(\mathcal{X}, \mathcal{A}, R, \rho)$ where:

1. **Context space** $\mathcal{X} \subset \mathbb{R}^{d_x}$: Compact space of user-query features (see DEF-1.1.0, EQ-1.4)
2. **Action space** $\mathcal{A} = [-a_{\max}, +a_{\max}]^K \subset \mathbb{R}^K$: Compact set of bounded boost weights
3. **Reward function** $R : \mathcal{X} \times \mathcal{A} \times \Omega \rightarrow \mathbb{R}$: Measurable in ω , integrable (see EQ-1.2, Standing Assumption)
4. **Context distribution** ρ : Probability measure on \mathcal{X} (the query/user arrival distribution)

This is a working definition. The measure-theoretic formalization (Borel σ -algebras on \mathcal{X} and \mathcal{A} , probability kernel $P(\omega | x, a)$, measurable policy class) appears in Chapter 2.

At each round $t = 1, 2, \dots$: - Observe context $x_t \sim \rho$ - Select action $a_t = \pi(x_t)$ (boost weights) - Rank products using score $s_i = r_{\text{ES}}(q, p_i) + a_t^\top \phi(p_i, u, q)$ - User interacts with ranking, generates outcome ω_t - Receive reward $R_t = R(x_t, a_t, \omega_t)$ - Update policy π

Objective: Maximize expected cumulative reward:

$$\max_{\pi} \mathbb{E}_{x \sim \rho, \omega} \left[\sum_{t=1}^T R(x_t, \pi(x_t), \omega_t) \right] \quad (1.7)$$

subject to constraints (1.3a-c).

Now the structure is clear: we make a **single decision** per context (choose boost weights), observe a **stochastic outcome** (user behavior), receive a **scalar reward**, and move to the next **independent context**. No sequential state transitions—that’s what makes it a “bandit” rather than a full MDP.

2.4.3 The Value Function

Define the **value** of a policy π as:

$$V(\pi) = \mathbb{E}_{x \sim \rho}[Q(x, \pi(x))] \quad (1.8)$$

where $Q(x, a) = \mathbb{E}_{\omega}[R(x, a, \omega)]$ is the **expected reward** for context x and action a . The **optimal value** is:

$$V^* = \max_{\pi} V(\pi) = \mathbb{E}_{x \sim \rho} \left[\max_{a \in \mathcal{A}} Q(x, a) \right] \quad (1.9)$$

and the **optimal policy** is:

$$\pi^*(x) = \arg \max_{a \in \mathcal{A}} Q(x, a) \quad (1.10)$$

Key observation: If we knew $Q(x, a)$ for all (x, a) , we’d simply evaluate it on a grid and pick the max. But Q is **unknown and expensive to estimate**—each evaluation requires a full search session with real users. This is the **exploration-exploitation tradeoff**:

- **Exploration:** Try diverse actions to learn $Q(x, a)$
- **Exploitation:** Use current Q estimate to maximize reward

2.4.4 Action Space Structure: Bounded Continuous

Unlike discrete bandits (finite arms), our action space $\mathcal{A} = [-a_{\max}, +a_{\max}]^K$ is **continuous and bounded**. This introduces both challenges and opportunities:

Challenges: - Cannot enumerate all actions - Need continuous optimization (gradient-based or derivative-free) - Exploration is harder (infinite actions to try)

Opportunities: - Smoothness: Nearby actions have similar rewards (we hope!) - Function approximation: Learn $Q(x, a)$ as a neural network - Gradient information: If Q is differentiable in a , use $\nabla_a Q$ to find $\arg \max$

Bounded actions are critical: Without bounds, the RL agent could set $w_{\text{discount}} = 10^6$ (destroying relevance) or $w_{\text{margin}} = -10^6$ (promoting loss-leaders indefinitely). Bounds enforce **safety**:

$$|a_k| \leq a_{\max} \quad \forall k \in \{1, \dots, K\} \quad (1.11)$$

Typical range: $a_{\max} \in [0.3, 1.0]$ (determined by domain experts).

2.4.5 Implementation: Bounded Action Space

The key operation is **clipping** uncalibrated policy outputs to the bounded space \mathcal{A} :

```
import numpy as np

# Project action onto A = [-a_max, +a_max] ⊂ (full class: Lab 1.7)
def clip_action(a, a_max=0.5):
    """Enforce #EQ-1.11 bounds. Critical for safety."""
    return np.clip(a, -a_max, a_max)

# Neural policy might output unbounded values
a_bad = np.array([1.2, -0.3, 0.8, -1.5, 0.4])
a_safe = clip_action(a_bad)  # -> [0.5, -0.3, 0.5, -0.5, 0.4]
```

	Action	Before	After Clipping
a_1	1.2	0.5	
a_2	-0.3	-0.3	
a_3	0.8	0.5	
a_4	-1.5	-0.5	
a_5	0.4	0.4	

Key takeaway: Always **clip actions before applying** them to the scoring function. Neural policies can output unbounded values; we must project them onto \mathcal{A} . Align `a_max` with `SimulatorConfig.action.a_max` in `zoosim/core/config.py` to ensure consistency. See **Lab 1.7** for the full `ActionSpace` class with sampling, validation, and volume computation.

Code $\leftarrow \rightarrow$ Env (clipping)

The production simulator (`MOD-zoosim.env`) enforces (1.11)1 action space bounds at ranking time.

- Action clipping: `np.clip(..., -a_max, +a_max)` in `zoosim/envs/search_env.py:85`
- Bound parameter: `SimulatorConfig.action.a_max` in `zoosim/core/config.py:229`
- Feature standardization toggle: `standardize_features` in `zoosim/core/config.py:231` (applied in env when enabled)

Keeping examples consistent with these guards avoids silent discrepancies between notebooks and the simulator.

2.4.6 Minimal End-to-End Check: One Step in the Simulator

Tie the concepts together by running a single simulated step with a bounded action.

```
import numpy as np
from zoosim.core import config
from zoosim.envs import ZooplusSearchEnv

cfg = config.load_default_config()  # uses SimulatorConfig.seed at `zoosim/core/config.py:252`
env = ZooplusSearchEnv(cfg, seed=cfg.seed)
state = env.reset()

# Zero action of correct dimensionality; env will clip if needed (see `zoosim/envs/search_env.py:85`).
action = np.zeros(cfg.action.feature_dim, dtype=float)
_, reward, done, info = env.step(action)

print(f"Reward: {reward:.3f}, done={done}")
print("Top-k ranking indices:", info["ranking"])  # shape aligns with `SimulatorConfig.top_k`
```

This verifies the scoring path: base relevance + bounded boosts → ranking → behavior simulation → reward aggregation.

Output (representative; actual values depend on seed and config):

```
Reward: ~27.0, done=True
Top-k ranking indices: [list of cfg.top_k integers]
```

2.4.6.1 Using the Gym Wrapper For RL loops and baselines, use the Gymnasium wrapper which exposes standard `reset`/`step` and action/observation spaces consistent with configuration.

```
import numpy as np
from zoosim.core import config
from zoosim.envs import GymZooplusEnv

cfg = config.load_default_config()
env = GymZooplusEnv(cfg, seed=cfg.seed)

obs, info = env.reset()
print("obs dim:", obs.shape) # |categories| + |query_types| + |segments|

# Zero action for consistent baseline (env clips incoming actions internally as well)
action = np.zeros(cfg.action.feature_dim, dtype=float)
obs2, reward, terminated, truncated, info2 = env.step(action)

print(f"reward={reward:.3f}, terminated={terminated}, truncated={truncated}")
```

This interface is used in tests and ensures actions stay within $[-a_{\max}, +a_{\max}]^K$ with observation encoding derived from configuration.

Output (representative; actual values depend on seed and config):

```
obs dim: (11,) # |categories| + |query_types| + |segments|
reward=~27.0, terminated=True, truncated=False
```

2.5 1.5 From Optimization to Learning: Why RL?

At this point, one might ask: **Why not just optimize equation (1.6) directly?** If we can evaluate $R(a, x)$ for any (a, x) , can we not use gradient descent?

2.5.1 The Sample Complexity Bottleneck

Problem: Evaluating $R(a, x)$ requires **running a live search session**: 1. Apply boost weights a to score products 2. Show ranked results to user 3. Wait for clicks/purchases 4. Compute $R = \alpha \cdot \text{GMV} + \dots$

This is **expensive and risky**: - **Expensive**: Each evaluation takes seconds (user interaction) and costs money (potential lost sales) - **Risky**: Trying bad actions (a) can hurt user experience and revenue - **Noisy**: User behavior is stochastic—one sample has high variance

Sample complexity estimate: Suppose we have $|\mathcal{X}| = 100$ contexts (user segments \times query types), $|\mathcal{A}| = 10^5$ discretized actions (gridding $K = 5$ boost features into 10 bins each), and need $G = 10$ gradient samples per action to estimate $\nabla_a R$ with low variance.

Naive grid search: Evaluate $R(x, a)$ for all (x, a) pairs: - Cost: $|\mathcal{X}| \cdot |\mathcal{A}| = 100 \cdot 10^5 = 10^7$ search sessions - At 1 session/second, this takes **116 days**

Gradient descent: Estimate $\nabla_a R$ for one context via finite differences: - Cost per iteration: $2K \cdot G = 2 \cdot 5 \cdot 10 = 100$ sessions (forward differences in K dimensions, G samples each) - For $T = 1000$ iterations to

converge: $100 \cdot 1000 = 10^5$ sessions per context - Total: $|\mathcal{X}| \cdot 10^5 = 100 \cdot 10^5 = 10^7$ sessions (same as grid search!)

RL with exploration: Learn $Q(x, a)$ via bandits with $\sim \sqrt{T}$ regret: - Cost: $T \sim 10^4$ sessions total (across all contexts, amortized) - Wallclock: **3 hours** at 1 session/second

This **1000x speedup** is why we use RL for search ranking.

Gradient-based optimization would require: - Thousands of evaluations per context x - Directional derivatives $\nabla_a R(a, x)$ via finite differences - No safety guarantees (could try catastrophically bad a)

This is **not feasible** in production.

2.5.2 RL as Sample-Efficient, Safe Exploration

Reinforcement learning provides:

1. **Off-policy learning:** Train on historical data (past search logs) without deploying new policies
2. **Exploration strategies:** Principled methods (UCB, Thompson Sampling) that balance exploration vs. exploitation
3. **Safety constraints:** Enforce bounds (1.11) and constraints (1.3a-c) during learning
4. **Function approximation:** Learn $Q(x, a)$ or $\pi(x)$ as neural networks, generalizing across contexts
5. **Continual learning:** Adapt to distribution shift (seasonality, new products) via online updates

The RL framework transforms our problem from: - **Black-box optimization** (expensive, unsafe, no generalization)

to: - **Function learning with feedback** (sample-efficient, safe, generalizes)

2.6 1.6 Roadmap: From Bandits to Deep RL

Chapter 0 provided an informal, code-first toy example; Chapters 1–3 now build the mathematical foundations that justify and generalize it. This section provides a **roadmap through the book** (the 4-part structure and what each chapter accomplishes). For the **roadmap through this chapter** specifically, see the section headers below.

2.6.1 Part I: Foundations (Chapters 1-3)

We've established the business problem and contextual bandit formulation (Chapter 1). To evaluate policies safely without online experiments, we need **measure-theoretic foundations** for off-policy evaluation (Chapter 2: absolute continuity, Radon-Nikodym derivatives). To extend beyond bandits to multi-step sessions, we need **Bellman operators and convergence theory** (Chapter 3: contractions, fixed points).

Chapter 1 (this chapter): Formulate search ranking as contextual bandit **Chapter 2:** Probability, measure theory, and click models (position bias, abandonment) **Chapter 3:** Operators and contractions (Bellman equation, convergence)

2.6.2 Part II: Simulator (Chapters 4-5)

Before implementing RL algorithms, we need a **realistic environment** to test them. Chapters 4-5 build a production-quality simulator with synthetic catalogs, users, queries, and behavior models. This enables safe offline experimentation before deploying to real search traffic.

Chapter 4: Catalog, users, queries—generative models for realistic environments **Chapter 5:** Position bias and counterfactuals—why we need off-policy evaluation (OPE)

2.6.3 Part III: Policies (Chapters 6-8)

With a simulator, we can now develop **algorithms**: discrete template bandits (Chapter 6), continuous action Q-learning (Chapter 7), and policy gradients (Chapter 8).

Hard constraint handling (feasibility filters for CM2 floors) and operational stability monitoring are treated in Chapter 10 (Guardrails); the underlying duality theory is developed in Appendix C, and the **primal--dual** optimization viewpoint is implemented in Chapter 14.

Chapter 6 develops bandits with formal regret bounds; Chapter 7 establishes convergence under realizability (but no regret guarantees for continuous actions); Chapter 8 proves the Policy Gradient Theorem and analyzes the theory-practice gap. All three provide PyTorch implementations.

Chapter 6: Discrete template bandits (LinUCB, Thompson Sampling over fixed strategies) **Chapter 7:** Continuous actions via $Q(x, a)$ regression (neural Q-functions) **Chapter 8:** Policy gradient methods (REINFORCE, PPO, theory-practice gap)

2.6.4 Part IV: Evaluation, Robustness & Multi-Episode MDPs (Chapters 9-11)

Before production deployment, we need **safety guarantees**: off-policy evaluation to test policies on historical data (Chapter 9), robustness checks and guardrails with production monitoring (Chapter 10), and the extension to multi-episode dynamics where user engagement compounds across sessions (Chapter 11).

Chapter 9: Off-policy evaluation (IPS, SNIPS, DR—how to test policies safely) **Chapter 10:** Robustness and guardrails (drift detection, stability metrics, hard feasibility filters for CM2 floors, A/B testing, monitoring) **Chapter 11:** Multi-episode MDPs (inter-session retention, hazard modeling, long-term user value)

2.6.5 The Journey Ahead

By the end of this chapter, we will: - **Prove** convergence of bandit algorithms under general conditions - **Implement** production-quality deep RL agents (NumPy/PyTorch) - **Understand** when theory applies and when it breaks (the deadly triad, function approximation divergence) - **Deploy** RL systems safely (OPE, constraints, monitoring)

Let's begin.

How to read this chapter on first pass.

Sections 1.1–1.6, 1.9, and 1.10 form the core path: they set up search as a constrained contextual bandit and explain why we use RL rather than static tuning. Sections 1.7–1.8 are advanced/optional previews of measure-theoretic foundations, the Bellman operator, and off-policy evaluation. Skim or skip these on first reading and return after Chapters 2–3.

2.7 1.7 (Advanced) Optimization Under Uncertainty and Off-Policy Evaluation

This section is optional on a first reading.

Readers primarily interested in the **contextual bandit formulation** and motivation for RL can safely skim this section and jump to §1.9 (Constraints) or Chapter 2. Here we take an early, slightly more formal look at:

- **Expected reward and well-posedness** (why the expectations we write down actually exist)
- **Off-policy evaluation (OPE)** at a *conceptual* level
- Two preview results: **existence of an optimal policy** and a **regret lower bound**

The full measure-theoretic machinery (Radon–Nikodym, conditional expectation) lives in **Chapter 2**. The full OPE toolbox (IPS, SNIPS, DR, FQE, SWITCH, MAGIC) lives in **Chapter 9**.

2.7.1 1.7.1 Expected Utility and Well-Defined Rewards

Up to now we've treated expressions like $\mathbb{E}[R(\mathbf{w}, x, \omega)]$ as if they were obviously meaningful. Let's make that explicit.

Recall the stochastic reward from section 1.2:

- Context $x \in \mathcal{X}$ (user, query, etc.)
- Action $a \in \mathcal{A}$ (boost weights \mathbf{w})
- Outcome $\omega \in \Omega$ (user behavior: clicks, purchases, abandonment)
- Reward $R(x, a, \omega) \in \mathbb{R}$ (scalarized GMV/CM2/STRAT/CLICKS)

We define the **expected utility** (Q -function) of action a in context x as

$$Q(x, a) := \mathbb{E}_{\omega \sim P(\cdot | x, a)}[R(x, a, \omega)]. \quad (1.12)$$

Here $P(\cdot | x, a)$ is the outcome distribution induced by showing the ranking determined by (x, a) in our click model.

To even *define* $Q(x, a)$, we need basic regularity conditions. These are made rigorous in Chapter 2 (Assumption 2.6.1); we preview them informally here:

Regularity conditions for well-defined rewards (informal):

1. **Measurability:** $R(x, a, \omega)$ is measurable as a function of ω .
2. **Integrability:** Rewards have finite expectation: $\mathbb{E}[|R(x, a, \omega)|] < \infty$.
3. **Coverage / overlap:** If the evaluation policy ever plays an action in a context, the logging policy must have taken that action with positive probability there. This is **absolute continuity** $\pi_{\text{eval}} \ll \pi_{\log}$, ensuring importance weights $\pi_{\text{eval}}(a | x)/\pi_{\log}(a | x)$ are finite.

Conditions (1)–(2) ensure $Q(x, a) = \mathbb{E}[R(x, a, \omega) | x, a]$ is a well-defined finite Lebesgue integral. Condition (3) is critical for **off-policy evaluation** (§1.7.2 below): when we estimate the value of a new policy using data from an old policy, we reweight observations by likelihood ratios. Absolute continuity guarantees these ratios exist (the denominator is never zero where the numerator is positive).

Continuous-action remark. Our action space $\mathcal{A} = [-a_{\max}, +a_{\max}]^K$ is continuous. In this case, $\pi_e(a | x)$ and $\pi_b(a | x)$ should be read as *densities* (Radon–Nikodym derivatives) with respect to Lebesgue measure on \mathcal{A} , and importance weights are density ratios. The coverage condition becomes a support condition: $\text{supp}(\pi_e(\cdot | x)) \subseteq \text{supp}(\pi_b(\cdot | x))$.

Chapter 2, §2.6 formalizes these conditions as **Assumption 2.6.1 (OPE Probability Conditions)** and proves that the IPS estimator is unbiased under these assumptions. For now, note that our search setting satisfies all three: rewards are bounded (GMV and CM2 are finite), and we'll use exploration policies (e.g., ε -greedy with $\varepsilon > 0$) that ensure coverage.

2.7.2 1.7.2 The Offline Evaluation Problem (Toy Cat-Food Example)

In §1.4 we defined the value of a policy π as

$$V(\pi) = \mathbb{E}_{x \sim \rho, \omega}[R(x, \pi(x), \omega)], \quad (1.7a)$$

where ρ is the context distribution (query/user stream).

So far we implicitly assumed we can just *deploy* any candidate policy π to estimate $V(\pi)$ online:

1. Pick boost weights $a = \pi(x)$.

2. Show ranking to users.
3. Observe reward $R(x, a, \omega)$.
4. Average over many sessions.

In a real search system, this is often **too risky**:

- Every exploratory policy hits **GMV** and **CM2**.
- It affects **real users** and competes with other experiments.
- It may violate **constraints** (CM2 floor, rank stability, strategic exposure).

This is where **off-policy evaluation (OPE)** enters:

Can we estimate $V(\pi_e)$ for a new evaluation policy π_e using only logs collected under an old behavior policy π_b ?

Formally, suppose we have a log

$$\mathcal{D} = (x_i, a_i, r_i)_{i=1}^n,$$

where $x_i \sim \rho$, $a_i \sim \pi_b(\cdot | x_i)$, and $r_i = R(x_i, a_i, \omega_i)$.

A **naïve idea** is to just average rewards in the logs:

$$\hat{V}_{\text{naive}} := \frac{1}{n} \sum_{i=1}^n r_i.$$

This clearly estimates $V(\pi_b)$, not $V(\pi_e)$.

2.7.2.1 Toy example: two cat-food templates Take a single query type “cat food” and two ranking templates:

- a_{GMV} — aggressive discount boosts (high GMV, risky CM2),
- a_{SAFE} — conservative boosts (lower GMV, safer CM2).

Consider:

- Logging policy π_b : always uses a_{SAFE} ,
- Evaluation policy π_e : would always use a_{GMV} .

The log contains n sessions:

$$\mathcal{D} = (x_i, a_i, r_i)_{i=1}^n, \quad a_i \equiv a_{\text{SAFE}}.$$

The empirical average

$$\hat{V}_{\text{naive}} = \frac{1}{n} \sum_{i=1}^n r_i$$

tells us how good a_{SAFE} is. It tells us **nothing** about a_{GMV} , because that action was never taken: there are *no facts in the data* about what would have happened under a_{GMV} .

Key lesson: OPE cannot recover counterfactuals from **purely deterministic logging** that never explores the actions of interest.

We need a way to reuse logs from π_b while “pretending” they came from π_e . That is exactly what **importance sampling** does.

A tiny NumPy sketch makes this concrete:

```

import numpy as np

# Logged under  $\pi_b$ : always choose SAFE (action 0)
logged_actions = np.array([0, 0, 0, 0, 0])
logged_rewards = np.array([0.8, 1.1, 0.9, 1.0, 1.2]) # CM2-safe template

# New policy  $\pi_e$ : always choose GMV-heavy (action 1)
def pi_b(a):
    return 1.0 if a == 0 else 0.0 # deterministic SAFE
def pi_e(a):
    return 1.0 if a == 1 else 0.0 # deterministic GMV

naive = logged_rewards.mean()
print(f"Naive log average: {naive:.3f} (this is V(pi_b), not V(pi_e))")

```

There is *no* way to estimate what would have happened under action 1 from this dataset: the required probabilities and rewards simply do not appear.

2.7.3 1.7.3 Importance Sampling at a High Level

To estimate $V(\pi_e)$ from data generated under π_b , we reweight logged samples by how much more (or less) likely they would be under π_e .

For a logged triplet (x, a, r) , define the **importance weight**

$$w(x, a) = \frac{\pi_e(a | x)}{\pi_b(a | x)}. \quad (1.7b)$$

Intuition:

- If $\pi_e(a | x) > \pi_b(a | x)$, then $w > 1$: this sample should count **more**, because π_e would have produced it more often.
- If $\pi_e(a | x) < \pi_b(a | x)$, then $w < 1$: it should count **less**.

The **inverse propensity scoring (IPS)** estimator for the value of π_e is

$$\hat{V}_{\text{IPS}}(\pi_e) = \frac{1}{n} \sum_{i=1}^n w(x_i, a_i) \cdot r_i = \frac{1}{n} \sum_{i=1}^n \frac{\pi_e(a_i | x_i)}{\pi_b(a_i | x_i)} \cdot r_i. \quad (1.7c)$$

Under the regularity conditions (measurability, integrability) and an additional **coverage** condition (next subsection), IPS is **unbiased**: in expectation, it recovers the true value $V(\pi_e)$ from data logged under π_b . Chapter 2, §2.6 formalizes these as **Assumption 2.6.1** and proves unbiasedness rigorously.

We will:

- Prove the general change-of-measure identity behind (1.7c) in **Chapter 2** (Radon–Nikodym).
- Implement IPS, SNIPS, DR, FQE, and friends in **Chapter 9**, including variance and diagnostics.

For this chapter, the only thing to remember is:

OPE \approx “**reweight logged rewards by importance weights**.”

2.7.4 1.7.4 Coverage / Overlap and Logging Design

The formula (1.7b) only makes sense when the denominator is non-zero whenever the numerator is:

$$\pi_e(a | x) > 0 \Rightarrow \pi_b(a | x) > 0. \quad (1.7d)$$

This is the **coverage** or **overlap** condition: any action that π_e might take in context x must have been tried with *some* positive probability by π_b .

If $\pi_b(a | x) = 0$ but $\pi_e(a | x) > 0$, the weight $w(x, a)$ would be infinite. Informally:

If the logging policy never took action a in context x , the data contains **no information** about that counterfactual.

For real systems, this translates into concrete requirements: avoid fully deterministic logging (use ε -greedy or mixture policies with $\varepsilon \in [0.01, 0.10]$), store propensities $\pi_b(a | x)$ alongside each interaction, and design logging with future evaluation policies in mind—if we plan to evaluate aggressive boost strategies later, we must explore them occasionally now.

Chapter 9, §9.5 develops these requirements into a full logging protocol with formal assumptions (common support, propensity tracking), diagnostics (effective sample size), and production implementation guidance. The key intuition: **if we never explore an action, we can never evaluate it offline.**

2.7.5 1.7.5 Preview: Existence of an Optimal Policy

In §1.4 we wrote

$$\pi^*(x) = \arg \max_{a \in \mathcal{A}} Q(x, a), \quad V^* = \max_{\pi} V(\pi),$$

as if the maximizer always existed and was a nice measurable function. In continuous spaces, this is surprisingly non-trivial.

Roughly, we need:

- A **compact** and nicely behaved action space \mathcal{A} ,
- A **measurable** and upper semicontinuous $Q(x, a)$,
- A bit of measure-theory to ensure the argmax can be chosen **measurably** in x .

Existence guarantee. Under mild topological conditions (compact action space, upper semicontinuous Q), a measurable optimal policy $\pi^*(x) = \arg \max_a Q(x, a)$ exists via measurable selection theorems—see **Chapter 2, §2.8.2 (Advanced: Measurable Selection)** for the Kuratowski–Ryll–Nardzewski theorem (Theorem 2.8.3). For our search setting—where $\mathcal{A} = [-a_{\max}, a_{\max}]^K$ is a compact box and scoring functions are continuous—this guarantees the optimization problem in §1.4 is well-posed: there exists a best policy π^* , and our learning algorithms will be judged by how close they get to it.

2.7.6 1.7.6 Preview: Regret and Fundamental Limits

The last concept we preview is **regret**—how far a learning algorithm falls short of the optimal policy over time.

For a fixed policy π and the optimal policy π^* , define the **instantaneous regret** at round t :

$$\text{regret}_t = Q(x_t, \pi^*(x_t)) - Q(x_t, \pi(x_t)), \quad (1.13)$$

and the **cumulative regret** over T rounds:

$$\text{Regret}_T = \sum_{t=1}^T \text{regret}_t. \quad (1.14)$$

We say an algorithm has **sublinear regret** if

$$\lim_{T \rightarrow \infty} \frac{\text{Regret}_T}{T} = 0, \quad (1.15)$$

i.e., average per-round regret goes to zero.

Information-theoretic lower bounds for stochastic bandits establish a fundamental limit on learning speed. **Theorem 6.0** (Minimax Lower Bound) in Chapter 6 states: for any learning algorithm and any time horizon T , there exists a K -armed bandit instance such that

$$\mathbb{E}[\text{Regret}_T] \geq c\sqrt{KT}$$

for a universal constant $c > 0$. No algorithm can do better than $\Omega(\sqrt{KT})$ regret uniformly over all bandit problems. We must pay at least this price to discover which arms are good. UCB and Thompson Sampling are “optimal” because they match this bound up to logarithmic factors. For contextual bandits, the lower bound becomes $\Omega(d\sqrt{T})$ where d is the feature dimension; see Chapter 6 and **Appendix D** for the complete treatment via Fano’s inequality and the data processing inequality. Here, the message is simply:

There is a built-in price for exploration, and even the best algorithm cannot beat it asymptotically.

2.7.7 1.7.7 Where the Real Math Lives

This section deliberately kept things at a **preview** level:

- We introduced **expected utility** $Q(x, a)$ and stated regularity conditions (measurability, integrability, coverage) to make expectations like (1.12) well-posed; these are formalized in Chapter 2 as Assumption 2.6.1.
- We sketched **off-policy evaluation** via importance sampling and stressed the coverage condition (1.7d).
- We previewed two structural results: existence of an optimal policy (discussed in §1.7.5, rigorous treatment in Ch2 §2.8.2 via measurable selection) and a fundamental regret lower bound ([THM-6.0] in Chapter 6, proof via Fano’s inequality in Appendix D).

The full story is split across later chapters:

- **Chapter 2** builds the measure-theoretic foundation (probability spaces, conditional expectation, Radon–Nikodym), and proves the change-of-measure identities that justify importance weights.
- **Chapter 6** develops bandit algorithms (LinUCB, Thompson Sampling) and proves regret upper bounds that match this lower-bound rate up to logs.
- **Chapter 9** turns IPS into a full-blown OPE toolbox, with model-based and doubly-robust estimators, variance analysis, and production diagnostics.

For the rest of this chapter, only the high-level picture is needed:

We treat search as a contextual bandit with a well-defined expected reward, we will sometimes need to evaluate policies **offline** via importance weights, and there are fundamental limits on how quickly any algorithm can learn.

2.8 1.8 (Advanced) Preview: Neural Q-Functions and Bellman Operators

How do we represent $Q(x, a)$ for high-dimensional \mathcal{X} (user embeddings, query text) and continuous \mathcal{A} ? Answer: **neural networks**.

Define a parametric Q-function:

$$Q_\theta(x, a) : \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R} \quad (1.16)$$

where $\theta \in \mathbb{R}^p$ are neural network weights. We'll learn θ to approximate the true $Q(x, a)$ via **regression**:

$$\min_{\theta} \mathbb{E}_{(x, a, r) \sim \mathcal{D}} [(Q_\theta(x, a) - r)^2] \quad (1.17)$$

where \mathcal{D} is a dataset of (x, a, r) triples from past search sessions.

If the number of contexts and actions were tiny, we could represent Q as a **table** $Q[x, a]$ and fit it directly by regression on observed rewards. Chapter 7 begins with such a tabular warm-up example before moving to neural networks that can handle high-dimensional \mathcal{X} and continuous \mathcal{A} .

2.8.1 Preview: The Bellman Operator (Chapter 3)

We've focused on contextual bandits—single-step decision making where each episode terminates after one action. But what if we extended to **multi-step reinforcement learning (MDPs)**? This preview provides the vocabulary for Exercise 1.5 and sets up Chapter 3.

In an MDP, actions have consequences that ripple forward: today's ranking affects whether the user returns tomorrow, builds a cart over multiple sessions, or churns. The value function must account for **future rewards**, not just immediate payoff.

The Bellman equation for an MDP value function is:

$$V(x) = \max_a \left\{ R(x, a) + \gamma \mathbb{E}_{x' \sim P(\cdot|x, a)} [V(x')] \right\} \quad (1.18)$$

where: - $P(x'|x, a)$ is the **transition probability** to next state x' given current state x and action a - $\gamma \in [0, 1]$ is a **discount factor** (future rewards are worth less than immediate ones) - The expectation is over the stochastic next state x'

Compact notation: We can write this as the **Bellman operator** \mathcal{T} :

$$(\mathcal{T}V)(x) := \max_a \{R(x, a) + \gamma \mathbb{E}_{x'}[V(x')]\} \quad (1.19)$$

The operator \mathcal{T} takes a value function $V : \mathcal{X} \rightarrow \mathbb{R}$ and produces a new value function $\mathcal{T}V$. The optimal value function V^* is the **fixed point** of \mathcal{T} :

$$V^* = \mathcal{T}V^* \Leftrightarrow V^*(x) = \max_a \{R(x, a) + \gamma \mathbb{E}_{x'}[V^*(x')]\} \quad (1.20)$$

How contextual bandits fit: In our single-step formulation, there is **no next state**—the episode ends after one search. Mathematically, this means $\gamma = 0$ (no future) or equivalently $P(x'|x, a) = \delta_{\text{terminal}}$ (deterministic transition to a terminal state with zero value). Then:

$$V(x) = \max_a \{R(x, a) + 0 \cdot \mathbb{E}[V(x')]\} = \max_a Q(x, a)$$

This is exactly equation (1.9)! **Contextual bandits are the $\gamma = 0$ special case of MDPs**.

Why the operator formulation matters: In Chapter 3, we'll prove that \mathcal{T} is a **contraction mapping** in $\|\cdot\|_\infty$, which guarantees: 1. **Existence and uniqueness** of V^* (Banach fixed-point theorem) 2. **Convergence** of iterative algorithms: $V_{k+1} = \mathcal{T}V_k$ converges to V^* geometrically 3. **Robustness:** Small errors in R or P lead to small errors in V^*

For now, just absorb the vocabulary: **Bellman operator**, **fixed point**, **discount factor**. These are the building blocks of dynamic programming and RL theory.

Looking ahead: Chapter 11 extends our search problem to **multi-episode MDPs** where user retention and session dynamics create genuine state transitions. There, we'll need the full Bellman machinery. But for the MVP (Chapters 1-8), contextual bandits suffice.

2.9 1.9 Constraints and Safety: Beyond Reward Maximization

Real-world RL requires **constrained optimization**. Maximizing (1.2) alone can lead to: - **Negative CM2**: Promoting loss-leaders to boost GMV - **Ignoring strategic products**: Optimizing short-term revenue at the expense of long-term goals - **Rank instability**: Reordering the top-10 drastically between queries, confusing users

We enforce constraints via **Lagrangian methods** (formalism in Chapter 3 §3.6; convex duality background in Appendix C; implementation in Chapter 10) and **rank stability penalties**.

2.9.1 Lagrangian Formulation

Transform constrained problem:

$$\begin{aligned} \max_{\pi} \quad & \mathbb{E}[R(\pi(x))] \\ \text{s.t.} \quad & \mathbb{E}[\text{CM2}(\pi(x))] \geq \tau_{\text{CM2}} \\ & \mathbb{E}[\text{STRAT}(\pi(x))] \geq \tau_{\text{STRAT}} \end{aligned} \tag{1.21}$$

into unconstrained:

$$\max_{\pi} \min_{\lambda \geq 0} \mathcal{L}(\pi, \lambda) = \mathbb{E}[R(\pi(x))] + \lambda_1(\mathbb{E}[\text{CM2}] - \tau_{\text{CM2}}) + \lambda_2(\mathbb{E}[\text{STRAT}] - \tau_{\text{STRAT}}) \tag{1.22}$$

where $\lambda = (\lambda_1, \lambda_2) \in \mathbb{R}_+^2$ are Lagrange multipliers. This is a **saddle-point problem**: maximize over π , minimize over λ .

Theorem 1.9.1 (Slater's Condition, informal). If there exists at least one policy that strictly satisfies all constraints (e.g., a policy with CM2 and exposure above the required floors and acceptable rank stability), then the **Lagrangian saddle-point problem**

$$\min_{\lambda \geq 0} \max_{\pi} \mathcal{L}(\pi, \lambda)$$

is equivalent to the original constrained optimization problem: they have the same optimal value.

Interpretation. Under mild convexity assumptions, we can treat Lagrange multipliers λ as “prices” for violating constraints and search for a saddle point instead of solving the constrained problem directly. **Appendix C** proves this rigorously (Theorem C.2.1) for the contextual bandit setting using the theory of randomized policies and convex duality ((Boyd and Vandenberghe 2004)). In Chapter 14 we exploit this to implement **primal--dual** constrained RL for search: we update the policy parameters to increase reward and constraint satisfaction (primal step) while adapting multipliers that penalize violations (dual step). Chapter 10 focuses instead on the production guardrail viewpoint (monitoring and fallback) rather than optimization over multipliers.

What this tells us:

Strong duality means we can solve the constrained problem (2.9.1) by solving the unconstrained Lagrangian (1.22) — no duality gap. Practically, this justifies **primal–dual algorithms**: alternate between improving the policy (primal) and adjusting constraint penalties (dual), confident that convergence to the saddle point yields the constrained optimum.

The strict feasibility requirement ($\exists \tilde{\pi}$ with slack in the CM2 constraint) is typically easy to verify: the baseline production policy usually satisfies constraints with margin. If no such policy exists, the constraints may be infeasible—one is asking for profitability floors that no ranking can achieve. **Appendix C, §C.4.3** discusses diagnosing infeasible constraint configurations: diverging dual variables, Pareto frontiers below constraint thresholds, and ε -relaxation remedies.

Implementation preview: In **Chapter 14**, we implement constraint-aware RL using primal–dual optimization (theory in **Appendix C, §C.5**): 1. **Primal step:** $\theta \leftarrow \theta + \eta \nabla_\theta \mathcal{L}(\theta, \lambda)$ (improve policy toward higher reward and constraint satisfaction) 2. **Dual step:** $\lambda \leftarrow \max(0, \lambda - \eta' \nabla_\lambda \mathcal{L}(\theta, \lambda))$ (tighten constraints if violated, relax if satisfied)

The saddle-point (θ^*, λ^*) satisfies the Karush-Kuhn-Tucker (KKT) conditions for the constrained problem (2.9.1). For now, just note that **constraints require dual variables** λ —we’re not just learning a policy, but also learning how to trade off GMV, CM2, and strategic exposure dynamically.

2.10 1.10 Summary and Looking Ahead

We’ve established the foundation:

What we have: - **Business problem:** Multi-objective search ranking with constraints - **Mathematical formulation:** Contextual bandit with $Q(x, a)$ to learn - **Action space:** Continuous bounded $\mathcal{A} = [-a_{\max}, +a_{\max}]^K$ - **Objective:** Maximize $\mathbb{E}[R]$ subject to CM2/exposure/stability constraints - **Regret limits (preview):** Bandit algorithms incur a $\tilde{\Omega}(\sqrt{KT})$ exploration cost; later bandit chapters formalize this lower bound and show algorithms that match it up to logs - **Implementation:** Tabular Q-table (baseline), preview of neural Q-function - **OPE foundations (conceptual):** Why absolute continuity and importance sampling matter for safe policy evaluation (full measure-theoretic treatment in Chapters 2 and 9)

What we need: - **Probability foundations** (Chapter 2): Measure theory for OPE reweighting; position bias models (PBM/DBN) for realistic user simulation; counterfactual reasoning to test “what if?” scenarios safely - **Convergence theory** (Chapter 3): Bellman operators, contraction mappings, fixed-point theorems for proving algorithm correctness - **Simulator** (Chapters 4-5): Realistic catalog/user/query/behavior models that mirror production search environments - **Algorithms** (Chapters 6-8): LinUCB, neural bandits, Lagrangian constraints for safe exploration and constrained optimization - **Evaluation** (Chapter 9): Off-policy evaluation (IPS, SNIPS, DR) for testing policies before deployment - **Deployment** (Chapters 10-11): Robustness, A/B testing, production ops for real-world systems

For Readers with Control Theory Background. Readers familiar with LQR, HJB equations, or optimal control will find **Appendix B** provides a detailed bridge to RL: we show how the discrete Bellman equation arises as a discretization of HJB, how policy gradients relate to Riccati solutions, and how Lyapunov analysis informs convergence proofs. That appendix also traces the lineage from classical control to modern deep RL algorithms (DDPG, PPO, SAC). Readers new to control theory may skip it for now and return when these connections appear in Chapters 8, 10, and 11.

2.10.1 Why Chapter 2 Comes Next

We’ve formulated search ranking as contextual bandits, but left two critical gaps unresolved:

1. **User behavior is a black box.** Section 1.3’s illustrative click model (position bias = $1/k$) was helpful pedagogically, but production search requires **rigorous click models** that capture examination, clicks, purchases, and abandonment. We need to formalize “How do users interact with rankings?” at the

level of **probability measures and stopping times**, not heuristics. Without this, our simulator won't reflect real user behavior, and algorithms trained in simulation will fail in production.

2. **We can't afford online-only learning.** Evaluating each policy candidate with real users (Section 1.5's "sample complexity bottleneck") is too expensive and risky. We need **off-policy evaluation (OPE)** to test policies on historical data logged under old policies. But OPE requires reweighting probabilities across different policies (importance sampling)—the weights $w(x, a) = \pi_{\text{eval}}(a|x)/\pi_{\log}(a|x)$ are only well-defined when both policies are absolutely continuous w.r.t. a common measure (the **coverage condition** in **Assumption 2.6.1** of Chapter 2, §2.6). This is **measure theory**, and it's not optional.

Chapter 2 addresses both gaps: We'll build **position-biased click models (PBM/DBN)** that mirror real user behavior with examination, relevance-dependent clicks, and session abandonment. Then we'll develop the **measure-theoretic foundations** (Radon-Nikodym derivatives, change of measure, importance sampling) that make OPE sound. This is not abstract mathematics for its own sake—it's the **foundation of safe RL deployment**.

By the end of Chapter 2, we will be able to:

- Simulate realistic user sessions with position bias and abandonment
- Formalize "what would have happened if we'd shown a different ranking?" (counterfactuals)
- Understand why naive off-policy estimates are biased and how to correct them

Let's build.

2.11 Exercises

Note. Readers who completed Chapter 0's toy bandit experiment should: (i) compare the regret curves from Exercise 0.3 to the $\tilde{\Omega}(\sqrt{KT})$ lower bound discussed in §1.7.6 (and revisited in Chapter 6); (ii) restate the Chapter 0 environment in this chapter's notation by identifying $(\mathcal{X}, \mathcal{A}, \rho, R)$.

Companion files for Chapter 1:

- Labs and tasks: `docs/book/ch01/exercises_labs.md`
- Written solutions: `docs/book/ch01/ch01_lab_solutions.md`
- Runnable reference implementation: `scripts/ch01/lab_solutions.py`
- Regression tests for chapter snippets: `tests/ch01/test_reward_examples.py`

Production Checklist (Chapter 1)

- **Seed deterministically:** `SimulatorConfig.seed` in `zoosim/core/config.py:252` and module-level RNGs.
- **Align action bounds:** `SimulatorConfig.action.a_max` in `zoosim/core/config.py:229`; examples should respect the same value.
- **Use config-driven weights:** `RewardConfig` for $(\alpha, \beta, \gamma, \delta)$; avoid hard-coded numbers.
- **Validate engagement weight:** Assert $\delta/\alpha \in [0.01, 0.10]$ in `zoosim/dynamics/reward.py:56` (see Section 1.2.1).
- **Monitor RPC:** Log $\text{RPC}_t = \sum \text{GMV}_i / \sum \text{CLICKS}_i$; alert if drops > 10% (clickbait detection).
- **Enforce constraints early:** Use hard feasibility filters for CM2 and exposure floors (Chapter 10, Exercise 10.3), or use Lagrange multipliers with `primal--dual` updates when optimizing under constraints (Appendix C; Chapter 14).
- **Ensure reproducible ranking:** Enable `ActionConfig.standardize_features` in `zoosim/core/config.py:231`.

Exercise 1.1 (Reward Function Sensitivity). [20 min] (a) Implement equation (1.2) with $(\alpha, \beta, \gamma, \delta) = (1, 0, 0, 0)$ (GMV-only) and $(0.3, 0.6, 0.1, 0)$ (profit-focused). Generate 1000 random outcomes and plot the reward distributions. (b) Compute the correlation between GMV and CM2 in the simulated data. Are they aligned or conflicting? (c) Find business weights that make the two strategies from Section 1.2 achieve equal reward.

Exercise 1.2 (Action Space Geometry). [30 min] (a) For $K = 2$ and $a_{\max} = 1$, plot the action space \mathcal{A} as a square $[-1, 1]^2$. (b) Sample 1000 random actions uniformly. How many are within the ℓ_2 ball $\|a\|_2 \leq 1$? (c) Modify `ActionSpace.sample()` to sample from the ℓ_∞ ball (current) vs. the ℓ_2 ball. Does this change the coverage of boost strategies?

Exercise 1.3 (Regret Bounds). [extended: 45 min] (a) Implement a naive **uniform exploration** policy that samples $a_t \sim \text{Uniform}(\mathcal{A})$ for T rounds. (b) Assume true $Q(x, a) = \mathbf{1}^\top x + \mathbf{1}^\top a + \epsilon$ where $\mathbf{1}^\top v := \sum_i v_i$ denotes the sum of components of vector v , and $\epsilon \sim \mathcal{N}(0, 0.1)$. Compute empirical regret Regret_T for $T = 100, 1000, 10000$. (c) Verify that $\text{Regret}_T/T \rightarrow \Delta$ where $\Delta = \max_a Q(x, a) - \mathbb{E}_a[Q(x, a)]$ (constant regret rate—suboptimal!). (d) **Challenge:** Implement ε -greedy (with $\varepsilon = 0.1$) and compare regret curves. Does it achieve sublinear regret?

Exercise 1.4 (Constraint Feasibility). [30 min] (a) Generate synthetic outcomes where CM2 is correlated with GMV: $CM2 = 0.25 \cdot GMV + \text{noise}$. (b) Find the minimum CM2 floor τ_{CM2} such that $\geq 90\%$ of sampled actions satisfy the constraint. (c) Plot the **Pareto frontier**: GMV vs. CM2 for different action distributions. Is it convex?

Exercise 1.5 (Bellman Equation for Bandits). [20 min] Show that the contextual bandit value function (equation 1.9) satisfies:

$$V(x) = \max_a Q(x, a) = \max_a \mathbb{E}_\omega[R(x, a, \omega)]$$

Prove this is a special case of the Bellman optimality equation:

$$V(x) = \max_a \{R(x, a) + \gamma \mathbb{E}_{x'}[V(x')]\}$$

when $\gamma = 0$ (no future states). What happens if $\gamma > 0$?

Hint for MDP extension: In the MDP Bellman equation, the term $\gamma \mathbb{E}_{x'}[V(x')]$ represents expected future value starting from next state x' (sampled from transition dynamics $P(x' | x, a)$). For contextual bandits, there is no next state—the episode terminates after one action. Setting $\gamma = 0$ eliminates future rewards, reducing to the bandit case. When $\gamma > 0$, we get multi-step RL with inter-session dynamics (Chapter 11).

Next Chapter: We'll develop the **measure-theoretic foundations** needed for off-policy evaluation, position bias models, and counterfactual reasoning.

3 Chapter 2 — Probability, Measure, and Click Models

Vlad Prytula

3.1 2.1 Motivation: Why Search Needs Measure Theory

This chapter develops the measure-theoretic probability framework— σ -algebras, measurable spaces, and Radon–Nikodym derivatives—that underlies off-policy evaluation (OPE) and, more broadly, reinforcement learning on general state and action spaces.

A natural question is why such machinery is needed for ranking. The answer is that OPE is a change-of-measure argument. When we compute an importance weight

$$w_t = \frac{\pi(a | x)}{\mu(a | x)},$$

we are computing a Radon–Nikodym derivative. On continuous representations (e.g., embeddings), point probabilities are typically zero, so ratios must be defined at the level of measures, not by naive counting. The purpose of this chapter is to make these ratios and expectations mathematically well-defined so that later estimators are theorems rather than heuristics.

The attribution puzzle. Consider a simple question: *What is the probability that a user clicks on the third-ranked product?*

In Chapter 0's toy simulator, we answered this with a lookup table: position 3 gets examination probability 0.7, product quality determines click probability given examination. In Chapter 1, we formalized rewards as expectations over stochastic outcomes ω . But we haven't yet made the **probability space** rigorous.

When the outcome space stops being finite — for example, **continuous** state/features (user embeddings $u \in \mathbb{R}^d$, product features $p \in \mathbb{R}^f$) or **infinite-horizon trajectories** in an RL formulation $(S_0, A_0, R_0, S_1, A_1, R_1, \dots)$ — the “probability = number of favourable outcomes \div number of possible outcomes” story breaks down. Naive counting no longer works; we need:

1. **Measure-theoretic probability** on general spaces
2. **Lebesgue integrals / expectations** to define values and policy gradients
3. **Product σ -algebras** to talk about probabilities on trajectories, stopping times, etc.
4. **Radon–Nikodym derivatives** for importance sampling and off-policy evaluation

The click model problem. Search systems must answer: *Given a ranking $\pi = (p_1, \dots, p_M)$, what is the distribution over click patterns $C \subseteq \{1, \dots, M\}$?*

Simple models like “top result gets 50% of clicks” are empirically false. Real click behavior exhibits:
- **Position bias:** Items ranked higher are examined more often, independent of quality
- **Cascade abandonment:** Users scan top-to-bottom, stopping when they find a satisfactory result or lose patience
- **Contextual heterogeneity:** Premium users have different click propensities than price hunters

The **Position Bias Model (PBM)** and **Dynamic Bayesian Network (DBN)** formalize these patterns using probability theory on discrete outcome spaces. But to **prove** properties (unbiasedness of estimators, convergence of learning algorithms), we need measure-theoretic foundations.

Chapter roadmap. This chapter builds the probability machinery for RL in continuous spaces:

- **Section 2.2–2.3:** Probability spaces, random variables, conditional expectation (Bourbaki–Kolmogorov rigorous treatment)
- **Section 2.4:** Filtrations and stopping times (for abandonment modeling)
- **Section 2.5:** Position Bias Model (PBM) and Dynamic Bayesian Networks (DBN) for clicks
- **Section 2.6:** Propensity scoring and unbiased estimation (foundation for off-policy learning)
- **Section 2.7:** Computational verification (NumPy experiments)
- **Section 2.8:** RL bridges (MDPs, policy evaluation, OPE preview)

Why this matters for RL. Chapter 1 used $\mathbb{E}[R | W]$ informally. Now we make it precise: expectations are **Lebesgue integrals** over probability measures, with $\mathbb{E}[R | W]$ a $\sigma(W)$ -measurable random variable and regular versions $\mathbb{E}[R | W = w]$ defined when standard Borel assumptions hold. Policy gradients (Chapter 8) require interchanging ∇_θ with \mathbb{E} —justified by Dominated Convergence. Off-policy evaluation (Chapter 9) uses importance sampling—defined via Radon–Nikodym derivatives. Without this chapter's foundations, those algorithms are heuristics. With them, they are theorems.

We begin.

How much measure theory is needed? (Reading guide)

Implementation-first reading: On a first pass, it is reasonable to skim §§2.2–2.4 (measure-theoretic foundations) and return when a later chapter invokes a specific result. The algorithm-facing core is:

- **§2.5 (Click Models):** Position Bias Model and DBN—these directly parameterize user behavior in the simulator
- **§2.6 (Propensity Scoring):** Foundation for importance weighting in off-policy evaluation (Chapter 9)
- **§2.7–2.8 (Computational Verification & RL Bridges):** NumPy experiments and connections to MDP formalism

Theory-first reading: §§2.2–2.4 provide the rigorous foundations that make policy gradient interchange (Chapter 8) and Radon–Nikodym importance weights (Chapter 9) theorems rather than heuristics. The proofs there are self-contained and follow Folland's *Real Analysis* (Folland 1999).

Navigation: If σ -algebras are heavy on a first reading, begin with §2.5 and return to §§2.2–2.4 as needed.

Assumptions (probability and RL foundations)

These assumptions apply throughout this chapter. - Spaces \mathcal{S} , \mathcal{A} , contexts \mathcal{X} , and outcome spaces are standard Borel (measurable subsets of Polish spaces, i.e. separable completely metrizable topological spaces). This guarantees existence of regular conditional probabilities and measurable stochastic kernels. - Rewards are integrable: $R \in L^1$. For discounted RL with $0 \leq \gamma < 1$, assume bounded rewards (or a uniform bound on expected discounted sums) so value iteration is well-defined. - Transition and policy kernels $P(\cdot | s, a)$ and $\pi(\cdot | s)$ are Markov kernels measurable in their arguments. - Off-policy evaluation (IPS): positivity/overlap - if $\pi(a | x) > 0$ then $\mu(a | x) > 0$ for the logging policy μ .

Background: Standard Borel and Polish Spaces

Polish space: A topological space that is separable (has a countable dense subset) and completely metrizable (admits a complete metric inducing its topology). Examples: \mathbb{R}^n , separable Hilbert spaces, the space of continuous functions $C([0, 1])$, discrete countable sets.

Standard Borel space: A measurable space (X, \mathcal{B}) isomorphic (as a measurable space) to a Borel subset of a Polish space equipped with its Borel σ -algebra. Equivalently: a measurable space that “looks like” \mathbb{R} , $[0, 1]$, \mathbb{N} , or a finite set from the measure-theoretic viewpoint.

Why this matters for RL: Standard Borel spaces enjoy three crucial properties:

1. **Regular conditional probabilities exist:** $\mathbb{P}(A | X = x)$ is well-defined as a function of x
2. **Measurable selection theorems apply:** Optimal policies $\pi^*(s) = \arg \max_a Q(s, a)$ are measurable functions
3. **Disintegration of measures:** Joint distributions factor cleanly into marginals and conditionals

Without these assumptions, pathological counterexamples exist where conditional expectations are undefined or optimal policies are non-measurable. The standard Borel assumption is the “fine print” that makes RL theory work.

Reference: (Kechris 1995, chap. 12) provides the definitive treatment. For RL applications, see (Bertsekas and Shreve 1996, Appendix C).

3.2 2.2 Probability Spaces and Random Variables

We start with Kolmogorov’s axiomatization of probability (1933), the foundation for modern stochastic processes and reinforcement learning.

3.2.1 2.2.1 Measurable Spaces and σ -Algebras

Definition 2.2.1 (Measurable Space)

A **measurable space** is a pair (Ω, \mathcal{F}) where: 1. Ω is a nonempty set (the **sample space**) 2. \mathcal{F} is a σ -algebra on Ω : a collection of subsets of Ω satisfying: - $\Omega \in \mathcal{F}$ - If $A \in \mathcal{F}$, then $A^c := \Omega \setminus A \in \mathcal{F}$ (closed under complements) - If $A_1, A_2, \dots \in \mathcal{F}$, then $\bigcup_{n=1}^{\infty} A_n \in \mathcal{F}$ (closed under countable unions)

Elements of \mathcal{F} are called **measurable sets** or **events**.

Example 2.2.1 (Finite outcome spaces). If $\Omega = \{\omega_1, \dots, \omega_N\}$ is finite, the **power set** $\mathcal{F} = 2^\Omega$ (all subsets) is a σ -algebra. This suffices for tabular RL and discrete click models.

Example 2.2.2 (Borel σ -algebra on \mathbb{R}). Let $\Omega = \mathbb{R}$. The **Borel σ -algebra** $\mathcal{B}(\mathbb{R})$ is the smallest σ -algebra containing all open intervals (a, b) . This enables probability on continuous spaces (e.g., user embeddings, boost weights).

Remark 2.2.1 (Why σ -algebras?). Why not allow *all* subsets as events? Two reasons:

1. **Pathological sets exist:** On \mathbb{R} , non-measurable sets (Vitali's construction) would violate additivity axioms if assigned probability
2. **Functional analysis:** Measurable functions (next) form well-behaved vector spaces; arbitrary functions do not

The σ -algebra structure ensures probability theory is **consistent** (no contradictions) and **complete** (all natural events are measurable).

Practical anchor: importance weights

In Chapter 9 we define the importance weight as a Radon-Nikodym derivative:

$$\rho = \frac{d\mathbb{P}^\pi}{d\mathbb{P}^\mu}.$$

Existence requires absolute continuity (overlap) $\mathbb{P}^\pi \ll \mathbb{P}^\mu$. See 2.3.5 for the canonical identity behind importance weighting.

3.2.2 2.2.2 Probability Measures

Definition 2.2.2 (Probability Measure)

A **probability measure** on (Ω, \mathcal{F}) is a function $\mathbb{P} : \mathcal{F} \rightarrow [0, 1]$ satisfying: 1. **Normalization:** $\mathbb{P}(\Omega) = 1$ 2. **Non-negativity:** $\mathbb{P}(A) \geq 0$ for all $A \in \mathcal{F}$ 3. **Countable additivity** (σ -additivity): For any countable sequence of **disjoint** events $A_1, A_2, \dots \in \mathcal{F}$ (i.e., $A_i \cap A_j = \emptyset$ for $i \neq j$),

$$\mathbb{P}\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mathbb{P}(A_n).$$

The triple $(\Omega, \mathcal{F}, \mathbb{P})$ is called a **probability space**.

Example 2.2.3 (Discrete uniform distribution). Let $\Omega = \{1, 2, \dots, N\}$, $\mathcal{F} = 2^\Omega$. Define $\mathbb{P}(A) = |A|/N$ for all $A \subseteq \Omega$. This is a probability measure (verify: normalization holds, countable additivity reduces to finite additivity since Ω is finite).

Example 2.2.4 (Uniform distribution on $[0, 1]$). Let $\Omega = [0, 1]$, $\mathcal{F} = \mathcal{B}([0, 1])$ (Borel sets). Define $\mathbb{P}((a, b)) = b - a$ for intervals $(a, b) \subseteq [0, 1]$. **Carathéodory's Extension Theorem** (Folland 1999, Theorem 1.14) says that any countably additive set function defined on an algebra (here, finite unions of intervals) extends uniquely to the σ -algebra it generates. Applying it here extends \mathbb{P} uniquely to all Borel sets, giving the **Lebesgue measure** restricted to $[0, 1]$.

Remark 2.2.2 (Necessity of countable additivity). Why require *countable* additivity rather than just finite additivity? Suppose $\mathbb{P}(\{x\}) > 0$ for all $x \in [0, 1]$. Define

$$A_n = \{x \in [0, 1] : \mathbb{P}(\{x\}) \geq 1/n\}.$$

For each n , A_n must be finite: otherwise, we could extract a countable subset $\{x_1, x_2, \dots\} \subseteq A_n$ and σ -additivity would give $\mathbb{P}(\bigcup_k \{x_k\}) = \sum_k \mathbb{P}(\{x_k\}) \geq \sum_k 1/n = \infty$, contradicting $\mathbb{P}([0, 1]) = 1$. But $\bigcup_n A_n = \{x : \mathbb{P}(\{x\}) > 0\}$ is a countable union of finite sets, hence countable. Thus at most countably many singletons can have positive measure.

For $[0, 1]$ with uncountably many points, if each singleton had positive measure, some A_n would be infinite—contradiction. Thus $\mathbb{P}(\{x\}) = 0$ for all but countably many x . This is why continuous distributions require σ -additivity: it forces “most” probability mass to spread across intervals rather than accumulate at points.

RL connection. This necessity propagates to off-policy evaluation: when actions live in continuous spaces $\mathcal{A} \subseteq \mathbb{R}^d$, we cannot define importance weights as ratios of point masses. Instead, the Radon-Nikodym theorem (Section 2.3) provides density-based weights $\rho(a | x) = \pi_1(a | x)/\pi_0(a | x)$ —a direct consequence of σ -additivity enabling absolute continuity.

3.2.3 2.2.3 Random Variables

Definition 2.2.3 (Random Variable)

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and (E, \mathcal{E}) a measurable space. A function $X : \Omega \rightarrow E$ is a **random variable** if it is **(\mathcal{F} , \mathcal{E})-measurable**: for all $A \in \mathcal{E}$,

$$X^{-1}(A) := \{\omega \in \Omega : X(\omega) \in A\} \in \mathcal{F}.$$

Intuition: Pre-images of measurable sets are measurable. This ensures $\mathbb{P}(X \in A)$ is well-defined for all events $A \in \mathcal{E}$.

Example 2.2.5 (Click indicator). In a search session, let Ω represent all possible user behaviors (examination patterns, clicks, purchases). Define $X_k : \Omega \rightarrow \{0, 1\}$ by $X_k(\omega) = 1$ if user clicks on result k under outcome ω , and $X_k(\omega) = 0$ otherwise. Then X_k is a random variable (discrete codomain).

Example 2.2.6 (GMV as a random variable). Let Ω be the space of all search sessions (rankings, clicks, purchases). Define $\text{GMV} : \Omega \rightarrow \mathbb{R}_+$ by summing purchase prices. Then GMV is a non-negative real-valued random variable.

Proposition 2.2.1 (Measurability of compositions). If $X : \Omega_1 \rightarrow \Omega_2$ is $(\mathcal{F}_1, \mathcal{F}_2)$ -measurable and $f : \Omega_2 \rightarrow \Omega_3$ is $(\mathcal{F}_2, \mathcal{F}_3)$ -measurable, then $f \circ X : \Omega_1 \rightarrow \Omega_3$ is $(\mathcal{F}_1, \mathcal{F}_3)$ -measurable.

Proof. For $A \in \mathcal{F}_3$,

$$(f \circ X)^{-1}(A) = X^{-1}(f^{-1}(A)).$$

Since f is measurable, $f^{-1}(A) \in \mathcal{F}_2$. Since X is measurable, $X^{-1}(f^{-1}(A)) \in \mathcal{F}_1$. \square

Remark 2.2.3 (Inverse-image composition technique). The proof uses the inverse-image composition identity $(f \circ X)^{-1}(A) = X^{-1}(f^{-1}(A))$ and closure of σ -algebras under inverse images. This “inverse-image trick” will reappear when showing measurability of stopped processes in Section 2.4.

Remark 2.2.4 (RL preview). In RL, states S_t , actions A_t , rewards R_t are all random variables on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ induced by the policy π and environment dynamics. Measurability ensures $\mathbb{P}(R_t > r)$ is well-defined for all thresholds r .

3.2.4 2.2.4 Expectation and Integration

Definition 2.2.4 (Expectation)

Let $X : \Omega \rightarrow \mathbb{R}$ be a random variable on $(\Omega, \mathcal{F}, \mathbb{P})$. The **expectation** (or **expected value**) of X is

$$\mathbb{E}[X] := \int_{\Omega} X d\mathbb{P},$$

where the integral is the **Lebesgue integral** with respect to the probability measure \mathbb{P} . We say X is **integrable** if $\mathbb{E}[|X|] < \infty$.

Construction (standard three-step approach, from (Folland 1999, chap. 2)): 1. **Simple functions:** For $s = \sum_{i=1}^n a_i \mathbf{1}_{A_i}$ with $A_i \in \mathcal{F}$ disjoint,

$$\int_{\Omega} s d\mathbb{P} := \sum_{i=1}^n a_i \mathbb{P}(A_i).$$

2. **Non-negative functions:** For $X \geq 0$, approximate by simple functions $s_n \uparrow X$:

$$\int_{\Omega} X d\mathbb{P} := \sup_n \int_{\Omega} s_n d\mathbb{P}.$$

3. **General functions:** Decompose $X = X^+ - X^-$ where $X^+ = \max(X, 0)$, $X^- = \max(-X, 0)$:

$$\int_{\Omega} X d\mathbb{P} := \int_{\Omega} X^+ d\mathbb{P} - \int_{\Omega} X^- d\mathbb{P}$$

provided both integrals are finite.

Example 2.2.7 (Finite sample space). Let $\Omega = \{\omega_1, \dots, \omega_N\}$ with $\mathbb{P}(\{\omega_i\}) = p_i$. Then

$$\mathbb{E}[X] = \sum_{i=1}^N X(\omega_i) p_i.$$

This is the familiar discrete expectation formula.

Example 2.2.8 (Continuous uniform on $[0, 1]$). Let $X(\omega) = \omega$ for $\omega \in [0, 1]$ with Lebesgue measure. Then

$$\mathbb{E}[X] = \int_0^1 x dx = \frac{1}{2}.$$

Theorem 2.2.2 (Linearity of Expectation)

If X, Y are integrable random variables and $\alpha, \beta \in \mathbb{R}$, then $\alpha X + \beta Y$ is integrable and

$$\mathbb{E}[\alpha X + \beta Y] = \alpha \mathbb{E}[X] + \beta \mathbb{E}[Y].$$

Proof. This follows from linearity of the Lebesgue integral (Folland 1999, Proposition 2.12). \square

Remark 2.2.5 (Linearity via simple-function approximation). The mechanism is the linearity of the Lebesgue integral, proved by reducing non-negative functions to increasing simple-function approximations and extending to integrable functions via $X = X^+ - X^-$. Naming the technique clarifies that no independence assumptions are needed—linearity is purely measure-theoretic.

Theorem 2.2.3 (Monotone Convergence Theorem)

Let $0 \leq X_1 \leq X_2 \leq \dots$ be a non-decreasing sequence of non-negative random variables with $X_n \rightarrow X$ pointwise. Then

$$\mathbb{E}[X] = \lim_{n \rightarrow \infty} \mathbb{E}[X_n].$$

Proof. Direct application of the Monotone Convergence Theorem for Lebesgue integration (Folland 1999, Theorem 2.14). \square

Remark 2.2.6 (Monotone convergence technique). The key mechanism is monotone convergence: approximate X by an increasing sequence $X_n \uparrow X$ of simple functions and pass the limit inside the integral. No domination is required; monotonicity alone suffices.

Remark 2.2.7 (Dominated convergence, informal). The **Dominated Convergence Theorem** complements monotone convergence: if $X_n \rightarrow X$ almost surely and there exists an integrable random variable Y with $|X_n| \leq Y$ for all n , then X is integrable and $\mathbb{E}[X_n] \rightarrow \mathbb{E}[X]$. Intuitively, a single integrable bound Y prevents “mass from escaping to infinity,” allowing us to interchange limit and expectation. In later chapters this justifies moving gradients or limits inside expectations when rewards or score functions are uniformly bounded.

Remark 2.2.8 (RL preview: reward expectations). In RL, the value function $V^\pi(s) = \mathbb{E}^\pi[\sum_{t=0}^{\infty} \gamma^t R_t | S_0 = s]$ is an expectation over trajectories. For this to be well-defined, we need R_t to be measurable and integrable. The Monotone Convergence Theorem 2.2.3 allows us to interchange limits and expectations when computing Bellman operator fixed points (Chapter 3).

3.2.5 2.2.5 Measurable Functions

Definition 2.2.5 (Measurable Function)

Let (E, \mathcal{E}) and (F, \mathcal{F}) be measurable spaces. A function $f : E \rightarrow F$ is **$(\mathcal{E}, \mathcal{F})$ -measurable** if for all $A \in \mathcal{F}$,

$$f^{-1}(A) := \{x \in E : f(x) \in A\} \in \mathcal{E}.$$

Remark 2.2.9 (Checking measurability via generators). If \mathcal{F} is generated by a collection \mathcal{G} (e.g., open intervals for Borel sets on \mathbb{R}), it suffices to check $f^{-1}(G) \in \mathcal{E}$ for all $G \in \mathcal{G}$.

Example 2.2.9 (Real-valued measurability). For $f : (E, \mathcal{E}) \rightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))$, measurability is equivalent to $f^{-1}((-\infty, a)) \in \mathcal{E}$ for all $a \in \mathbb{R}$.

This definition justifies the **random variable** definition (2.2.3): a random variable is simply a measurable map from (Ω, \mathcal{F}) into a codomain measurable space.

3.2.6 2.2.6 Segment Distributions (Finite Spaces)

Definition 2.2.6 (Segment distribution)

Let $\mathcal{S}_{\text{seg}} = \{s_1, \dots, s_K\}$ be a finite set of user segments equipped with the power-set σ -algebra $2^{\mathcal{S}_{\text{seg}}}$. A **segment distribution** is a probability measure \mathbb{P}_{seg} on \mathcal{S}_{seg} . Equivalently, it is a probability vector $\mathbf{p}_{\text{seg}} \in \Delta_K$ such that $\mathbb{P}_{\text{seg}}(\{s_i\}) = (\mathbf{p}_{\text{seg}})_i$ and $\sum_{i=1}^K (\mathbf{p}_{\text{seg}})_i = 1$.

Remark 2.2.10 (Simulator connection). In our simulator, \mathcal{S}_{seg} is the finite set of segment labels (e.g., `price_hunter`, `premium`), and \mathbf{p}_{seg} is sampled by `zoosim/world/users.py::sample_user`.

3.3 2.3 Conditional Probability and Conditional Expectation

Click models require **conditional probabilities**: the probability of clicking given examination, the probability of examination given position. We formalize this rigorously.

3.3.1 2.3.1 Conditional Probability Given an Event

Definition 2.3.1 (Conditional Probability)

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $B \in \mathcal{F}$ with $\mathbb{P}(B) > 0$. For any event $A \in \mathcal{F}$, the **conditional probability** of A given B is

$$\mathbb{P}(A | B) := \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}.$$

Theorem 2.3.1 (Law of Total Probability)

Let $B_1, B_2, \dots \in \mathcal{F}$ be a countable partition of Ω (disjoint events with $\bigcup_n B_n = \Omega$) such that $\mathbb{P}(B_n) > 0$ for all n . Then for any event $A \in \mathcal{F}$,

$$\mathbb{P}(A) = \sum_{n=1}^{\infty} \mathbb{P}(A | B_n) \mathbb{P}(B_n).$$

Proof.

Step 1 (Partition property): Since $\{B_n\}$ partition Ω and are disjoint,

$$A = A \cap \Omega = A \cap \left(\bigcup_{n=1}^{\infty} B_n \right) = \bigcup_{n=1}^{\infty} (A \cap B_n),$$

with the sets $A \cap B_n$ pairwise disjoint.

Step 2 (Apply σ -additivity): By countable additivity of \mathbb{P} ,

$$\mathbb{P}(A) = \mathbb{P}\left(\bigcup_{n=1}^{\infty}(A \cap B_n)\right) = \sum_{n=1}^{\infty}\mathbb{P}(A \cap B_n).$$

Step 3 (Substitute definition of conditional probability): By Definition 2.3.1, $\mathbb{P}(A \cap B_n) = \mathbb{P}(A | B_n)\mathbb{P}(B_n)$. Substituting:

$$\mathbb{P}(A) = \sum_{n=1}^{\infty}\mathbb{P}(A | B_n)\mathbb{P}(B_n).$$

□

Remark 2.3.1 (The partition technique). This proof uses the **partition technique**: decompose a complex event into disjoint cases, apply additivity, and sum. We'll use this repeatedly when analyzing click cascades (Section 2.5).

Example 2.3.1 (Click given examination). In a search session, let $E_k = \{\text{user examines result } k\}$ and $C_k = \{\text{user clicks result } k\}$. The **examination-conditioned click probability** is

$$\mathbb{P}(C_k | E_k) = \frac{\mathbb{P}(C_k \cap E_k)}{\mathbb{P}(E_k)}.$$

This is the foundation of the Position Bias Model (PBM, Section 2.5).

3.3.2 2.3.2 Conditional Expectation Given a σ -Algebra

For RL applications (policy evaluation, off-policy estimation), we need conditional expectation **with respect to a σ -algebra**, not just a single event. This is more abstract but essential.

Definition 2.3.2 (Conditional Expectation Given σ -Algebra)

Let X be an integrable random variable on $(\Omega, \mathcal{F}, \mathbb{P})$ and $\mathcal{G} \subseteq \mathcal{F}$ a sub- σ -algebra. The **conditional expectation** of X given \mathcal{G} , denoted $\mathbb{E}[X | \mathcal{G}]$, is the unique (up to \mathbb{P} -almost everywhere equality) \mathcal{G} -measurable random variable Y satisfying:

1. **Measurability:** Y is \mathcal{G} -measurable
2. **Partial averaging:** For all $A \in \mathcal{G}$,

$$\int_A Y d\mathbb{P} = \int_A X d\mathbb{P}.$$

Intuition: $\mathbb{E}[X | \mathcal{G}]$ is the “best \mathcal{G} -measurable approximation” to X . It averages X over the “unobservable” parts not captured by \mathcal{G} .

Example 2.3.2 (Trivial cases). - If $\mathcal{G} = \{\emptyset, \Omega\}$ (trivial σ -algebra), then $\mathbb{E}[X | \mathcal{G}] = \mathbb{E}[X]$ (constant function). - If $\mathcal{G} = \mathcal{F}$ (full σ -algebra), then $\mathbb{E}[X | \mathcal{G}] = X$ (no averaging).

Theorem 2.3.2 (Tower Property)

Let $\mathcal{G} \subseteq \mathcal{H} \subseteq \mathcal{F}$ be nested σ -algebras. Then

$$\mathbb{E}[\mathbb{E}[X | \mathcal{H}] | \mathcal{G}] = \mathbb{E}[X | \mathcal{G}].$$

Proof. Let $Y = \mathbb{E}[X | \mathcal{H}]$ and $Z = \mathbb{E}[X | \mathcal{G}]$. For any $A \in \mathcal{G}$, since $\mathcal{G} \subseteq \mathcal{H}$ we have

$$\int_A Y d\mathbb{P} = \int_A X d\mathbb{P} = \int_A Z d\mathbb{P}.$$

Define $W := \mathbb{E}[Y | \mathcal{G}]$. By the defining property of conditional expectation, W is the unique \mathcal{G} -measurable random variable such that $\int_A W d\mathbb{P} = \int_A Y d\mathbb{P}$ for all $A \in \mathcal{G}$. Since Z also satisfies $\int_A Z d\mathbb{P} = \int_A Y d\mathbb{P}$ for all $A \in \mathcal{G}$, uniqueness implies $W = Z$ almost surely. Hence $\mathbb{E}[\mathbb{E}[X | \mathcal{H}] | \mathcal{G}] = \mathbb{E}[X | \mathcal{G}]$. \square

Remark 2.3.3 (Tower as projection/uniqueness). The technique is the projection/uniqueness property of conditional expectation: $\mathbb{E}[\cdot | \mathcal{G}]$ is the L^1 projection onto \mathcal{G} -measurable functions characterized by matching integrals on sets in \mathcal{G} . This viewpoint will reappear in martingale proofs.

Theorem 2.3.3 (Existence and Uniqueness of Conditional Expectation)

Let $X \in L^1(\Omega, \mathcal{F}, \mathbb{P})$ and $\mathcal{G} \subseteq \mathcal{F}$ a sub- σ -algebra. Then $\mathbb{E}[X | \mathcal{G}]$ exists and is unique up to \mathbb{P} -almost sure equality.

Proof. This is a deep result from measure theory, proven via the **Radon-Nikodym Theorem** (Folland 1999, Theorem 3.8). Informally, Radon-Nikodym says that if a (finite) measure ν is absolutely continuous with respect to another measure \mathbb{P} , then there exists an integrable density h such that $\nu(A) = \int_A h d\mathbb{P}$ for all A ; we write $h = d\nu/d\mathbb{P}$. We cite this result and defer the full proof to standard references. The key idea: define a signed measure $\nu(A) = \int_A X d\mathbb{P}$ for $A \in \mathcal{G}$. This measure is absolutely continuous with respect to \mathbb{P} restricted to \mathcal{G} . The Radon-Nikodym Theorem provides the density $d\nu/d\mathbb{P}$, which is precisely $\mathbb{E}[X | \mathcal{G}]$. \square

Remark 2.3.2 (Radon-Nikodym preview). Existence and uniqueness of conditional expectations ultimately rest on the Radon-Nikodym theorem 2.3.4. The same theorem yields the importance weights used in off-policy evaluation; see 2.3.5.

Code note: In `zoosim`, the IPS estimator computes `weights` (the importance-weighted ratios) implementing the Radon-Nikodym weight from 2.3.5. If overlap fails—i.e., $\pi_0(a | x) = 0$ while $\pi_1(a | x) > 0$ —then the weight is undefined (formally infinite), and estimators based on it are ill-posed; implementations will either error or exhibit uncontrolled variance.

Theorem 2.3.4 (Radon-Nikodym)

Let μ and ν be σ -finite measures on (Ω, \mathcal{F}) with $\nu \ll \mu$ (absolute continuity: $\mu(A) = 0 \Rightarrow \nu(A) = 0$ for all $A \in \mathcal{F}$). Then there exists a non-negative measurable function $f : \Omega \rightarrow [0, \infty)$ such that for all $A \in \mathcal{F}$:

$$\nu(A) = \int_A f d\mu.$$

The function f , unique μ -a.e., is called the **Radon-Nikodym derivative** and written $f = \frac{d\nu}{d\mu}$.

Proof. See (Folland 1999, Theorem 3.8). \square

Remark 2.3.5 (Importance sampling as change of measure). Let μ and ν be probability measures on a measurable space $(\mathcal{A}, \mathcal{E})$ with $\nu \ll \mu$. For any μ -integrable function f ,

$$\int_{\mathcal{A}} f(a) \nu(da) = \int_{\mathcal{A}} f(a) \frac{d\nu}{d\mu}(a) \mu(da).$$

In off-policy evaluation, for each fixed context x we take $\mu(\cdot) := \pi_0(\cdot | x)$ (logging policy) and $\nu(\cdot) := \pi_1(\cdot | x)$ (evaluation policy). The **importance weight** is the Radon-Nikodym derivative

$$\rho(a | x) := \frac{d\pi_1(\cdot | x)}{d\pi_0(\cdot | x)}(a),$$

which reduces to the ratio $\pi_1(a | x)/\pi_0(a | x)$ in the finite-action case. Absolute continuity $\pi_1(\cdot | x) \ll \pi_0(\cdot | x)$ is exactly the overlap condition: if $\pi_1(a | x) > 0$ then $\pi_0(a | x) > 0$.

Remark 2.3.6 (Conditioning on a random variable vs a value). We write $\mathbb{E}[R | W]$ for the $\sigma(W)$ -measurable conditional expectation. When evaluating at a value w , we use a regular conditional distribution $\mathbb{P}(R \in \cdot | W = w)$ (which exists under the standard Borel assumption) and set

$$\mathbb{E}[R | W = w] := \int r d\mathbb{P}(R \in dr | W = w).$$

If w is a deterministic parameter (not a random variable), $\mathbb{E}[R \mid w]$ denotes a function of w rather than a conditional expectation in the measure-theoretic sense.

3.4 2.4 Filtrations and Stopping Times

Session abandonment in search is a **sequential stopping problem**: users scan results top-to-bottom, stopping when satisfied or losing patience. Formalizing this requires **filtrations** and **stopping times**.

3.4.1 2.4.1 Filtrations

Definition 2.4.1 (Filtration)

A **filtration** on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is a sequence of σ -algebras $\{\mathcal{F}_t\}_{t=0}^{\infty}$ satisfying:

$$\mathcal{F}_0 \subseteq \mathcal{F}_1 \subseteq \mathcal{F}_2 \subseteq \dots \subseteq \mathcal{F}.$$

Intuition: \mathcal{F}_t represents “information available up to time t ”. As t increases, more information is revealed.

Example 2.4.1 (Search session filtration). In a search session with M results, let \mathcal{F}_k be the σ -algebra generated by examination and click outcomes for positions $1, \dots, k$:

$$\mathcal{F}_k = \sigma(E_1, C_1, E_2, C_2, \dots, E_k, C_k).$$

At stage k , the user has seen results 1 through k ; outcomes at positions $k+1, \dots, M$ are not yet revealed.

Definition 2.4.2 (Adapted Process)

A sequence of random variables $\{X_t\}_{t=0}^{\infty}$ is **adapted** to filtration $\{\mathcal{F}_t\}$ if X_t is \mathcal{F}_t -measurable for all t .

Intuition: X_t depends only on information available up to time t (no “looking into the future”).

3.4.2 2.4.2 Stopping Times

Definition 2.4.3 (Stopping Time)

Let $\{\mathcal{F}_t\}$ be a filtration on $(\Omega, \mathcal{F}, \mathbb{P})$. A random variable $\tau : \Omega \rightarrow \mathbb{N} \cup \{\infty\}$ is a **stopping time** if for all $t \in \mathbb{N}$,

$$\{\tau \leq t\} \in \mathcal{F}_t.$$

In discrete time this is equivalent to requiring $\{\tau = t\} \in \mathcal{F}_t$ for all t .

Intuition: The event “we stop at time t ” is determined by information available **up to and including** time t . No future information is used to decide when to stop.

Example 2.4.2 (First click is a stopping time). Define

$$\tau = \min\{k \geq 1 : C_k = 1\},$$

the first position where the user clicks (or $\tau = \infty$ if no clicks). Then τ is a stopping time: $\{\tau = k\} = \{C_1 = 0, \dots, C_{k-1} = 0, C_k = 1\} \in \mathcal{F}_k$.

Example 2.4.3 (Abandonment stopping time). Model session abandonment as

$$\tau = \min\{k \geq 1 : E_k = 0\},$$

the first position the user does not examine (or $\tau = \infty$ if user examines all M results). This is a stopping time: $\{\tau = k\} = \{E_1 = 1, \dots, E_{k-1} = 1, E_k = 0\} \in \mathcal{F}_k$.

Non-Example 2.4.1 (Last click is NOT a stopping time). Define $\tau = \max\{k : C_k = 1\}$, the position of the last click. This is **not** a stopping time: to know $\{\tau = k\}$, we must verify $C_{k+1} = 0, \dots, C_M = 0$, requiring future information beyond time k .

Theorem 2.4.1 (Measurability at a Stopping Time)

If $\{X_t\}$ is adapted to $\{\mathcal{F}_t\}$ and τ is a stopping time, then X_τ (defined as $X_\tau(\omega) = X_{\tau(\omega)}(\omega)$ when $\tau(\omega) < \infty$) is measurable with respect to the stopped σ -algebra

$$\mathcal{F}_\tau := \{A \in \mathcal{F} : A \cap \{\tau \leq t\} \in \mathcal{F}_t \text{ for all } t\}.$$

Proof.

Step 1 (Reduce to Borel preimages). It suffices to show $\{X_\tau \in B\} \in \mathcal{F}_\tau$ for all Borel $B \subseteq \mathbb{R}$, since X_τ is real-valued.

Step 2 (Verify the defining condition). Fix $t \in \mathbb{N}$. We show $\{X_\tau \in B\} \cap \{\tau \leq t\} \in \mathcal{F}_t$. Decompose:

$$\{X_\tau \in B\} \cap \{\tau \leq t\} = \bigcup_{k=0}^t (\{\tau = k\} \cap \{X_k \in B\}).$$

Indeed, on $\{\tau = k\}$ we have $X_\tau = X_k$, and on $\{\tau \leq t\}$ only the indices $k \leq t$ contribute.

Step 3 (Measurability of each slice). Since τ is a stopping time, $\{\tau \leq k\} \in \mathcal{F}_k$ for each k . For $k = 0$ we have $\{\tau = 0\} = \{\tau \leq 0\} \in \mathcal{F}_0$. For $k \geq 1$,

$$\{\tau = k\} = \{\tau \leq k\} \setminus \{\tau \leq k-1\} \in \mathcal{F}_k.$$

By adaptation, $\{X_k \in B\} \in \mathcal{F}_k$. Therefore $\{\tau = k\} \cap \{X_k \in B\} \in \mathcal{F}_k \subseteq \mathcal{F}_t$ for each $k \leq t$.

Step 4 (Conclusion). The union in Step 2 is finite, hence lies in \mathcal{F}_t . Since this holds for all t , we have $\{X_\tau \in B\} \in \mathcal{F}_\tau$. \square

Remark 2.4.2 (Stopping-time measurability technique). The method slices $\{X_\tau \in B\}$ along deterministic times and uses adaptation/stopping-time properties to establish measurability on each slice. This is the **inverse-image + partition** technique, mirroring Remark 2.2.3 and Remark 2.3.1.

Remark 2.4.1 (RL preview: episodic termination). In RL, episode length is often a stopping time: $\tau = \min\{t : \text{terminal state reached}\}$. The return $G = \sum_{t=0}^\tau \gamma^t R_t$ is \mathcal{F}_τ -measurable. For infinite-horizon discounted settings, we need $\tau = \infty$ with probability 1 (continuing tasks).

3.5 2.5 Click Models for Search

We now apply probability theory to model **click behavior** in ranked search. The Position Bias Model (PBM) and Dynamic Bayesian Network (DBN) are foundational for search evaluation and off-policy learning.

3.5.1 2.5.1 The Position Bias Model (PBM)

Motivation. Empirical observation: top-ranked results receive disproportionately more clicks, **even when relevance is controlled**. A product ranked at position 1 gets 30% CTR; the same product at position 5 gets 8% CTR. This is **position bias**: users are more likely to examine top positions, independent of content quality.

Definition 2.5.1 (Position Bias Model)

Let $\pi = (p_1, \dots, p_M)$ be a ranking of M products. For each position $k \in \{1, \dots, M\}$, define: - $E_k \in \{0, 1\}$: User examines result at position k (1 = examine, 0 = skip) - $C_k \in \{0, 1\}$: User clicks on result at position k (1 = click, 0 = no click) - $\text{rel}(p_k)$: Relevance (or attractiveness) of product p_k at position k

The **Position Bias Model (PBM)** assumes:

1. Examination is position-dependent only:

$$\mathbb{P}(E_k = 1) = \theta_k,$$

where $\theta_k \in [0, 1]$ is the **examination probability** at position k , independent of the product.

2. Click requires examination and relevance:

$$C_k = E_k \cdot \text{Bernoulli}(\text{rel}(p_k)),$$

i.e.,

$$\mathbb{P}(C_k = 1 | E_k = 1) = \text{rel}(p_k), \quad \mathbb{P}(C_k = 1 | E_k = 0) = 0.$$

3. Independence across positions: Conditioned on the ranking π , the events $(E_1, C_1), (E_2, C_2), \dots$ are independent.

Click probability formula:

$$\mathbb{P}(C_k = 1) = \mathbb{P}(C_k = 1 | E_k = 1)\mathbb{P}(E_k = 1) = \text{rel}(p_k) \cdot \theta_k. \quad (2.1)$$

Example 2.5.1 (PBM parametrization). Suppose examination probabilities decay exponentially with position:

$$\theta_k = \theta_1 \cdot e^{-\lambda(k-1)}, \quad \lambda > 0.$$

For $\theta_1 = 0.9$ and $\lambda = 0.3$: - Position 1: $\theta_1 = 0.90$ - Position 2: $\theta_2 = 0.67$ - Position 3: $\theta_3 = 0.50$ - Position 5: $\theta_5 = 0.27$

A product with $\text{rel}(p) = 0.5$ gets: - At position 1: $\mathbb{P}(C_1 = 1) = 0.5 \times 0.90 = 0.45$ - At position 5: $\mathbb{P}(C_5 = 1) = 0.5 \times 0.27 = 0.135$

Same product, 3× difference in CTR due to position bias alone.

Remark 2.5.1 (Why PBM?). The independence assumption (3) is **empirically false**: users often stop after finding a satisfactory result, inducing **negative dependence** across positions. Despite this, PBM is analytically tractable and a good first-order model. The DBN model (next) relaxes independence. Note: independence is **not** required for the single-position marginal (2.1); it becomes relevant for multi-position events.

3.5.2 2.5.2 The Dynamic Bayesian Network (DBN) Model

The **cascade hypothesis** (Craswell et al. 2008): users scan top-to-bottom, clicking on attractive results, and **stopping** after a satisfactory click. This induces dependence: if position 2 is clicked and satisfies the user, positions 3– M are never examined.

Definition 2.5.2 (Dynamic Bayesian Network Model for Clicks)

For each position $k \in \{1, \dots, M\}$, define: - $E_k \in \{0, 1\}$: Examination at position k - $C_k \in \{0, 1\}$: Click at position k - $S_k \in \{0, 1\}$: User is satisfied after examining position k (1 = satisfied, stops; 0 = continues)

Convention: S_k is defined only when $E_k = 1$; by convention set $S_k = 0$ when $E_k = 0$ so the cascade is well-defined.

The **DBN cascade model** specifies:

1. Examination cascade:

$$\mathbb{P}(E_1 = 1) = 1 \quad (\text{user always examines first result}),$$

$$\mathbb{P}(E_{k+1} = 1 | E_k = 1, S_k = 0) = 1, \quad \mathbb{P}(E_{k+1} = 1 | \text{otherwise}) = 0. \quad (2.2)$$

Intuition: User examines next position if current position was examined but user is not satisfied.

2. Click given examination:

$$\mathbb{P}(C_k = 1 \mid E_k = 1) = \text{rel}(p_k), \quad \mathbb{P}(C_k = 1 \mid E_k = 0) = 0.$$

3. Satisfaction given click:

$$\mathbb{P}(S_k = 1 \mid C_k = 1) = s(p_k), \quad \mathbb{P}(S_k = 1 \mid C_k = 0) = 0,$$

where $s(p_k) \in [0, 1]$ is the **satisfaction probability** for product p_k .

4. **Abandonment:** Define stopping time

$$\tau = \min\{k : S_k = 1 \text{ or } k = M\},$$

the first position where user is satisfied (or end of list).

Key difference from PBM: Examination at position $k + 1$ depends on outcomes at position k (via S_k). This is a **Markov chain** over positions, not independent Bernoullis.

Proposition 2.5.1 (Marginal examination probability in DBN). Under the DBN model, the probability of examining position k is

$$\mathbb{P}(E_k = 1) = \prod_{j=1}^{k-1} [1 - \text{rel}(p_j) \cdot s(p_j)]. \quad (2.3)$$

Proof.

Step 1 (Base case): $\mathbb{P}(E_1 = 1) = 1$ by model definition. The formula gives $\prod_{j=1}^0 [\dots] = 1$ (empty product), so $k = 1$ holds.

Step 2 (Recursive structure): User examines position k if and only if they examined all positions $1, \dots, k-1$ without being satisfied. By EQ-2.2, $E_k = 1$ iff $E_{k-1} = 1$ and $S_{k-1} = 0$.

Step 3 (Probability of satisfaction given examination): Along the cascade, given examination at position j , satisfaction occurs iff the user clicks AND is satisfied given the click:

$$\mathbb{P}(S_j = 1 \mid E_j = 1) = \mathbb{P}(C_j = 1 \mid E_j = 1) \cdot s(p_j) = \text{rel}(p_j) \cdot s(p_j).$$

So $\mathbb{P}(S_j = 0 \mid E_j = 1) = 1 - \text{rel}(p_j) \cdot s(p_j)$.

Step 4 (Chain rule via cascade): Since examination at position k requires not being satisfied at all $j < k$:

$$\mathbb{P}(E_k = 1) = \prod_{j=1}^{k-1} \mathbb{P}(S_j = 0 \mid E_j = 1) = \prod_{j=1}^{k-1} [1 - \text{rel}(p_j) \cdot s(p_j)].$$

□

Remark 2.5.2 (Examination decay in DBN). By (2.3), examination probability **decays multiplicatively** with position. Each unsatisfactory result provides another chance to abandon. If all products have $\text{rel}(p) \cdot s(p) = 0.2$, then: - $\mathbb{P}(E_1 = 1) = 1.0$ - $\mathbb{P}(E_2 = 1) = 0.8 \cdot 0.8 = 0.64$ - $\mathbb{P}(E_5 = 1) = 0.41$

This is empirically more accurate than PBM's position-only dependence.

Remark 2.5.3 (Stopping time interpretation). The stopping position

$$\tau = \min\{k : S_k = 1 \text{ or } k = M\}$$

from Definition 2.5.2 is a stopping time with respect to the filtration $\mathcal{F}_k = \sigma(E_1, C_1, S_1, \dots, E_k, C_k, S_k)$. This connects to Section 2.4: user behavior is a stopped random process.

3.5.3 2.5.3 Comparing PBM and DBN

Trade-offs:

Property	PBM	DBN (Cascade)
Independence	Yes (positions independent)	No (cascade dependence)
Realism	Low (ignores abandonment)	High (models stopping)
Analytic tractability	High (closed-form CTR)	Medium (requires recursion)
Parameter estimation	Easy (linear regression)	Harder (EM algorithm)

When to use PBM: Offline analysis, A/B test design, approximate CTR modeling. Fast, simple, interpretable.

When to use DBN: Off-policy evaluation, counterfactual ranking, realistic simulation. More accurate but computationally expensive.

Chapter 0 connection: The toy simulator in Chapter 0 used a simplified PBM (fixed examination probabilities θ_k , independent clicks). The production simulator `zoosim` implements a richer **Utility-Based Cascade Model** (§2.5.4), configurable via `zoosim/core/config.py`. This production model reproduces PBM's marginal factorization under a parameter specialization (Proposition 2.5.4) and exhibits cascade-style dependence driven by an internal state, analogous in spirit to DBN.

Remark 2.5.5 (Limitations relative to the simulator). PBM and DBN are analytically valuable but omit mechanisms that matter in `zoosim/dynamics/behavior.py`:

- **User heterogeneity:** segment-dependent preference parameters (price, private label, category affinities)
- **Continuous internal state:** a real-valued satisfaction/patience state rather than a binary stop indicator
- **Purchases and saturation:** purchase events and hard caps (e.g., max purchases) that influence termination
- **Query-typed position bias:** different position-bias curves by query class, not a single $\{\theta_k\}$

These omissions are benign for closed-form derivations (e.g., (2.1), (2.3)) but become first-order in production evaluation and simulation.

Code \leftrightarrow Config (position bias and satisfaction)

PBM and DBN parameters map to configuration fields:

- Examination bias vectors: `BehaviorConfig.pos_bias` in `zoosim/core/config.py:180-186`
- Satisfaction dynamics: `BehaviorConfig.satisfaction_gain`, `BehaviorConfig.satisfaction_decay`, `BehaviorConfig.abandonment_threshold`, `BehaviorConfig.post_purchase_fatigue` in `zoosim/core/config.py:175-179`

Code \leftrightarrow Behavior (Stopping Times & Satisfaction)

The abstract stopping time τ from 2.4.3 is implemented concretely in the user session loop:

- **Implementation:** `zoosim/dynamics/behavior.py` inside `simulate_session`
- **The Filtration:** The loop state (current `satisfaction`, `purchase_count`) represents \mathcal{F}_t .
- **The Stopping Rule:**

```

# The stopping time tau implementation
if rng.random() > examine_prob: break      # Abandonment (PBM/DBN)
if satisfaction < abandonment_threshold: break # Satisfaction termination
if purchase_count >= purchase_limit: break    # Saturation

```

- **Integration:** The `SessionOutcome` returned is the stopped process X_τ .

3.5.4 2.5.4 The Utility-Based Cascade Model (Production Model)

The PBM and DBN models above are valuable for theoretical analysis and algorithm design, but our production simulator implements a richer model that combines the best of both paradigms with economically meaningful user preferences. This section formalizes the **Utility-Based Cascade Model** implemented in `zoosim/dynamics/behavior.py` and establishes its relationship to the textbook models.

Why formalize the production model? Without this bridge, students would learn theory (PBM/DBN) they cannot verify in the codebase, and practitioners would use code they cannot connect to guarantees. The core principle of this book—*theory and code in constant dialogue*—demands that our production simulator have rigorous mathematical foundations.

Definition 2.5.3 (Utility-Based Cascade Model)

Let user u have preference parameters $(\theta_{\text{price}}, \theta_{\text{pl}}, \theta_{\text{cat}})$ where $\theta_{\text{cat}} \in \mathbb{R}^{|\mathcal{C}|}$ encodes category affinities. For a ranking (p_1, \dots, p_M) in response to query q , define the session dynamics:

1. **Latent utility at position k :**

$$U_k = \alpha_{\text{rel}} \cdot \text{match}(q, p_k) + \alpha_{\text{price}} \cdot \theta_{\text{price}} \cdot \log(1 + \text{price}_k) + \alpha_{\text{pl}} \cdot \theta_{\text{pl}} \cdot \mathbf{1}_{\text{is_pl}(p_k)} + \alpha_{\text{cat}} \cdot \theta_{\text{cat}}(\text{cat}_k) + \varepsilon_k \quad (2.4)$$

where $\text{match}(q, p_k) = \cos(\phi_q, \phi_{p_k})$ is semantic similarity (Chapter 5), cat_k is the category of product p_k , and $\varepsilon_k \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_u^2)$ is utility noise.

2. **Click probability given examination:**

$$\mathbb{P}(C_k = 1 \mid E_k = 1, U_k) = \sigma(U_k) := \frac{1}{1 + e^{-U_k}} \quad (2.5)$$

3. **Examination probability (cascade with satisfaction):**

$$\mathbb{P}(E_k = 1 \mid \mathcal{F}_{k-1}) = \sigma(\text{pos_bias}_k(q) + \beta_{\text{exam}} \cdot S_{k-1}) \quad (2.6)$$

where $\text{pos_bias}_k(q)$ depends on query type and position, and S_{k-1} is the running satisfaction state.

4. **Satisfaction dynamics:**

$$S_k = S_{k-1} + \gamma_{\text{gain}} \cdot U_k \cdot C_k - \gamma_{\text{decay}} \cdot (1 - C_k) - \gamma_{\text{fatigue}} \cdot B_k \quad (2.7)$$

where $B_k \in \{0, 1\}$ indicates purchase at position k , and γ_{fatigue} captures post-purchase satiation.

5. **Stopping time:**

$$\tau = \min\{k : E_k = 0 \text{ or } S_k < \theta_{\text{abandon}} \text{ or } \sum_{j \leq k} B_j \geq n_{\text{max}}\} \quad (2.8)$$

The session terminates at the first position where examination fails, satisfaction drops below threshold, or the purchase limit is reached.

Why this model? The Utility-Based Cascade captures three phenomena that pure PBM and DBN miss:

- **User heterogeneity:** Different users have different price sensitivities (θ_{price}), brand preferences (θ_{pl}), and category affinities (θ_{cat}). A premium user clicks expensive items; a price hunter clicks discounts. The utility structure EQ-2.4 makes this heterogeneity explicit.

- **Satisfaction dynamics:** Unlike DBN’s binary satisfaction, our running state S_k accumulates positive utility on clicks and decays on non-clicks. This models realistic shopping fatigue: a user who sees several irrelevant results becomes less likely to continue, even if they haven’t yet clicked.
- **Purchase satiation:** The γ_{fatigue} term captures the observation that users who just bought something are less likely to continue browsing. This is economically significant for GMV optimization.

Proposition 2.5.4 (Nesting relations)

The Utility-Based Cascade Model contains PBM as a parameter specialization (at the level of per-position marginals) and, in general, induces cascade-style dependence through its internal state.

(a) PBM marginal factorization. Set $\alpha_{\text{price}} = \alpha_{\text{pl}} = \alpha_{\text{cat}} = 0$, $\sigma_u = 0$, $\beta_{\text{exam}} = 0$, $\gamma_{\text{gain}} = \gamma_{\text{decay}} = \gamma_{\text{fatigue}} = 0$, and $\theta_{\text{abandon}} = -\infty$ with $n_{\max} = \infty$ (no termination from purchases). Then for each position k ,

$$\mathbb{P}(C_k = 1) = \theta_k \cdot \text{rel}(p_k),$$

where $\theta_k := \sigma(\text{pos_bias}_k(q))$ and $\text{rel}(p_k) := \sigma(\alpha_{\text{rel}} \cdot \text{match}(q, p_k))$. This matches the PBM marginal formula (2.1) under the above identification.

(b) Cascade dependence (DBN-like mechanism). If $\beta_{\text{exam}} \neq 0$ and the state S_k evolves nontrivially, then the examination probability at position k depends on the past through S_{k-1} . In particular, in general the pairs (E_k, C_k) are not independent across positions. The DBN model is a discrete-state, hard-stopping cascade driven by a binary satisfaction variable; Definition 2.5.3 should be viewed as a smooth state-space cascade rather than a distributionally identical reduction.

Proof. For (a), under the stated specialization, Definition 2.5.3(3) yields $\mathbb{P}(E_k = 1 \mid \mathcal{F}_{k-1}) = \sigma(\text{pos_bias}_k(q)) =: \theta_k$, independent of the past. Definition 2.5.3(1) makes $U_k = \alpha_{\text{rel}} \cdot \text{match}(q, p_k)$ deterministic, hence Definition 2.5.3(2) gives $\mathbb{P}(C_k = 1 \mid E_k = 1) = \sigma(U_k) =: \text{rel}(p_k)$. Therefore $\mathbb{P}(C_k = 1) = \mathbb{P}(C_k = 1 \mid E_k = 1)\mathbb{P}(E_k = 1) = \theta_k \text{rel}(p_k)$.

For (b), Definition 2.5.3(4) implies S_{k-1} is \mathcal{F}_{k-1} -measurable and depends on prior clicks/purchases. By Definition 2.5.3(3), $\mathbb{P}(E_k = 1 \mid \mathcal{F}_{k-1})$ depends on S_{k-1} , hence on past outcomes, which induces dependence across positions. \square

Proposition 2.5.5 (Stopping Time Validity)

The stopping time τ from EQ-2.8 is a valid stopping time with respect to the natural filtration $\mathcal{F}_k = \sigma(E_1, C_1, B_1, S_1, \dots, E_k, C_k, B_k, S_k)$.

Proof. We verify that $\{\tau \leq k\} \in \mathcal{F}_k$ for all $k \geq 1$. The event $\{\tau \leq k\}$ is the union:

$$\{\tau \leq k\} = \bigcup_{j=1}^k \left(\{E_j = 0\} \cup \{S_j < \theta_{\text{abandon}}\} \cup \left\{ \sum_{\ell \leq j} B_\ell \geq n_{\max} \right\} \right).$$

Each component event at position $j \leq k$ is determined by $(E_1, \dots, E_j, C_1, \dots, C_j, B_1, \dots, B_j, S_1, \dots, S_j)$, all of which are \mathcal{F}_k -measurable for $j \leq k$. The union of \mathcal{F}_k -measurable events is \mathcal{F}_k -measurable. \square

Remark 2.5.4 (Why this proof matters). The stopping time validity ensures that the session outcome $X_\tau = (C_1, \dots, C_\tau, B_1, \dots, B_\tau)$ is a well-defined random variable on the underlying probability space. This is essential for defining rewards (Chapter 1) and value functions (Chapter 3) rigorously. Without this guarantee, the “GMV of a session” would be mathematically undefined.

Code <-> Theory (Complete Mapping for Utility-Based Cascade)

Every term in Definition 2.5.3 maps directly to `BehaviorConfig` and `behavior.py`:

Theory Symbol	Code Reference	Default Value
α_{rel}	BehaviorConfig.alpha_rel	1.0
α_{price}	BehaviorConfig.alpha_price	0.8
α_{pl}	BehaviorConfig.alpha_pl	1.2
α_{cat}	BehaviorConfig.alpha_cat	0.6
σ_u	BehaviorConfig.sigma_u	0.8
$\text{pos_bias}_k(q)$	BehaviorConfig.pos_bias[query_type_id]	
β_{exam}	hardcoded 0.2 in behavior.py:91	0.2
γ_{gain}	BehaviorConfig.satisfaction_gain	
γ_{decay}	BehaviorConfig.satisfaction_decay	
γ_{fatigue}	BehaviorConfig.post_purchase_fatigue	
θ_{abandon}	BehaviorConfig.abandonment_threshold	
n_{max}	BehaviorConfig.max_purchases	3

Implementation location: zoosim/dynamics/behavior.py:67-118 (`simulate_session` function).

We have now formalized three click models with increasing realism: PBM (§2.5.1) for analytical tractability, DBN (§2.5.2) for cascade dynamics, and the Utility-Based Cascade (§2.5.4) for production simulation. The nesting property (Proposition 2.5.4) ensures that insights from the simpler models transfer to the richer one. Next, we turn to off-policy evaluation, where all three models serve as the outcome distribution $P(\cdot | x, a)$ in importance sampling.

3.6 2.6 Unbiased Estimation via Propensity Scoring

A central challenge in RL for search: we observe clicks under a **logging policy** (current production ranking), but want to evaluate a **new policy** (candidate ranking) without deploying it. This requires **off-policy evaluation (OPE)** via **propensity scoring**.

Throughout this section, we write contexts as $x \sim \mathcal{D}$ for a distribution \mathcal{D} on \mathcal{X} , propensities as $\pi_0(a | x)$ and $\pi_1(a | x)$, and we reserve ρ for importance weights (Radon-Nikodym derivatives) as in 2.3.5.

3.6.1 2.6.1 The Counterfactual Evaluation Problem

Setup: - Logging policy π_0 generates ranking $\pi_0(x)$ for context x (user, query) - We observe outcomes $(x, \pi_0(x), C_{\pi_0(x)})$ where C is the click pattern - We want to estimate performance of **new policy** π_1 that would produce ranking $\pi_1(x)$ - **Challenge:** We never observe $C_{\pi_1(x)}$ (user didn't see π_1 's ranking)

Naive approach fails: Simply averaging rewards $R(x, \pi_0(x))$ under the logging policy does **not** estimate $\mathbb{E}[R(x, \pi_1(x))]$ because rankings differ.

Propensity scoring solution: Reweight observations by the **likelihood ratio** of policies producing the same ranking.

3.6.2 2.6.2 Propensity Scores and Inverse Propensity Scoring (IPS)

To formally define the IPS estimator and prove its unbiasedness, we first state the regularity conditions required for off-policy evaluation.

Assumption 2.6.1 (OPE Probability Conditions).

For all $(x, a) \in \mathcal{X} \times \mathcal{A}$:

1. **Measurability:** $R(x, a, \omega)$ is measurable as a function of ω .
2. **Integrability:** $\mathbb{E}[|R(x, a, \omega)|] < \infty$ (finite first moment).
3. **Overlap (policy absolute continuity):** For each context x , the evaluation policy $\pi_1(\cdot | x)$ is absolutely continuous with respect to the logging policy $\pi_0(\cdot | x)$, written $\pi_1(\cdot | x) \ll \pi_0(\cdot | x)$. In the finite-action case this is the support condition $\pi_1(a | x) > 0 \Rightarrow \pi_0(a | x) > 0$.

Conditions (1)–(2) ensure $Q(x, a) := \mathbb{E}[R(x, a, \omega) | x, a]$ is a well-defined finite expectation. Condition (3) is the **coverage** or **overlap** assumption: it guarantees that the importance weight is well-defined. In the finite-action case this weight is the ratio $\pi_1(a | x)/\pi_0(a | x)$ in (2.9); in general it is the Radon–Nikodym derivative $d\pi_1(\cdot | x)/d\pi_0(\cdot | x)$.

Remark 2.6.1a (Why overlap?). Off-policy evaluation reweights logged actions: we estimate the value of π_1 using data collected under π_0 . In the finite-action case, IPS uses the ratio $\pi_1(a | x)/\pi_0(a | x)$. For general action spaces, this ratio is replaced by the Radon–Nikodym derivative $d\pi_1(\cdot | x)/d\pi_0(\cdot | x)$. The overlap condition $\pi_1(\cdot | x) \ll \pi_0(\cdot | x)$ is exactly what guarantees that this derivative exists.

Remark 2.6.1b (Verification for our setting). In the search ranking simulator (Chapters 4–5): condition (1) holds because rewards aggregate measurable click outcomes; condition (2) holds because rewards have **finite first moments**—prices are lognormal (finite moments), purchases per session are bounded by `BehaviorConfig.max_purchases`, and click counts are bounded by `top_k`; condition (3) requires sufficient **exploration** in the logging policy—e.g., an ε -greedy policy with $\varepsilon > 0$ ensures all actions have positive probability, satisfying coverage.

Definition 2.6.1 (Propensity Score)

Let π_0 be a stochastic logging policy that produces ranking $a \in \mathcal{A}$ for context x with probability $\pi_0(a | x)$. The **propensity score** of action (ranking) a in context x is the conditional probability $\pi_0(a | x)$.

Definition 2.6.2 (Inverse Propensity Scoring Estimator)

Let $(x_1, a_1, r_1), \dots, (x_N, a_N, r_N)$ be logged data collected under policy π_0 , where $a_i \sim \pi_0(\cdot | x_i)$ and $r_i = R(x_i, a_i, \omega_i)$ is the observed reward. The **IPS estimator** for the expected reward under new policy π_1 is

$$\hat{V}_{\text{IPS}}(\pi_1) := \frac{1}{N} \sum_{i=1}^N \frac{\pi_1(a_i | x_i)}{\pi_0(a_i | x_i)} r_i. \quad (2.9)$$

Theorem 2.6.1 (Unbiasedness of IPS)

Under Assumption 2.6.1 (OPE Probability Conditions) and assuming **correct logging** (observed actions a_i are sampled from $\pi_0(\cdot | x_i)$), the IPS estimator is **unbiased**:

$$\mathbb{E}[\hat{V}_{\text{IPS}}(\pi_1)] = V(\pi_1) := \mathbb{E}_{x \sim \mathcal{D}, a \sim \pi_1(\cdot | x)}[R(x, a)].$$

Proof.

Step 1 (Expand expectation over data and outcomes): The expectation is over contexts $x_i \sim \mathcal{D}$, actions $a_i \sim \pi_0(\cdot | x_i)$, and outcomes ω drawn from the environment:

$$\mathbb{E}[\hat{V}_{\text{IPS}}(\pi_1)] = \mathbb{E}_{x \sim \mathcal{D}} \left[\mathbb{E}_{a \sim \pi_0(\cdot | x)} \left[\mathbb{E}_{\omega} \left[\frac{\pi_1(a | x)}{\pi_0(a | x)} R(x, a, \omega) | x, a \right] \right] \right].$$

Since the importance ratio depends only on (x, a) , we can take it outside the inner expectation and define the conditional mean reward $\mu(x, a) := \mathbb{E}_{\omega}[R(x, a, \omega) | x, a]$. For brevity, write $R(x, a) := \mu(x, a)$ in the steps below.

Step 2 (Rewrite inner expectation as sum): For a discrete action space,

$$\mathbb{E}_{a \sim \pi_0(\cdot|x)} \left[\frac{\pi_1(a|x)}{\pi_0(a|x)} R(x, a) \right] = \sum_a \pi_0(a|x) \cdot \frac{\pi_1(a|x)}{\pi_0(a|x)} R(x, a).$$

Step 3 (Cancel propensities):

$$= \sum_a \pi_1(a|x) R(x, a) = \mathbb{E}_{a \sim \pi_1(\cdot|x)} [R(x, a)].$$

Step 4 (Substitute into outer expectation):

$$\mathbb{E}[\hat{V}_{\text{IPS}}(\pi_1)] = \mathbb{E}_{x \sim \mathcal{D}} \left[\mathbb{E}_{a \sim \pi_1(\cdot|x)} [R(x, a)] \right] = V(\pi_1).$$

□

Remark 2.6.1 (Importance sampling mechanism). This proof is a finite-action instantiation of the Radon-Nikodym identity in 2.3.5. For each fixed context x , define $\mu(a) := \pi_0(a|x)$ and $\nu(a) := \pi_1(a|x)$ on \mathcal{A} . The weight $\rho(a|x) = d\nu/d\mu$ satisfies

$$\sum_{a \in \mathcal{A}} \rho(a|x) R(x, a) \mu(a) = \sum_{a \in \mathcal{A}} R(x, a) \nu(a),$$

which is exactly the algebra used in Steps 2-3.

Remark 2.6.2 (High variance caveat). While IPS is unbiased, it has **high variance** when π_1 and π_0 differ substantially (i.e., when $\pi_1(a|x)/\pi_0(a|x)$ is large for some (x, a)). This is the **curse of importance sampling**. Chapter 9 introduces variance-reduction techniques: **capping**, **doubly robust estimation**, and **SWITCH estimators**.

Definition 2.6.3 (Clipped IPS)

For a cap $c > 0$, the **clipped IPS** estimator is

$$\hat{V}_{\text{clip}}(\pi_1) := \frac{1}{N} \sum_{i=1}^N \min \left\{ c, \frac{\pi_1(a_i|x_i)}{\pi_0(a_i|x_i)} \right\} r_i. \quad (2.10)$$

Definition 2.6.4 (Self-normalized IPS, SNIPS)

The **SNIPS** estimator normalizes by the sum of weights:

$$\hat{V}_{\text{SNIPS}}(\pi_1) := \frac{\sum_{i=1}^N \frac{\pi_1(a_i|x_i)}{\pi_0(a_i|x_i)} r_i}{\sum_{i=1}^N \frac{\pi_1(a_i|x_i)}{\pi_0(a_i|x_i)}}. \quad (2.11)$$

Remark 2.6.5 (SNIPS properties). SNIPS reduces variance but loses unbiasedness; under mild regularity it is consistent as $N \rightarrow \infty$. Clipped IPS (2.10) trades bias for variance: for nonnegative rewards, clipping induces **negative bias** (the estimator systematically underestimates). Formal bias and consistency results, along with numerical experiments illustrating the bias-variance trade-off, live in **Chapter 9** (Off-Policy Evaluation), specifically PROP-9.6.1 and Lab 9.5.

3.6.3 2.6.3 Propensities for Ranked Lists

For search ranking, the action space \mathcal{A} consists of **permutations** of M products: $|\mathcal{A}| = M!$. Computing exact propensities $\pi_0(a|x)$ for full rankings is intractable when M is large (e.g., $M = 50 \Rightarrow 50! \approx 10^{64}$ rankings).

Position-based approximation (Plackett–Luce model): Let $w_\pi(p | x) > 0$ be a positive weight for product p under policy π in context x (for a real-valued score $s_\pi(p | x)$, a standard choice is $w_\pi(p | x) = \exp(s_\pi(p | x))$). Approximate the ranking distribution via sequential sampling. Let R_k be the set of remaining items after positions $1, \dots, k - 1$ have been chosen: $R_k := \{p : p \notin \{p_1, \dots, p_{k-1}\}\}$. Then

$$\pi(p_k | x, p_1, \dots, p_{k-1}) = \frac{w_\pi(p_k | x)}{\sum_{p \in R_k} w_\pi(p | x)}. \quad (2.12)$$

This gives propensity for full ranking $a = (p_1, \dots, p_M)$:

$$\pi(a | x) = \prod_{k=1}^M \frac{w_\pi(p_k | x)}{\sum_{p \in R_k} w_\pi(p | x)}. \quad (2.13)$$

Practical simplification (top- K propensity): Only reweight top K positions (e.g., $K = 5$), treating lower positions as fixed:

$$\pi_0^{(K)}(a | x) := \prod_{k=1}^K \frac{w_{\pi_0}(p_k | x)}{\sum_{j=k}^M w_{\pi_0}(p_j | x)}.$$

This reduces computational cost while retaining most signal (users rarely examine beyond position 5–10).

Remark 2.6.4 (Approximation bias). Plackett–Luce and top- K truncations approximate true ranking propensities and can introduce bias in IPS. Doubly robust estimators (Chapter 9) mitigate bias by combining propensity weighting with outcome models.

Counterexample 2.6.1 (Factorization bias under item-position weights). Consider two items A, B with logging scores $s_0(A) = 2, s_0(B) = 1$ and target scores $s_1(A) = 1, s_1(B) = 2$. Under Plackett–Luce,

$$\mu((A, B)) = \frac{2}{3}, \quad \mu((B, A)) = \frac{1}{3}, \quad \pi((A, B)) = \frac{1}{3}, \quad \pi((B, A)) = \frac{2}{3}.$$

Let reward R be 1 if the top item is A and 0 otherwise. The true value is $V(\pi) = \frac{1}{3}$. From these ranking probabilities, we derive item-position marginals:

$$\begin{aligned} \mu(A@1) &= \frac{2}{3}, \quad \mu(B@2) = \frac{2}{3}, \quad \mu(B@1) = \frac{1}{3}, \quad \mu(A@2) = \frac{1}{3} \\ \pi(A@1) &= \frac{1}{3}, \quad \pi(B@2) = \frac{1}{3}, \quad \pi(B@1) = \frac{2}{3}, \quad \pi(A@2) = \frac{2}{3} \end{aligned}$$

The **item-position factorization** that uses per-position marginals yields

$$\tilde{w}(A, B) = \frac{\pi(A@1)}{\mu(A@1)} \cdot \frac{\pi(B@2)}{\mu(B@2)} = \frac{1/3}{2/3} \cdot \frac{1/3}{2/3} = \frac{1}{4}, \quad \tilde{w}(B, A) = \frac{2/3}{1/3} \cdot \frac{2/3}{1/3} = 4.$$

Hence $\mathbb{E}_\mu[\tilde{w}R] = \frac{2}{3} \cdot \frac{1}{4} \cdot 1 + \frac{1}{3} \cdot 4 \cdot 0 = \frac{1}{6} \neq V(\pi) = \frac{1}{3}$. The factorization produces **biased IPS** because item-position marginals ignore the correlation structure of full rankings. List-level propensities (product of conditionals, (2.13)) avoid this pitfall.

Remark 2.6.3 (Chapter 9 preview). Off-policy evaluation in production search systems uses **clipped IPS**, **doubly robust estimators**, or **learned propensities** from logged data. The full treatment lives in Chapter 9 (Off-Policy Evaluation), with implementation in `zoosim/evaluation/ope.py`.

3.7 Computational Illustrations

We verify the theory numerically using simple Python experiments.

3.7.1 2.7.1 Simulating PBM and DBN Click Models

We generate synthetic click data under PBM and DBN models and verify that marginal probabilities match theoretical predictions.

```
import numpy as np
from typing import Tuple, List

# Set seed for reproducibility
np.random.seed(42)

# =====
# PBM: Position Bias Model
# =====

def simulate_pbm(
    relevance: np.ndarray, # relevance[k] = rel(p_k) in [0, 1]
    exam_probs: np.ndarray, # exam_probs[k] = theta_k
    n_sessions: int = 10000
) -> Tuple[np.ndarray, np.ndarray]:
    """Simulate click data under Position Bias Model (PBM).

    Mathematical correspondence: Implements Definition 2.5.1 (PBM).

    Args:
        relevance: Product relevance at each position, shape (M,)
        exam_probs: Examination probabilities theta_k, shape (M,)
        n_sessions: Number of independent sessions to simulate

    Returns:
        examinations: Binary matrix (n_sessions, M), E_k = 1 if examined
        clicks: Binary matrix (n_sessions, M), C_k = 1 if clicked
    """
    M = len(relevance)
    examinations = np.random.binomial(1, exam_probs, size=(n_sessions, M))
    clicks = examinations * np.random.binomial(1, relevance, size=(n_sessions, M))
    return examinations, clicks

# Example: 10 results with decaying examination and varying relevance
M = 10
relevance = np.array([0.9, 0.8, 0.7, 0.5, 0.6, 0.3, 0.4, 0.2, 0.3, 0.1])
theta_1 = 0.9
decay = 0.25
exam_probs = theta_1 * np.exp(-decay * np.arange(M))

print("== Position Bias Model (PBM) ===")
print(f'Relevance: {relevance}')
print(f'Examination probabilities: {exam_probs.round(3)}')

# Simulate
E_pbm, C_pbm = simulate_pbm(relevance, exam_probs, n_sessions=50000)

# Verify theoretical vs empirical CTR
theoretical_ctr = relevance * exam_probs
```

```

empirical_ctr = C_pbm.mean(axis=0)

print("\nPosition | Rel | Exam | Theory CTR | Empirical CTR | Match?")
print("-" * 65)
for k in range(M):
    match = "OK" if abs(theoretical_ctr[k] - empirical_ctr[k]) < 0.01 else "FAIL"
    print(f"{k+1:8d} | {relevance[k]:.2f} | {exam_probs[k]:.2f} | "
          f"{theoretical_ctr[k]:10.3f} | {empirical_ctr[k]:13.3f} | {match}")

# Output:
# Position | Rel | Exam | Theory CTR | Empirical CTR | Match?
# -----
#      1 | 0.90 | 0.90 |      0.810 |      0.811 | OK
#      2 | 0.80 | 0.70 |      0.560 |      0.560 | OK
#      3 | 0.70 | 0.54 |      0.378 |      0.379 | OK
#      4 | 0.50 | 0.42 |      0.210 |      0.211 | OK
#      5 | 0.60 | 0.33 |      0.198 |      0.197 | OK
# ... (positions 6-10 omitted for brevity)

# =====
# DBN: Dynamic Bayesian Network (Cascade Model)
# =====

def simulate_dbn(
    relevance: np.ndarray,           # relevance[k] = rel(p_k)
    satisfaction: np.ndarray,         # satisfaction[k] = s(p_k)
    n_sessions: int = 10000
) -> Tuple[np.ndarray, np.ndarray, np.ndarray, np.ndarray]:
    """Simulate click data under DBN cascade model.

    Mathematical correspondence: Implements Definition 2.5.2 (DBN).
    """

    Args:
        relevance: Product relevance, shape (M,)
        satisfaction: Satisfaction probability s(p), shape (M,)
        n_sessions: Number of sessions

    Returns:
        examinations: (n_sessions, M), E_k
        clicks: (n_sessions, M), C_k
        satisfied: (n_sessions, M), S_k
        stop_positions: (n_sessions,), tau (stopping time)
    """
    M = len(relevance)
    E = np.zeros((n_sessions, M), dtype=int)
    C = np.zeros((n_sessions, M), dtype=int)
    S = np.zeros((n_sessions, M), dtype=int)
    tau = np.full(n_sessions, M, dtype=int) # Default: examine all

    for i in range(n_sessions):
        for k in range(M):
            # Always examine first; cascade rule for k > 0
            if k == 0:
                E[i, k] = 1

```

```

        else:
            # Examine if previous not satisfied
            if S[i, k-1] == 0:
                E[i, k] = 1
            else:
                break # Stop cascade

        # Click given examination
        if E[i, k] == 1:
            C[i, k] = np.random.binomial(1, relevance[k])

        # Satisfaction given click
        if C[i, k] == 1:
            S[i, k] = np.random.binomial(1, satisfaction[k])
            if S[i, k] == 1:
                tau[i] = k # Stopped here
                break

    return E, C, S, tau

# Example: Same relevance, add satisfaction probabilities
satisfaction = np.array([0.6, 0.5, 0.7, 0.8, 0.6, 0.9, 0.7, 0.8, 0.9, 1.0])

print("\n\n==== Dynamic Bayesian Network (DBN Cascade) ===")
print(f'Relevance: {relevance}')
print(f'Satisfaction: {satisfaction}')

# Simulate
E_dbn, C_dbn, S_dbn, tau_dbn = simulate_dbn(relevance, satisfaction, n_sessions=50000)

# Verify examination probabilities match Proposition 2.5.1 [EQ-2.3]
def theoretical_exam_dbn(relevance, satisfaction, k):
    """Compute P(E_k = 1) using Proposition 2.5.1."""
    if k == 0:
        return 1.0
    prob = 1.0
    for j in range(k):
        prob *= (1 - relevance[j] * satisfaction[j])
    return prob

empirical_exam = E_dbn.mean(axis=0)
theoretical_exam = np.array([theoretical_exam_dbn(relevance, satisfaction, k) for k in range(M)])

print("\nPosition | Rel | Sat | Theory Exam | Empirical Exam | Match?")
print("-" * 68)
for k in range(M):
    match = "OK" if abs(theoretical_exam[k] - empirical_exam[k]) < 0.01 else "FAIL"
    print(f'{k+1:8d} | {relevance[k]:.2f} | {satisfaction[k]:.2f} | '
          f'{theoretical_exam[k]:11.3f} | {empirical_exam[k]:14.3f} | {match}')


# Output:
# Position | Rel | Sat | Theory Exam | Empirical Exam | Match?
# -----

```

```

#      1 / 0.90 / 0.60 /      1.000 /      1.000 / OK
#      2 / 0.80 / 0.50 /      0.460 /      0.460 / OK
#      3 / 0.70 / 0.70 /      0.276 /      0.277 / OK
#      4 / 0.50 / 0.80 /      0.140 /      0.140 / OK
# ... (examination decays rapidly as satisfied users stop)

# Abandonment statistics
# Note: tau is 0-based index; add 1 for position (rank)
print(f"\n\nMean stopping position (1-based): {tau_dbn.mean() + 1:.2f}")
print(f"% sessions satisfied at position 1: {(tau_dbn == 0).mean() * 100:.1f}%")
print(f"% sessions exhausting list without satisfaction: {(tau_dbn == M).mean() * 100:.1f}%")

# Output:
# Mean stopping position (1-based): 3.34
# % sessions satisfied at position 1: 48.6%
# % sessions exhausting list without satisfaction: 5.2%

```

Key observations: 1. **PBM verification:** Empirical CTR matches $\text{rel}(p_k) \cdot \theta_k$ within 0.01 (Monte Carlo error) 2. **DBN cascade:** Examination probability decays rapidly due to satisfaction-induced stopping 3. **Early satisfaction:** ~50% satisfied at position 1; only ~5% exhaust list without satisfaction

This confirms Definitions 2.5.1 (PBM) and 2.5.2 (DBN), and Proposition 2.5.1 (DBN examination formula).

Remark 2.7.1 (Confidence intervals). For Bernoulli CTR estimates with n sessions, a 95% normal approximation interval is $\hat{p} \pm 1.96\sqrt{\hat{p}(1 - \hat{p})}/n$. With $n = 50,000$, the tolerance < 0.01 used above lies within the corresponding confidence intervals.

3.7.2 2.7.2 Verifying IPS Unbiasedness

We simulate off-policy evaluation: collect data under logging policy π_0 , estimate performance of new policy π_1 using IPS, and verify unbiasedness.

```

# =====
# Off-Policy Evaluation: IPS Estimator
# =====

def simulate_context_bandit(
    n_contexts: int,
    n_actions: int,
    n_samples: int,
    pi_logging,           # Callable: pi_logging(x) returns action probs
    pi_target,            # Callable: pi_target(x) returns action probs
    reward_fn,            # Callable: reward_fn(x, a) returns mean reward
    seed: int = 42
) -> Tuple[float, float, float]:
    """Simulate contextual bandit and estimate target policy value via IPS.

```

Mathematical correspondence: Implements Theorem 2.6.1 (IPS unbiasedness).

Returns:

- true_value: True expected reward under target policy*
- ips_estimate: IPS estimate from logged data*
- naive_estimate: Naive average (biased)*

```
rng = np.random.default_rng(seed)
```

```

# Collect logged data under pi_logging
contexts = rng.integers(0, n_contexts, size=n_samples)
logged_rewards = []
importance_weights = []

for x in contexts:
    # Sample action from logging policy
    pi_log_probs = pi_logging(x)
    a = rng.choice(n_actions, p=pi_log_probs)

    # Observe reward (with noise)
    mean_reward = reward_fn(x, a)
    r = mean_reward + rng.normal(0, 0.1) # Add Gaussian noise
    logged_rewards.append(r)

    # Compute importance weight
    pi_tgt_probs = pi_target(x)
    w = pi_tgt_probs[a] / pi_log_probs[a]
    importance_weights.append(w)

# IPS estimator [EQ-2.9]
ips_estimate = np.mean(np.array(logged_rewards) * np.array(importance_weights))

# Naive estimator (biased)
naive_estimate = np.mean(logged_rewards)

# Compute true expected reward under target policy (ground truth)
true_value = 0.0
for x in range(n_contexts):
    pi_tgt_probs = pi_target(x)
    for a in range(n_actions):
        true_value += (1 / n_contexts) * pi_tgt_probs[a] * reward_fn(x, a)

return true_value, ips_estimate, naive_estimate

# Example: 5 contexts, 3 actions
n_contexts, n_actions = 5, 3

# Define reward function: action 0 good for contexts 0-1, action 2 good for contexts 3-4
def reward_fn(x, a):
    rewards = [
        [1.0, 0.3, 0.2], # context 0
        [0.9, 0.4, 0.1], # context 1
        [0.5, 0.6, 0.4], # context 2
        [0.2, 0.3, 0.9], # context 3
        [0.1, 0.2, 1.0], # context 4
    ]
    return rewards[x][a]

# Logging policy: uniform random (safe but inefficient)
def pi_logging(x):
    return np.array([1/3, 1/3, 1/3])

```

```

# Target policy: greedy (optimal action per context)
def pi_target(x):
    optimal_actions = [0, 0, 1, 2, 2] # Best action per context
    probs = np.zeros(n_actions)
    probs[optimal_actions[x]] = 1.0
    return probs

print("\n\n==== Off-Policy Evaluation: IPS Unbiasedness ===")

# Run multiple trials to estimate bias and variance
n_trials = 500
true_values = []
ips_estimates = []
naive_estimates = []

for trial in range(n_trials):
    true_val, ips_est, naive_est = simulate_context_bandit(
        n_contexts, n_actions, n_samples=1000,
        pi_logging=pi_logging, pi_target=pi_target,
        reward_fn=reward_fn, seed=trial
    )
    true_values.append(true_val)
    ips_estimates.append(ips_est)
    naive_estimates.append(naive_est)

true_value = true_values[0] # Should be constant
ips_mean = np.mean(ips_estimates)
ips_std = np.std(ips_estimates)
naive_mean = np.mean(naive_estimates)
naive_std = np.std(naive_estimates)

print(f"True target policy value: {true_value:.3f}")
print(f"\nIPS Estimator:")
print(f"  Mean: {ips_mean:.3f} (bias: {ips_mean - true_value:.4f})")
print(f"  Std: {ips_std:.3f}")
print(f"  Unbiased? {'PASS' if abs(ips_mean - true_value) < 0.02 else 'FAIL'}")
print(f"\nNaive Estimator (biased):")
print(f"  Mean: {naive_mean:.3f} (bias: {naive_mean - true_value:.4f})")
print(f"  Std: {naive_std:.3f}")
print(f"  Biased? {'PASS (expected)' if abs(naive_mean - true_value) > 0.05 else 'FAIL (unexpected)'}")

# Output:
# True target policy value: 0.820
#
# IPS Estimator:
#   Mean: 0.821 (bias: 0.0010)
#   Std: 0.087
#   Unbiased? PASS
#
# Naive Estimator (biased):
#   Mean: 0.507 (bias: -0.3130)
#   Std: 0.018
#   Biased? PASS (expected)

```

Key results: 1. **IPS is unbiased:** Mean IPS estimate \approx true value (bias < 0.01), confirming Theorem 2.6.1 2. **Naive estimator is biased:** Underestimates target policy value by ~30% (logging policy is uniform, target is greedy) 3. **Variance tradeoff:** IPS has higher variance (std = 0.087) than naive (std = 0.018) due to importance weights

This validates the theoretical unbiasedness result while illustrating the **bias-variance tradeoff:** IPS removes bias at the cost of increased variance.

Code <-> Env/Reward (session step and aggregation)

The end-to-end simulator routes theory to code: - Env step calls behavior: zoosim/envs/search_env.py:93-100 (behavior.simulate_session) - Reward aggregation per (1.2): zoosim/dynamics/reward.py:60-65 - Env returns ranking, clicks, buys: zoosim/envs/search_env.py:113-120

3.7.3 Verifying the Tower Property Numerically

We illustrate the Tower Property 2.3.2 by constructing nested σ -algebras via simple groupings and verifying

$$\mathbb{E}[\mathbb{E}[Z | \mathcal{H}] | \mathcal{G}] = \mathbb{E}[Z | \mathcal{G}]$$

numerically.

```
import numpy as np

np.random.seed(42)
N = 50_000

# Contexts and nested sigma-algebras via groupings
x = np.random.randint(0, 10, size=N)      # contexts 0..9
G = x % 2                                # coarse sigma-algebra: parity (2 groups)
H = x % 4                                # finer sigma-algebra: mod 4 (4 groups)

# Random variable Z depending on context with noise
Z = 2.0 * x + np.random.normal(0.0, 1.0, size=N)

# Compute E[Z | H] for each sample by replacing Z with the H-group mean
E_Z_given_H_vals = np.array([Z[H == h].mean() for h in range(4)])
E_Z_given_H = E_Z_given_H_vals[H]

# Left-hand side: E[E[Z | H] | G] - average E_Z_given_H within each G group
lhs = np.array([E_Z_given_H[G == g].mean() for g in range(2)])

# Right-hand side: E[Z | G] - average Z within each G group
rhs = np.array([Z[G == g].mean() for g in range(2)])

print("Group g | E[E[Z|H]|G=g] | E[Z|G=g] | Match?")
print("-" * 58)
for g in range(2):
    match = "OK" if abs(lhs[g] - rhs[g]) < 1e-2 else "FAIL"
    print(f" {g:5d} | {lhs[g]:16.4f} | {rhs[g]:14.4f} | {match}")

# Output:
# Group g | E[E[Z|H]|G=g] | E[Z|G=g] | Match?
```

```

# -----
#   0   /     8.9196 /     8.9206 /  OK
#   1   /    13.9180 /    13.9190 /  OK

```

The numerical experiment confirms the Tower Property: averaging the conditional expectation $\mathbb{E}[Z | \mathcal{H}]$ over the coarser \mathcal{G} equals $\mathbb{E}[Z | \mathcal{G}]$.

Code <-> Theory (Tower Property)

This numerical check verifies 2.3.2 (Tower Property) by constructing nested σ -algebras via parity (#groups=2) and mod-4 (#groups=4) partitions and confirming $\mathbb{E}[\mathbb{E}[Z | \mathcal{H}] | \mathcal{G}] = \mathbb{E}[Z | \mathcal{G}]$.

3.8 2.8 Application Bridge to RL

We've built measure-theoretic probability foundations. Now we connect to reinforcement learning.

Before diving into MDPs, we establish a key integrability result that ensures reward expectations are well-defined.

Proposition 2.8.1 (Score Integrability)

Under the standard Borel assumptions (see §2.1 assumptions box), the base relevance score function $s : \mathcal{Q} \times \mathcal{P} \rightarrow \mathbb{R}$ satisfies:

1. **Measurability:** s is $(\mathcal{B}(\mathcal{Q}) \otimes \mathcal{B}(\mathcal{P}), \mathcal{B}(\mathbb{R}))$ -measurable
2. **Square-integrability:** Under the simulator-induced distribution, $s \in L^2$

Proof.

Step 1 (Score decomposition). The simulator's relevance score decomposes as

$$s(q, p) = s_{\text{sem}}(q, p) + s_{\text{lex}}(q, p) + \varepsilon,$$

where s_{sem} is the cosine similarity between query and product embeddings, $s_{\text{lex}} = \log(1 + \text{overlap}(q, p))$ is the lexical overlap component, and $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ is independent observation noise.

Step 2 (Measurability). The cosine similarity $s_{\text{sem}} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [-1, 1]$ is continuous (hence Borel measurable) away from the origin. The logarithm $\log : (0, \infty) \rightarrow \mathbb{R}$ is continuous. Compositions and sums of Borel-measurable functions are Borel measurable ((Folland 1999, Proposition 2.6)). The noise ε is measurable as a random variable by construction. Thus s is $(\mathcal{B}(\mathcal{Q}) \otimes \mathcal{B}(\mathcal{P}) \otimes \mathcal{B}(\mathbb{R}), \mathcal{B}(\mathbb{R}))$ -measurable.

Step 3 (Finite second moments). We verify each component:

- *Semantic component:* $|s_{\text{sem}}(q, p)| \leq 1$, so $s_{\text{sem}}^2 \leq 1$.
- *Lexical component:* The overlap count is bounded by token-set sizes: $\text{overlap}(q, p) \leq \min(|q|, |p|) \leq M$ where M is the maximum query/product token count in the simulator. Thus $s_{\text{lex}}^2 \leq (\log(1+M))^2 < \infty$.
- *Noise component:* $\mathbb{E}[\varepsilon^2] = \sigma^2 < \infty$ by assumption.

Step 4 (Square-integrability of sum). By independence of ε from (q, p) and the elementary inequality $(a + b + c)^2 \leq 3(a^2 + b^2 + c^2)$,

$$\mathbb{E}[s(Q, P)^2] \leq 3(\mathbb{E}[s_{\text{sem}}^2] + \mathbb{E}[s_{\text{lex}}^2] + \mathbb{E}[\varepsilon^2]) \leq 3(1 + (\log(1+M))^2 + \sigma^2) < \infty.$$

Thus $s \in L^2$ under the simulator-induced distribution. \square

Remark 2.8.1a (Boundedness not required). The OPE machinery (Theorem 2.6.1) requires only integrability, not boundedness. Our scores are square-integrable but **not** bounded to $[0, 1]$ —the Gaussian noise component is unbounded. This is typical of realistic relevance models where measurement noise and model uncertainty introduce unbounded perturbations.

Consequence for OPE (Theorem 2.6.1): The integrability assumption in Theorem 2.6.1 is satisfied when rewards have **finite first moments**. Since $R(x, a, \omega)$ aggregates GMV (lognormal prices with finite moments), CM2 (bounded margin rates), and clicks (bounded by `top_k`)—all with finite expectations—the IPS estimator is well-defined.

Code <-> Theory (Score Distribution)

Lab 2.2 verifies Proposition 2.8.1 empirically. The implementation in `zoosim/ranking/relevance.py` combines:

- Cosine similarity (bounded $[-1, 1]$)
- Lexical overlap $\log(1 + \text{overlap})$ (bounded by token-set sizes)
- Gaussian noise (unbounded but integrable)

Scores are NOT constrained to $[0, 1]$; empirically they cluster near 0 with std ~ 0.2 .

3.8.1 2.8.1 MDPs as Probability Spaces

Markov Decision Processes (MDPs), the canonical RL framework (Chapter 3), are probability spaces with structure.

Definition 2.8.1 (MDP, informal preview). An MDP is a tuple $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ where: - \mathcal{S} : State space (measurable space) - \mathcal{A} : Action space (measurable space) - $P(\cdot | s, a)$: Markov transition kernel on \mathcal{S} (for each (s, a) , $P(\cdot | s, a)$ is a probability measure on \mathcal{S} , and $(s, a) \mapsto P(B | s, a)$ is measurable for each measurable $B \subseteq \mathcal{S}$) - $R : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$: measurable one-step reward function (the realized reward random variables are $R_t := R(S_t, A_t)$ on the induced trajectory space) - $\gamma \in [0, 1]$: Discount factor

A policy $\pi : \mathcal{S} \rightarrow \Delta(\mathcal{A})$ maps states to probability distributions over actions. Together with initial state distribution ρ_0 , this defines a **probability space over trajectories**:

$$\Omega = (\mathcal{S} \times \mathcal{A})^\infty, \quad \mathbb{P}^\pi = \text{measure induced by } \rho_0, \pi, P.$$

The **value function** is an expectation over this space:

$$V^\pi(s) := \mathbb{E}^\pi \left[\sum_{t=0}^{\infty} \gamma^t R_t \mid S_0 = s \right] = \mathbb{E}^\pi \left[\sum_{t=0}^{\infty} \gamma^t R(S_t, A_t) \mid S_0 = s \right].$$

What we've learned enables: - **Measurability**: S_t, A_t, R_t are random variables (Section 2.2.3) - **Conditional expectation**: $V^\pi(s) = \mathbb{E}[G_0 \mid S_0 = s]$ is well-defined (Section 2.3.2) - **Infinite sums**: Monotone Convergence Theorem 2.2.3 justifies interchanging \sum and \mathbb{E} - **Filtrations**: $\mathcal{F}_t = \sigma(S_0, A_0, \dots, S_t, A_t)$ models “information up to time t ” (Section 2.4.1)

Chapter 3 makes this rigorous and proves convergence of value iteration via contraction mappings.

Remark 2.8.1b (Uncountable trajectory space). Even when per-step state and action spaces are finite, the space of infinite-horizon trajectories $\Omega = (\mathcal{S} \times \mathcal{A} \times \mathbb{R})^\mathbb{N}$ is uncountable (same cardinality as $[0, 1]$). There is no meaningful “uniform counting” on Ω ; probabilities must be defined as measures on σ -algebras.

Proposition 2.8.2 (Bellman measurability and contraction) .

Assume standard Borel state/action spaces, bounded measurable rewards $r(s, a)$, measurable Markov kernel $P(\cdot | s, a)$, measurable policy kernel $\pi(\cdot | s)$, and discount $0 \leq \gamma < 1$. Then on $(B_b(\mathcal{S}), \|\cdot\|_\infty)$, - the policy evaluation operator

$$(\mathcal{T}^\pi V)(s) := \int_{\mathcal{A}} r(s, a) \pi(da | s) + \gamma \int_{\mathcal{A}} \int_{\mathcal{S}} V(s') P(ds' | s, a) \pi(da | s) \quad (2.14)$$

maps bounded measurable functions to bounded measurable functions and satisfies $\|\mathcal{T}^\pi V - \mathcal{T}^\pi W\|_\infty \leq \gamma \|V - W\|_\infty$; - the control operator

$$(\mathcal{T}V)(s) := \sup_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right\}$$

is a γ -contraction under the same boundedness conditions; measurability of $\mathcal{T}V$ may require additional topological assumptions (e.g., compact \mathcal{A} , upper semicontinuity) or a measurable selection theorem.

Proof sketch. Measurability is preserved under integration against Markov kernels; boundedness follows from bounded r and V . The contraction bound follows from the triangle inequality and linearity of the integral. \square

Remark 2.8.2 (Control operator) . For the control operator

$$(\mathcal{T}V)(s) := \sup_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right\},$$

measurability of $\mathcal{T}V$ can require additional topological assumptions (e.g., compact \mathcal{A} and upper semicontinuity) or application of a measurable selection theorem. Contraction still holds under boundedness and $0 \leq \gamma < 1$. The measurable selection theorem needed for the control operator appears in **§2.8.2 (Advanced: Measurable Selection and Optimal Policies)** below.

3.8.2 2.8.2 (Advanced) Measurable Selection and Optimal Policies

This section is optional on a first reading. It addresses the topological fine print that ensures optimal policies $\pi^(s) = \arg \max_a Q(s, a)$ are well-defined measurable functions in continuous state and action spaces. Readers primarily interested in finite action spaces (Chapters 6, 8) can safely skip this and return when studying continuous actions (Chapter 7).*

In Remark 2.8.2 above, we noted that the control Bellman operator

$$(\mathcal{T}V)(s) = \sup_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right\}$$

requires additional care to ensure measurability of $\mathcal{T}V$. The issue is subtle but fundamental to continuous-space RL.

The problem. For each state s , the Bellman optimality equation requires finding $a^*(s) = \arg \max_a Q(s, a)$. But knowing that a maximum *exists* at each s (e.g., by compactness and continuity) doesn't guarantee that the mapping $s \mapsto a^*(s)$ is *measurable*—and if it's not measurable, the “optimal policy” cannot be evaluated as a random variable. We couldn't take expectations like $\mathbb{E}[R(S, \pi^*(S))]$ because π^* would be ill-defined measure-theoretically.

Why this is subtle. The supremum of measurable functions is measurable—this is a standard result in measure theory. But the **argmax** (the action achieving the supremum) need not be measurable. Geometrically, the set of maximizers

$$A^*(s) = \{a \in \mathcal{A} : Q(s, a) = \sup_{a' \in \mathcal{A}} Q(s, a')\}$$

can vary wildly with s in continuous spaces. Selecting one element from each set $A^*(s)$ in a measurable way is non-trivial—this is an Axiom of Choice problem constrained by measurability requirements. Without structure, pathological examples exist where no measurable selector is possible.

The solution. The following theorem packages the conditions under which measurable optimal policies exist:

Theorem 2.8.3 (Kuratowski–Ryll–Nardzewski Selection, specialized to RL).

Let \mathcal{S} be a standard Borel space and \mathcal{A} a compact metric space. Suppose $Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ satisfies:

(A1) Joint measurability: Q is Borel measurable in (s, a)

(A2) Upper semicontinuity: For each fixed $s \in \mathcal{S}$, the map $a \mapsto Q(s, a)$ is upper semicontinuous

Then there exists a Borel measurable function $\pi^* : \mathcal{S} \rightarrow \mathcal{A}$ such that

$$Q(s, \pi^*(s)) = \sup_{a \in \mathcal{A}} Q(s, a) \quad \text{for all } s \in \mathcal{S}.$$

That is, a **measurable optimal selector** (greedy policy) exists.

Proof sketch. Assumption (A2) plus compactness of \mathcal{A} ensure the supremum is attained at each s (Weierstrass theorem). The challenge is proving that some selector is measurable. Under standard Borel state spaces and compact metric action spaces, the Kuratowski–Ryll–Nardzewski measurable selection theorem ((Kuratowski and Ryll-Nardzewski 1965)) guarantees that every non-empty-valued, closed-valued measurable correspondence admits a measurable selector. The set-valued map $s \mapsto A^*(s)$ (maximizers) is closed-valued by upper semicontinuity and measurable by joint measurability of Q . Applying the theorem yields a measurable π^* . See (Kechris 1995, sec. 36) for the full descriptive set theory machinery. \square

What this guarantees for RL. This theorem ensures:

1. **Bellman optimality operator is well-defined:** The pointwise maximum $(\mathcal{T}V)(s) = \max_a \{r(s, a) + \gamma \mathbb{E}[V(S') | s, a]\}$ produces a measurable function $\mathcal{T}V : \mathcal{S} \rightarrow \mathbb{R}$ when V is measurable.
2. **Optimal policies are random variables:** The greedy policy $\pi^*(s) \in \arg \max_a Q(s, a)$ is a measurable function, so we can evaluate expectations like $\mathbb{E}_{S \sim \rho_0}[R(S, \pi^*(S))]$ when S is drawn from an initial state distribution ρ_0 .
3. **Value iteration convergence machinery works:** Chapter 3 proves that iterating $V_{n+1} = \mathcal{T}V_n$ converges to the unique fixed point V^* . Measurability of \mathcal{T} at each step is essential for this operator-theoretic argument.

When this theorem matters in our book:

- **Finite action spaces:** Trivially satisfied. If $\mathcal{A} = \{a_1, \dots, a_M\}$ is finite, compactness is automatic and argmax is trivially measurable (just pick the first maximizer in some fixed ordering). No sophisticated machinery needed.
- **Discrete template bandits (Chapter 6):** Our template library has $|\mathcal{A}| = 25$ templates. Theorem 2.8.3 is overkill—measurability is immediate.
- **Continuous boost actions (Chapter 7):** When we learn $Q(x, a)$ for $a \in [-a_{\max}, a_{\max}]^K$ (continuous action space), this theorem becomes essential. Neural Q-networks approximate Q as $Q_\theta(x, a)$; upper semicontinuity (A2) may fail in practice (neural nets are not inherently u.s.c.), requiring care in implementation.
- **General state/action spaces:** In extensions to continuous state representations (e.g., learned embeddings $x \in \mathbb{R}^d$), the standard Borel assumption on \mathcal{S} becomes critical. Pathological spaces exist where measurable selection fails without these topological conditions.

Practical takeaway. In the finite-action and compact-action settings emphasized early in this book, measurability of greedy selectors is immediate; the selection theorem becomes essential primarily when passing to genuinely continuous action spaces. On a first reading, we may treat the set-theoretic details as background and focus on the consequences stated above.

References: The original Kuratowski–Ryll–Nardzewski theorem appears in (Kuratowski and Ryll-Nardzewski 1965). For textbook treatments: (Kechris 1995, sec. 36) provides the definitive descriptive set theory perspective; (Bertsekas and Shreve 1996, chap. 7) develops the RL-specific machinery and verifies standard Borel conditions for typical RL state/action spaces.

3.8.3 Click Models as Contextual Bandits

The **contextual bandit** (one-step MDP, no state transitions) is the foundation for Chapters 6–8:

Setup: - Context $x \sim \mathcal{D}$ (user, query) - Policy $\pi : \mathcal{X} \rightarrow \Delta(\mathcal{A})$ selects action (boost weights) $a \sim \pi(\cdot | x)$
- Outcome $\omega \sim P(\cdot | x, a)$ drawn from click model (PBM or DBN) - Reward $R(x, a, \omega)$ aggregates GMV, CM2, clicks (Chapter 1, (1.2))

Goal: Learn policy π^* maximizing

$$V(\pi) = \mathbb{E}_{x \sim \mathcal{D}, a \sim \pi(\cdot | x), \omega \sim P(\cdot | x, a)} [R(x, a, \omega)].$$

Click models provide $P(\cdot | x, a)$: - PBM (Section 2.5.1): $\omega = (E_1, C_1, \dots, E_M, C_M)$ with independent examination/click - DBN (Section 2.5.2): $\omega = (E_1, C_1, S_1, \dots)$ with cascade stopping

Propensity scores (Section 2.6) enable off-policy learning: - Collect data under exploration policy π_0 (e.g., ϵ -greedy, Thompson Sampling) - Estimate $V(\pi_1)$ for candidate policies via IPS (2.9) - Select best policy without online deployment risk

Chapter connections: - **Chapter 6** (Discrete Template Bandits): Tabular policies, finite action space $|\mathcal{A}| = 25$ - **Chapter 7** (Continuous Actions via Q-learning): Regression over $Q(x, a) = \mathbb{E}[R | x, a]$ - **Chapter 10** (Guardrails): Production constraints—CM2 floors, $\Delta\text{Rank}@k$ stability, safe fallback (CMDP theory in §3.6) - **Chapter 9** (Off-Policy Evaluation): Production IPS, SNIPS, doubly robust estimators

All rely on the probability foundations built in this chapter.

3.8.4 Forward References

Chapter 3 — Stochastic Processes & Bellman Foundations: - Bellman operators as contractions in function spaces (operator theory) - Value iteration convergence via **Banach Fixed-Point Theorem** - Filtrations $\{\mathcal{F}_t\}$ and martingale convergence theorems

Chapter 4 — Catalog, Users, Queries: - Generative models for contexts $x = (u, q)$ with distributional realism - Deterministic generation via seeds (reproducibility) - Feature engineering $\phi_k(p, u, q)$ as random variables

Chapter 5 — Relevance, Features, Reward: - Reward function $R(x, a, \omega)$ implementation using click model outcomes ω - Verification that $\mathbb{E}[R | x, a]$ is well-defined and integrable - Conditional expectation structure for model-based value estimation

Chapter 9 — Off-Policy Evaluation: - IPS, SNIPS, doubly robust estimators (extending Section 2.6)
- Variance reduction via capping, control variates - Propensity estimation from logged data (when π_0 is unknown)

Chapter 11 — Multi-Episode MDP: - Stopping times τ for session termination (extending Section 2.4.2)
- Inter-session dynamics: state transitions $s_{t+1} = f(s_t, \omega_t)$ - Retention modeling via survival analysis

3.9 Production Checklist

Production Checklist (Chapter 2)

Configuration alignment:

The simulator implements the **Utility-Based Cascade Model** (§2.5.4). Under a parameter specialization it reproduces PBM's marginal factorization (Proposition 2.5.4), and in general it exhibits cascade-style dependence through an internal state.

- **Position bias:** `BehaviorConfig.pos_bias` in `zoosim/core/config.py:180–186` — dictionary

- mapping query types to position bias vectors (PBM-like behavior)
- Satisfaction dynamics:** `BehaviorConfig.satisfaction_decay` and `satisfaction_gain` in `zoosim/core/config.py:175-176` — state-driven cascade dependence (DBN-like mechanism)
- Abandonment threshold:** `BehaviorConfig.abandonment_threshold` in `zoosim/core/config.py:177` — session termination condition
- Seeds:** `SimulatorConfig.seed` in `zoosim/core/config.py:252` for reproducible click patterns

Implementation modules:

- `zoosim/dynamics/behavior.py`: Implements cascade session simulation via `simulate_session()` — combines PBM position bias with DBN-style satisfaction/abandonment dynamics
- `zoosim/core/config.py`: `BehaviorConfig` dataclass with utility weights (`alpha_*`), satisfaction parameters, and position bias vectors
- `zoosim/evaluation/ope.py` (Chapter 9): Implements IPS, SNIPS, PDIS, and DR estimators from Definitions 2.6.1–2.6.2

Tests:

- `tests/ch09/test_ope.py`: Verifies OPE estimator behavior
- `tests/ch02/test_behavior.py`: Verifies position bias monotonicity (click rates decrease with position); does NOT verify exact PBM/DBN equation matches
- `tests/ch02/test_segment_sampling.py`: Verifies segment frequencies converge to configured probabilities

Score distribution (Lab 2.2):

- Lab 2.2 validates integrability; scores are NOT bounded to $[0, 1]$
- Empirically, scores cluster near 0 with $\text{std} \sim 0.2$

Reward moments:

- GMV/CM2 have finite moments (lognormal prices); not bounded
- Click counts bounded by `top_k`

Assertions:

- Check $0 \leq \theta_k \leq 1$ for all position bias values
- Check positivity assumption $\pi_0(a | x) > 0$ when computing IPS weights

3.10 2.10 Exercises

Exercise 2.1 (Measurability, 10 min). Let $X : \Omega \rightarrow \mathbb{R}$ and $Y : \Omega \rightarrow \mathbb{R}$ be random variables on $(\Omega, \mathcal{F}, \mathbb{P})$. Prove that $Z = X + Y$ is also a random variable.

Exercise 2.2 (Conditional probability computation, 15 min). In the PBM model, suppose $\text{rel}(p_3) = 0.6$ and $\theta_3 = 0.5$. Compute: 1. $\mathbb{P}(C_3 = 1)$ 2. $\mathbb{P}(E_3 = 1 | C_3 = 1)$ 3. $\mathbb{P}(C_3 = 1 | E_3 = 1)$

Exercise 2.3 (DBN cascade probability, 20 min). In the DBN model, suppose $M = 3$ with: - $\text{rel}(p_1) = 0.8$, $s(p_1) = 0.5$ - $\text{rel}(p_2) = 0.6$, $s(p_2) = 0.7$ - $\text{rel}(p_3) = 0.9$, $s(p_3) = 0.9$

Compute: 1. $\mathbb{P}(E_2 = 1)$ 2. $\mathbb{P}(E_3 = 1)$ 3. $\mathbb{P}(\tau = 1)$ (probability user stops at position 1)

Exercise 2.4 (IPS estimator properties, 20 min). Prove that if $\pi_1 = \pi_0$ (target equals logging), then $\hat{V}_{\text{IPS}}(\pi_1)$ reduces to the naive sample mean, and has lower variance than the general IPS estimator.

Exercise 2.5 (Stopping time verification, 15 min). Show that $\tau = \max\{k : C_k = 1\}$ (position of last click) is **not** a stopping time, by constructing a specific example where $\{\tau = 2\}$ requires knowledge of C_3 .

Exercise 2.6 (RL bridge: Bellman operator as conditional expectation, 20 min). Let $V : \mathcal{S} \rightarrow \mathbb{R}$ be a value function. The Bellman operator $\mathcal{T}^\pi V$ is defined as

$$(\mathcal{T}^\pi V)(s) = \mathbb{E}_{a \sim \pi(\cdot|s)} [R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot|s, a)} [V(s')]].$$

Show that this is a **conditional expectation**: $(\mathcal{T}^\pi V)(s) = \mathbb{E}[R_0 + \gamma V(S_1) | S_0 = s]$ under policy π .

Exercise 2.7 (Code: Variance of IPS, 30 min). Extend the IPS experiment in Section 2.7.2. Vary the divergence between π_0 and π_1 (e.g., make π_1 increasingly greedy while π_0 remains uniform). Plot IPS variance vs policy divergence (measured by KL divergence $D_{\text{KL}}(\pi_1 \parallel \pi_0)$). Verify that variance increases as policies diverge.

3.10.1 Labs

- Lab 2.1 — Segment Mix Sanity Check: sample thousands of users via `zoosim.users` and verify empirical frequencies converge to the segment distribution \mathbf{p}_{seg} from 2.2.6.
 - Lab 2.2 — Query Measure and Base Score Integration: connect the PBM/DBN derivations to simulator base scores by logging statistics from `zoosim.queries` and `zoosim.relevance`.
 - Lab 2.3 — Textbook Click Model Verification: verify PBM and DBN toy simulators match the closed-form predictions from (2.1) and (2.3).
 - Lab 2.4 — Nesting Verification ([PROP-2.5.4]): show that the Utility-Based Cascade reduces to PBM under the parameter specialization in 2.5.4.
 - Lab 2.5 — Utility-Based Cascade Dynamics ([DEF-2.5.3]): empirically validate position decay, satisfaction dynamics, and stopping conditions from [EQ-2.4]–[EQ-2.8].
-

3.11 Chapter Summary

What we built: 1. **Probability spaces** ($\Omega, \mathcal{F}, \mathbb{P}$): Sample spaces, σ -algebras, probability measures 2. **Random variables and expectations:** Measurable functions, Lebesgue integration, linearity 3. **Conditional probability:** Conditional expectation given σ -algebras, Tower Property 4. **Filtrations and stopping times:** Sequential information, abandonment as stopped processes 5. **Click models for search:** PBM (position bias), DBN (cascade), theoretical formulas vs empirical validation 6. **Propensity scoring:** Unbiased off-policy estimation via IPS, importance sampling mechanism

Why it matters for RL: - **Chapter 1's rewards are now rigorous:** $\mathbb{E}[R \mid W]$ is a $\sigma(W)$ -measurable conditional expectation, and (under standard Borel assumptions) $\mathbb{E}[R \mid W = w] = \int r d\mathbb{P}(R \in dr \mid W = w)$ is a regular conditional expectation. - **Chapter 3's Bellman operators are measurable:** Value functions are conditional expectations - **Chapters 6–8's bandits have formal semantics:** Contexts, actions, outcomes are random variables - **Chapter 9's off-policy evaluation is justified:** IPS unbiasedness proven via measure theory under positivity and integrability; clipped IPS incurs negative bias and SNIPS trades bias for variance.

Next chapter: We develop stochastic processes, Markov chains, Bellman operators, and contraction mappings, and we prove value iteration convergence via the Banach fixed-point theorem.

Central lesson: Reinforcement learning is applied probability theory: algorithms are expectations, policies are conditional distributions, and convergence proofs rely on measure-theoretic limit theorems. This chapter supplies the hypotheses required for those results.

3.12 References

The primary references for this chapter are:

- (Folland 1999) — Measure theory, integration, conditional expectation
- (Durrett 2019) — Stochastic processes, filtrations, stopping times, martingales
- (Craswell et al. 2008) — Click models for web search (PBM, DBN)
- (Chapelle and Zhang 2009) — Unbiased learning to rank via propensity scoring
- (Wang et al. 2016) — Position bias in contextual bandits for search

Full bibliography lives in `docs/references.bib`.

4 Chapter 3 — Stochastic Processes and Bellman Foundations

Vlad Prytula

4.1 3.1 Motivation: From Single Queries to Sequential Sessions

Chapter 1 formalized search ranking as a contextual bandit: observe context x (user segment, query type), select action a (boost weights), and observe an immediate reward $R(x, a, \omega)$. This abstraction is appropriate when each query can be treated as an independent decision, and when myopic objectives (GMV, CM2, clicks) are sufficient proxies for long-run value.

In deployed systems, user behavior is sequential. Actions taken on one query influence the distribution of future queries, clicks, and purchases within a session, and they can shape return probability across sessions. A user may refine a query after inspecting a ranking; a cart may accumulate over several steps; satisfaction may drift and eventually trigger abandonment. These are precisely the phenomena that a single-step model cannot represent.

Mathematically, the missing ingredient is **state**: a variable S_t that summarizes the relevant history at time t (cart, browsing context, latent satisfaction, recency). Once we represent the interaction as a controlled stochastic process $(S_0, A_0, R_0, S_1, A_1, R_1, \dots)$, the central objects of reinforcement learning become well-defined:

- **Value functions** $V^\pi(s)$ and $Q^\pi(s, a)$, which measure expected cumulative reward under a policy π
- **Bellman operators** \mathcal{T}^π and \mathcal{T} , which encode the dynamic programming principle as fixed-point equations

The guiding question of this chapter is structural: under what assumptions does repeated Bellman backup converge, and why does it converge to the optimal value function? The answer is an operator-theoretic one: the discounted Bellman operator is a contraction in the sup-norm, so it has a unique fixed point and value iteration converges to it.

We develop these foundations in the following order:

1. Section 3.2–3.3: Stochastic processes, filtrations, stopping times (measure-theoretic rigor for sequential randomness)
2. Section 3.4: Markov Decision Processes (formal definition, standard Borel assumptions)
3. Section 3.5: Bellman operators and value functions (from intuition to operators on function spaces)
4. Section 3.6: Contraction mappings and Banach fixed-point theorem (complete proof, step-by-step)
5. Section 3.7: Value iteration convergence (why dynamic programming works)
6. Section 3.8: Connection to bandits (the $\gamma = 0$ special case from Chapter 1)
7. Section 3.9: Computational verification (NumPy experiments)
8. Section 3.10: RL bridges (preview of Chapter 11’s multi-episode formulation)

By the end of this chapter, we understand:

- Why value iteration converges exponentially fast (contraction mapping theorem)
- How to prove convergence of RL algorithms rigorously (fixed-point theory)
- When the bandit formulation is sufficient and when MDPs are necessary
- The mathematical foundations that justify TD-learning, Q-learning, and policy gradients

Prerequisites. This chapter assumes:

- Measure-theoretic probability from Chapter 2 (probability spaces, random variables, conditional expectation)
- Familiarity with supremum norm and function spaces (we will introduce contraction mappings from first principles)

4.2 3.2 Stochastic Processes: Modeling Sequential Randomness

Definition 3.2.1 (Stochastic Process)

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, $T \subseteq \mathbb{R}_+$ an index set (often $T = \mathbb{N}$ or $T = [0, \infty)$), and (E, \mathcal{E}) a measurable space. A **stochastic process** is a collection of random variables $\{X_t : t \in T\}$ where each $X_t : \Omega \rightarrow E$ is $(\mathcal{F}, \mathcal{E})$ -measurable.

Notation: We write $(X_t)_{t \in T}$ or simply (X_t) when T is clear from context.

Intuition: A stochastic process is a **time-indexed family of random variables**. Each X_t represents the state of a system at time t . For a fixed $\omega \in \Omega$, the mapping $t \mapsto X_t(\omega)$ is a **sample path** or **trajectory**.

Example 3.2.1 (User satisfaction process). Let $E = [0, 1]$ represent satisfaction levels. Define $S_t : \Omega \rightarrow [0, 1]$ as the user's satisfaction after the t -th query in a session. Then $(S_t)_{t=0}^T$ is a stochastic process modeling satisfaction evolution.

Example 3.2.2 (RL trajectory). In a Markov Decision Process, the sequence $(S_0, A_0, R_0, S_1, A_1, R_1, \dots)$ is a stochastic process where: - $S_t \in \mathcal{S}$ (state space) - $A_t \in \mathcal{A}$ (action space) - $R_t \in \mathbb{R}$ (reward)

Each component is a random variable, and their joint distribution is induced by the policy π and environment dynamics P .

Standing convention (Discrete time). Throughout this chapter we work in discrete time with index set $T = \mathbb{N}$. Continuous-time analogues require additional measurability notions (e.g., predictable processes and optional σ -algebras), which we do not pursue here.

4.2.1 3.2.1 Filtrations and Adapted Processes

Definition 3.2.2 (Filtration)

A **filtration** on $(\Omega, \mathcal{F}, \mathbb{P})$ is a collection $(\mathcal{F}_t)_{t \in T}$ of sub- σ -algebras of \mathcal{F} satisfying:

$$\mathcal{F}_s \subseteq \mathcal{F}_t \subseteq \mathcal{F} \quad \text{for all } s \leq t.$$

Intuition: \mathcal{F}_t represents the **information available at time t** . The inclusion $\mathcal{F}_s \subseteq \mathcal{F}_t$ captures the idea that information accumulates over time: we never “forget” past observations.

Example 3.2.3 (Natural filtration). Given a stochastic process (X_t) , the **natural filtration** is:

$$\mathcal{F}_t := \sigma(X_s : s \leq t),$$

the smallest σ -algebra making all X_s with $s \leq t$ measurable. This represents “all information revealed by observing (X_0, X_1, \dots, X_t) .”

We write

$$\mathcal{F}_\infty := \sigma \left(\bigcup_{t \in T} \mathcal{F}_t \right)$$

for the terminal σ -algebra generated by the filtration.

Definition 3.2.3 (Adapted Process)

A stochastic process (X_t) is **adapted** to the filtration (\mathcal{F}_t) if X_t is \mathcal{F}_t -measurable for all $t \in T$.

Intuition: Adaptedness means “the value of X_t is determined by information available at time t .” This is the mathematical formalization of **causality**: X_t cannot depend on future information \mathcal{F}_s with $s > t$.

Remark 3.2.1 (Adapted vs. predictable). In continuous-time stochastic calculus, there is a stronger notion called **predictable** (measurable with respect to \mathcal{F}_{t-} , the left limit). For discrete-time RL, adapted suffices.

Remark 3.2.2 (RL policies must be adapted). In reinforcement learning, a policy $\pi(a|h_t)$ at time t must depend only on the **history** $h_t = (s_0, a_0, r_0, \dots, s_t)$ available at t , not on future states s_{t+1}, s_{t+2}, \dots . This is precisely the adaptedness condition: π_t is \mathcal{F}_t -measurable where $\mathcal{F}_t = \sigma(h_t)$.

4.2.2 3.2.2 Stopping Times

Definition 3.2.4 (Stopping Time)

Let (\mathcal{F}_t) be a filtration on $(\Omega, \mathcal{F}, \mathbb{P})$. A random variable $\tau : \Omega \rightarrow T \cup \{\infty\}$ is a **stopping time** if:

$$\{\tau \leq t\} \in \mathcal{F}_t \quad \text{for all } t \in T.$$

Intuition: A stopping time is a **random time** whose occurrence is determined by information available *up to that time*. The event “ τ has occurred by time t ” must be \mathcal{F}_t -measurable—we can decide whether to stop using only observations (X_0, \dots, X_t) , without peeking into the future.

Example 3.2.4 (Session abandonment). Define:

$$\tau := \inf\{t \geq 0 : S_t < \theta\},$$

the first time user satisfaction S_t drops below threshold θ . This is a stopping time: to check “ $\tau \leq t$ ” (user has abandoned by time t), we only need to observe (S_0, \dots, S_t) . We do not need to know future satisfaction S_{t+1}, S_{t+2}, \dots .

Example 3.2.5 (Purchase event). Define τ as the first time the user makes a purchase. This is a stopping time: the event “ $\tau = t$ ” means “user purchased at time t , having not purchased before”—determined by history up to t .

Non-Example 3.2.6 (Last time satisfaction peaks). Define $\tau := \sup\{t : S_t = \max_{s \leq T} S_s\}$ (the last time satisfaction reaches its maximum over $[0, T]$). This is **NOT** a stopping time: to determine “ $\tau = t$,” we need to know future values S_{t+1}, \dots, S_T to verify satisfaction never exceeds S_t afterward.

Proposition 3.2.1 (Measurability of stopped processes)

Assume $T = \mathbb{N}$. If (X_t) is adapted to (\mathcal{F}_t) and τ is a stopping time, then $X_\tau \mathbf{1}_{\{\tau < \infty\}}$ is \mathcal{F}_∞ -measurable.

Proof. **Step 1** (Indicator decomposition). Write:

$$X_\tau \mathbf{1}_{\{\tau < \infty\}} = \sum_{t=0}^{\infty} X_t \mathbf{1}_{\{\tau = t\}}.$$

Step 2 (Measurability of indicators). For each $t \in \mathbb{N}$, the event $\{\tau = t\}$ belongs to \mathcal{F}_t . Indeed, $\{\tau = 0\} = \{\tau \leq 0\} \in \mathcal{F}_0$, and for $t \geq 1$,

$$\{\tau = t\} = \{\tau \leq t\} \cap \{\tau \leq t-1\}^c \in \mathcal{F}_t,$$

since $\{\tau \leq t\} \in \mathcal{F}_t$ and $\{\tau \leq t-1\} \in \mathcal{F}_{t-1} \subseteq \mathcal{F}_t$.

Step 3 (Measurability of $X_t \mathbf{1}_{\{\tau=t\}}$). Since X_t is \mathcal{F}_t -measurable and $\{\tau = t\} \in \mathcal{F}_t$, the product $X_t \mathbf{1}_{\{\tau=t\}}$ is \mathcal{F}_t -measurable, hence \mathcal{F}_∞ -measurable.

Step 4 (Countable sum). A countable sum of measurable functions is measurable, so the right-hand side of Step 1 is \mathcal{F}_∞ -measurable; hence $X_\tau \mathbf{1}_{\{\tau < \infty\}}$ is \mathcal{F}_∞ -measurable. \square

Remark 3.2.3 (The indicator technique). The proof uses the **indicator decomposition**: write a stopped process as a sum over stopping events. This technique will reappear when proving optional stopping theorems for martingales (used in stochastic approximation convergence proofs, deferred to later chapters).

Remark 3.2.4 (RL preview: Episode termination). In episodic RL, the terminal time T is often a stopping time: the episode ends when the agent reaches a terminal state (e.g., user completes purchase or abandons

session). The return $G_0 = \sum_{t=0}^{T-1} \gamma^t R_t$ depends on T , which is random. Proposition 3.2.1 ensures G_0 is well-defined as a random variable.

4.3 3.3 Markov Chains and the Markov Property

Before defining MDPs, we introduce **Markov chains**—stochastic processes with memoryless transitions.

Definition 3.3.1 (Markov Chain)

A discrete-time stochastic process $(X_t)_{t \in \mathbb{N}}$ taking values in a countable or general measurable space (E, \mathcal{E}) is a **Markov chain** (with respect to its natural filtration $\mathcal{F}_t := \sigma(X_0, \dots, X_t)$) if:

$$\mathbb{P}(X_{t+1} \in A \mid \mathcal{F}_t) = \mathbb{P}(X_{t+1} \in A \mid X_t) \quad \text{for all } A \in \mathcal{E}, t \geq 0. \quad (3.1)$$

This is the **Markov property**: the future X_{t+1} is conditionally independent of the past (X_0, \dots, X_{t-1}) given the present X_t .

Intuition: “The future depends on the present, not on how we arrived at the present.”

Example 3.3.1 (Random walk). Let (ξ_t) be i.i.d. random variables with $\mathbb{P}(\xi_t = +1) = \mathbb{P}(\xi_t = -1) = 1/2$. Define $X_t = \sum_{s=0}^{t-1} \xi_s$ (cumulative sum). Then:

$$X_{t+1} = X_t + \xi_t,$$

so X_{t+1} depends only on X_t and the new increment ξ_t (independent of history). This is a Markov chain.

Example 3.3.2 (User state transitions). In an e-commerce session, let $X_t \in \{\text{browsing, engaged, ready_to_buy, abandoned}\}$ be the user’s state after t queries. If transitions depend only on current state (not on the path taken to reach it), then (X_t) is a Markov chain.

Non-Example 3.3.3 (ARMA processes violate the Markov property). Consider $X_t = 0.5X_{t-1} + 0.3X_{t-2} + \varepsilon_t$ where ε_t is white noise. Given only X_t , the distribution of X_{t+1} depends on X_{t-1} (through the 0.3 term), violating the Markov property (3.1). To restore Markovianity, **augment the state**: define $\tilde{X}_t = (X_t, X_{t-1})$. Then \tilde{X}_{t+1} depends only on \tilde{X}_t , so (\tilde{X}_t) is Markov. This **state augmentation** technique is fundamental in RL—frame stacking in video games (Remark 3.4.1), LSTM hidden states, and user history embeddings all restore the Markov property by expanding what we call “state.”

Definition 3.3.2 (Transition Kernel)

The **transition kernel** (or **transition probability**) of a Markov chain is:

$$P(x, A) := \mathbb{P}(X_{t+1} \in A \mid X_t = x), \quad x \in E, A \in \mathcal{E}.$$

For time-homogeneous chains, P is independent of t .

Properties: 1. For each $x \in E$, $A \mapsto P(x, A)$ is a probability measure on (E, \mathcal{E}) 2. For each $A \in \mathcal{E}$, $x \mapsto P(x, A)$ is measurable

Remark 3.3.1 (Standard Borel assumption). For general state spaces, we require E to be a **standard Borel space** (a measurable subset of a Polish space, i.e., separable complete metric space). This ensures:

- Transition kernels $P(x, A)$ are well-defined and measurable
- Regular conditional probabilities exist
- Optimal policies can be chosen measurably

All finite and countable spaces are standard Borel. \mathbb{R}^n with Borel σ -algebra is standard Borel. This covers essentially all RL applications.

4.4 3.4 Markov Decision Processes: The RL Framework

Definition 3.4.1 (Markov Decision Process)

A **Markov Decision Process (MDP)** is a tuple $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ where:

1. \mathcal{S} is the **state space** (a standard Borel space)
2. \mathcal{A} is the **action space** (a standard Borel space)
3. $P(\cdot | s, a)$ is a **Markov kernel** from $(\mathcal{S} \times \mathcal{A}, \mathcal{B}(\mathcal{S}) \otimes \mathcal{B}(\mathcal{A}))$ to $(\mathcal{S}, \mathcal{B}(\mathcal{S}))$: $P(B | s, a)$ is the probability of transitioning to a Borel set $B \subseteq \mathcal{S}$ when taking action a in state s
4. $R : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow \mathbb{R}$ is the **reward function**: $R(s, a, s')$ is the reward obtained from transition (s, a, s')
5. $\gamma \in [0, 1]$ is the **discount factor**

Structural assumptions: - For each (s, a) , $B \mapsto P(B | s, a)$ is a probability measure on $(\mathcal{S}, \mathcal{B}(\mathcal{S}))$ - For each $B \in \mathcal{B}(\mathcal{S})$, $(s, a) \mapsto P(B | s, a)$ is measurable - R is bounded and measurable: $|R(s, a, s')| \leq R_{\max} < \infty$ for all (s, a, s')

Notation: - We write the bounded measurable one-step expected reward as

$$r(s, a) := \int_{\mathcal{S}} R(s, a, s') P(ds' | s, a).$$

When \mathcal{S} is finite, integrals against $P(\cdot | s, a)$ reduce to sums: $\int_{\mathcal{S}} f(s') P(ds' | s, a) = \sum_{s' \in \mathcal{S}} P(s' | s, a) f(s')$.

- When \mathcal{S} and \mathcal{A} are finite, we represent P as a tensor $P \in [0, 1]^{|\mathcal{S}| \times |\mathcal{A}| \times |\mathcal{S}|}$ with $P_{s,a,s'} = P(s' | s, a)$

Definition 3.4.2 (Policy)

A **(stationary Markov) policy** is a **stochastic kernel** $\pi(\cdot | s)$ from $(\mathcal{S}, \mathcal{B}(\mathcal{S}))$ to $(\mathcal{A}, \mathcal{B}(\mathcal{A}))$ such that: - For each $s \in \mathcal{S}$, $B \mapsto \pi(B | s)$ is a probability measure on $(\mathcal{A}, \mathcal{B}(\mathcal{A}))$ - For each $B \in \mathcal{B}(\mathcal{A})$, $s \mapsto \pi(B | s)$ is $\mathcal{B}(\mathcal{S})$ -measurable

We write integrals against the policy as $\pi(da | s)$. When \mathcal{A} is finite, $\pi(a | s)$ is a mass function and $\int_{\mathcal{A}} f(a) \pi(da | s) = \sum_{a \in \mathcal{A}} f(a) \pi(a | s)$.

Deterministic policies: A policy is deterministic if $\pi(\cdot | s)$ is a point mass for all s . We identify deterministic policies with measurable functions $\pi : \mathcal{S} \rightarrow \mathcal{A}$, with the induced kernel $\pi(da | s) = \delta_{\pi(s)}(da)$.

Assumption 3.4.1 (Markov assumption).

The MDP satisfies: 1. **Transition Markov property**: $\mathbb{P}(S_{t+1} \in B | s_0, a_0, \dots, s_t, a_t) = P(B | s_t, a_t)$ 2. **Reward Markov property**: $\mathbb{E}[R_t | s_0, a_0, \dots, s_t, a_t, s_{t+1}] = R(s_t, a_t, s_{t+1})$

These properties ensure that **state s_t summarizes all past information relevant for predicting the future**. This is crucial: if the state does not satisfy the Markov property, the MDP framework breaks down.

Remark 3.4.1 (State design in practice). Real systems rarely have perfectly Markovian observations. Practitioners construct **augmented states** to restore the Markov property:

- **Frame stacking** in video games: stack last 4 frames to capture velocity
- **LSTM hidden states**: recurrent network state becomes part of MDP state
- **User history embeddings**: include session features (past clicks, queries) in context vector

This is a modeling choice rather than a theorem, but it is essential for applying MDP theory in practice.

4.4.1 3.4.1 Value Functions

Definition 3.4.3 (State-Value Function)

Given a policy π and initial state $s \in \mathcal{S}$, the **state-value function** is:

$$V^\pi(s) := \mathbb{E}^\pi \left[\sum_{t=0}^{\infty} \gamma^t R_t \middle| S_0 = s \right], \quad (3.2)$$

where the expectation is over trajectories $(S_0, A_0, R_0, S_1, A_1, R_1, \dots)$ generated by policy π and transition kernel P : - $S_0 = s$ (initial state) - $A_t \sim \pi(\cdot | S_t)$ (actions sampled from policy) - $S_{t+1} \sim P(\cdot | S_t, A_t)$ (states transition according to dynamics) - $R_t = R(S_t, A_t, S_{t+1})$ (rewards realized from transitions)

Notation: The superscript \mathbb{E}^π emphasizes that the expectation is under the probability measure \mathbb{P}^π induced by policy π and dynamics P . Existence and uniqueness of this trajectory measure (built from the initial state, the policy kernel, and the transition kernel) can be formalized via the Ionescu–Tulcea extension theorem; Chapter 2 gives the measurable construction of MDP trajectories.

Well-definedness: Since $\gamma < 1$ and $|R_t| \leq R_{\max}$, the series converges absolutely:

$$\left| \sum_{t=0}^{\infty} \gamma^t R_t \right| \leq \sum_{t=0}^{\infty} \gamma^t R_{\max} = \frac{R_{\max}}{1-\gamma} < \infty.$$

Thus $V^\pi(s)$ is well-defined and $|V^\pi(s)| \leq R_{\max}/(1-\gamma)$ for all s, π .

Definition 3.4.4 (Action-Value Function)

Given a policy π , state s , and action a , the **action-value function** (or **Q-function**) is:

$$Q^\pi(s, a) := \mathbb{E}^\pi \left[\sum_{t=0}^{\infty} \gamma^t R_t \mid S_0 = s, A_0 = a \right]. \quad (3.3)$$

This is the expected return starting from state s , taking action a , then following policy π .

Relationship:

$$V^\pi(s) = \int_{\mathcal{A}} Q^\pi(s, a) \pi(da \mid s), \quad (3.4)$$

When \mathcal{A} is finite, the integral reduces to the familiar sum $\sum_{a \in \mathcal{A}} \pi(a \mid s) Q^\pi(s, a)$.

Definition 3.4.5 (Optimal Value Functions)

The **optimal state-value function** is:

$$V^*(s) := \sup_{\pi} V^\pi(s), \quad (3.5)$$

and the **optimal action-value function** is:

$$Q^*(s, a) := \sup_{\pi} Q^\pi(s, a). \quad (3.6)$$

Remark 3.4.2 (Existence of optimal policies and measurable selection). In finite action spaces, optimal actions exist statewise and the Bellman optimality operator can be written with max. In general Borel state-action spaces, the optimality operator is stated with sup, and existence of a **deterministic stationary** optimal policy can require additional topological conditions (e.g., compact \mathcal{A} and upper semicontinuity) or a measurable selection theorem.

Chapter 2 discusses this fine print and gives a measurable formulation of the Bellman operators; see also (Puterman 2014, Theorem 6.2.10) for a comprehensive treatment. In this chapter, we focus on statements and proofs that do not require selecting maximizers: operator well-definedness on bounded measurable functions and contraction in $\|\cdot\|_\infty$.

4.5 3.5 Bellman Equations

The Bellman equations provide **recursive characterizations** of value functions. These are the cornerstone of RL theory.

Theorem 3.5.1 (Bellman Expectation Equation)

For any policy π , the value function V^π satisfies:

$$V^\pi(s) = \int_{\mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V^\pi(s') P(ds' | s, a) \right] \pi(da | s), \quad (3.7)$$

where $r(s, a) = \int_{\mathcal{S}} R(s, a, s') P(ds' | s, a)$ as in 3.4.1.

Equivalently, in operator notation:

$$V^\pi = \mathcal{T}^\pi V^\pi, \quad (3.8)$$

where \mathcal{T}^π is the **Bellman expectation operator** for policy π :

$$(\mathcal{T}^\pi V)(s) := \int_{\mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] \pi(da | s). \quad (3.9)$$

Proof. **Step 1** (Decompose the return). By definition (3.2),

$$V^\pi(s) = \mathbb{E}^\pi \left[\sum_{t=0}^{\infty} \gamma^t R_t \middle| S_0 = s \right].$$

Separate the first reward from the tail:

$$V^\pi(s) = \mathbb{E}^\pi \left[R_0 + \gamma \sum_{t=1}^{\infty} \gamma^{t-1} R_t \middle| S_0 = s \right].$$

Step 2 (Tower property). Apply the law of total expectation (tower property) conditioning on (A_0, S_1) :

$$V^\pi(s) = \mathbb{E}^\pi \left[\mathbb{E}^\pi \left[R_0 + \gamma \sum_{t=1}^{\infty} \gamma^{t-1} R_t \middle| S_0 = s, A_0, S_1 \right] \right].$$

Step 3 (Markov property). Since $R_0 = R(S_0, A_0, S_1)$ is determined by (S_0, A_0, S_1) , and future rewards (R_1, R_2, \dots) depend only on S_1 onward (Markov property [ASM-3.4.1]), we have:

$$\mathbb{E}^\pi \left[R_0 + \gamma \sum_{t=1}^{\infty} \gamma^{t-1} R_t \middle| S_0 = s, A_0 = a, S_1 = s' \right] = R(s, a, s') + \gamma V^\pi(s').$$

Step 4 (Integrate over actions and next states). Taking expectations over $A_0 \sim \pi(\cdot | s)$ and $S_1 \sim P(\cdot | s, a)$:

$$V^\pi(s) = \int_{\mathcal{A}} \int_{\mathcal{S}} [R(s, a, s') + \gamma V^\pi(s')] P(ds' | s, a) \pi(da | s).$$

Rearranging:

$$V^\pi(s) = \int_{\mathcal{A}} \left[\underbrace{\int_{\mathcal{S}} R(s, a, s') P(ds' | s, a)}_{=: r(s, a)} + \gamma \int_{\mathcal{S}} V^\pi(s') P(ds' | s, a) \right] \pi(da | s),$$

which is (3.7). \square

Remark 3.5.1 (The dynamic programming principle). The proof uses the **principle of optimality**: breaking the infinite-horizon return into immediate reward plus discounted future value. This is the essence of dynamic programming. The Markov property 3.4.1 is crucial—without it, $V^\pi(s')$ would depend on the history leading to s' , and the recursion would fail.

Theorem 3.5.2 (Bellman Optimality Equation)

The optimal value function V^* satisfies:

$$V^*(s) = \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V^*(s') P(ds' | s, a) \right], \quad (3.10)$$

or in operator notation:

$$V^* = \mathcal{T}V^*, \quad (3.11)$$

where \mathcal{T} is the **Bellman optimality operator**:

$$(\mathcal{T}V)(s) := \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right]. \quad (3.12)$$

Proof. **Step 1** (Control dominates evaluation). For any bounded measurable function V and any policy π , we have, for each $s \in \mathcal{S}$,

$$(\mathcal{T}^\pi V)(s) = \int_{\mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] \pi(da | s) \leq \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] = (\mathcal{T}V)(s).$$

Step 2 (Fixed point characterization of the optimal value). Section 3.7 shows that \mathcal{T} is a γ -contraction on $(B_b(\mathcal{S}), \|\cdot\|_\infty)$, hence has a unique fixed point \bar{V} by 3.6.2. Similarly, for each policy π , the evaluation operator \mathcal{T}^π is a γ -contraction (the proof is the same as for 3.7.1, without the supremum), hence has a unique fixed point V^π .

By Step 1, $(\mathcal{T}^\pi)^k V \leq \mathcal{T}^k V$ for all k and all $V \in B_b(\mathcal{S})$. Taking $k \rightarrow \infty$ yields $V^\pi \leq \bar{V}$, hence $\sup_\pi V^\pi \leq \bar{V}$ pointwise.

Discounted dynamic-programming theory shows that the fixed point \bar{V} coincides with the optimal value function V^* defined in (3.5), and therefore satisfies $V^* = \mathcal{T}V^*$; see (Puterman 2014, Theorem 6.2.10) for the measurable-selection details behind this identification. This gives (3.11) and the pointwise form (3.10). \square

Note on proof structure. This proof invokes 3.7.1 (Bellman contraction) and 3.6.2 (Banach fixed-point), which we establish in Section 3.6–3.7. We state the optimality equation here because it is conceptually fundamental—*this is the equation RL algorithms solve*. The existence and uniqueness of V^* follow once we prove \mathcal{T} is a contraction in Section 3.7.

Remark 3.5.2 (Suprema, maximizers, and greedy policies). Equation (3.10) is stated with sup because the supremum need not be attained without additional assumptions. In finite action spaces, or under compactness/upper-semicontinuity conditions, the supremum is attained and we may write max.

When a measurable maximizer exists, we can extract a deterministic greedy policy via:

$$\pi^*(s) \in \arg \max_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V^*(s') P(ds' | s, a) \right].$$

Without measurable maximizers, we work with ε -optimal selectors and interpret (3.10) as a value characterization; Chapter 2 discusses the measurable-selection fine print in more detail.

Remark 3.5.3 (CMDPs and regret: where the details live). Many practical ranking problems impose constraints (e.g., CM2 floors, exposure parity). **Constrained MDPs** (CMDPs) handle these by introducing

Lagrange multipliers that convert the constrained problem into an unconstrained MDP with modified rewards $r_\lambda = r - \lambda c$ —the Bellman theory of this section then applies directly to the relaxed problem. Appendix C develops the full CMDP framework with rigorous duality and algorithms; see THM-C.2.1, COR-C.3.1, and [ALG-C.5.1]. Chapter 10 treats constraints operationally as production guardrails, while Chapter 14 implements soft constraint optimization via primal–dual methods.

Regret guarantees are developed in Chapter 6 (e.g., THM-6.1, [THM-6.2]) with information-theoretic lower bounds in Appendix D ([THM-D.3.1]).

Once we compute V^* (via value iteration, which we will prove converges next), extracting the optimal policy is straightforward.

4.6 3.6 Contraction Mappings and the Banach Fixed-Point Theorem

The Bellman operator \mathcal{T} is a **contraction mapping**. This fundamental property guarantees: 1. Existence and uniqueness of the fixed point $V^* = \mathcal{T}V^*$ 2. Convergence of value iteration: $V_{k+1} = \mathcal{T}V_k \rightarrow V^*$ exponentially fast

We now develop this theory rigorously.

4.6.1 3.6.1 Normed Spaces and Contractions

Definition 3.6.1 (Normed Vector Space)

A **normed vector space** is a pair $(V, \|\cdot\|)$ where V is a vector space (over \mathbb{R} or \mathbb{C}) and $\|\cdot\| : V \rightarrow \mathbb{R}_+$ is a **norm** satisfying: 1. **Positive definiteness**: $\|v\| = 0 \iff v = 0$ 2. **Homogeneity**: $\|\alpha v\| = |\alpha| \|v\|$ for all scalars α 3. **Triangle inequality**: $\|u + v\| \leq \|u\| + \|v\|$ for all $u, v \in V$

Definition 3.6.2 (Supremum Norm)

For bounded measurable functions $f : \mathcal{S} \rightarrow \mathbb{R}$, the **supremum norm** (or ∞ -norm) is:

$$\|f\|_\infty := \sup_{s \in \mathcal{S}} |f(s)|. \quad (3.13)$$

We write $B_b(\mathcal{S})$ for the space of bounded measurable functions:

$$B_b(\mathcal{S}) := \{f : \mathcal{S} \rightarrow \mathbb{R} \text{ measurable} : \|f\|_\infty < \infty\}.$$

Then $(B_b(\mathcal{S}), \|\cdot\|_\infty)$ is a normed vector space.

Proposition 3.6.1 (Completeness of $(B_b(\mathcal{S}), \|\cdot\|_\infty)$)

The space $(B_b(\mathcal{S}), \|\cdot\|_\infty)$ is **complete**: every Cauchy sequence converges.

Proof. **Step 1** (Cauchy implies pointwise Cauchy). Let (f_n) be a Cauchy sequence in $B_b(\mathcal{S})$. For each $s \in \mathcal{S}$,

$$|f_n(s) - f_m(s)| \leq \|f_n - f_m\|_\infty \rightarrow 0 \quad \text{as } n, m \rightarrow \infty.$$

Thus $(f_n(s))$ is a Cauchy sequence in \mathbb{R} . Since \mathbb{R} is complete, $f_n(s) \rightarrow f(s)$ for some $f(s) \in \mathbb{R}$.

Step 2 (Uniform boundedness and measurability). Since (f_n) is Cauchy, it is bounded: $\sup_n \|f_n\|_\infty \leq M < \infty$. Thus $|f(s)| = \lim_n |f_n(s)| \leq M$ for all s , so $\|f\|_\infty \leq M < \infty$. Since each f_n is measurable and $f_n \rightarrow f$ pointwise, the limit f is measurable.

Step 3 (Uniform convergence). Given $\epsilon > 0$, choose N such that $\|f_n - f_m\|_\infty < \epsilon$ for all $n, m \geq N$. Fixing $n \geq N$ and taking $m \rightarrow \infty$:

$$|f_n(s) - f(s)| = \lim_{m \rightarrow \infty} |f_n(s) - f_m(s)| \leq \epsilon \quad \text{for all } s.$$

Thus $\|f_n - f\|_\infty \leq \epsilon$ for all $n \geq N$, proving $f_n \rightarrow f$ in $\|\cdot\|_\infty$. \square

Remark 3.6.1 (Banach spaces and uniform convergence). A complete normed space is called a **Banach space**. Proposition 3.6.1 shows $B_b(\mathcal{S})$ is a Banach space—this is essential for applying the Banach fixed-point theorem.

A crucial subtlety: Step 3 establishes **uniform convergence**, where $\sup_s |f_n(s) - f(s)| \rightarrow 0$. This is strictly stronger than **pointwise convergence** (where each $f_n(s) \rightarrow f(s)$ individually, which Step 1 provides). The space of bounded functions is complete under uniform convergence but *not* under pointwise convergence—a sequence of bounded continuous functions can converge pointwise to an unbounded or discontinuous function. This distinction matters: the Banach fixed-point theorem requires completeness in the norm topology, and value iteration convergence guarantees 3.7.3 are statements about uniform convergence over all states.

Definition 3.6.3 (Contraction Mapping)

Let $(V, \|\cdot\|)$ be a normed space. A mapping $T : V \rightarrow V$ is a **γ -contraction** if there exists $\gamma \in [0, 1)$ such that:

$$\|T(f) - T(g)\| \leq \gamma \|f - g\| \quad \text{for all } f, g \in V. \quad (3.14)$$

Intuition: T brings points closer together by a factor $\gamma < 1$. The distance between $T(f)$ and $T(g)$ is strictly smaller than the distance between f and g (unless $f = g$).

Example 3.6.1 (Scalar contraction). Let $V = \mathbb{R}$ with norm $|x|$. Define $T(x) = \frac{1}{2}x + 1$. Then:

$$|T(x) - T(y)| = \left| \frac{1}{2}(x - y) \right| = \frac{1}{2}|x - y|,$$

so T is a $1/2$ -contraction.

Non-Example 3.6.2 (Expansion). Define $T(x) = 2x$. Then $|T(x) - T(y)| = 2|x - y|$, so T is an **expansion**, not a contraction.

4.6.2 3.6.2 Banach Fixed-Point Theorem

Theorem 3.6.2 (Banach Fixed-Point Theorem)

Let $(V, \|\cdot\|)$ be a complete normed space (Banach space) and $T : V \rightarrow V$ a γ -contraction with $\gamma \in [0, 1)$. Then:

1. **Existence:** T has a **unique fixed point** $v^* \in V$ satisfying $T(v^*) = v^*$
2. **Convergence:** For any initial point $v_0 \in V$, the sequence $v_{k+1} = T(v_k)$ converges to v^*
3. **Rate:** The convergence is **exponential**:

$$\|v_k - v^*\| \leq \frac{\gamma^k}{1 - \gamma} \|T(v_0) - v_0\| \quad (3.15)$$

Proof. We prove each claim step-by-step.

Proof of (1): Uniqueness Suppose $T(v^*) = v^*$ and $T(w^*) = w^*$ are two fixed points. Then:

$$\|v^* - w^*\| = \|T(v^*) - T(w^*)\| \leq \gamma \|v^* - w^*\|.$$

Since $\gamma < 1$, this implies $\|v^* - w^*\| = 0$, hence $v^* = w^*$. \square (Uniqueness)

Proof of (2): Convergence to a fixed point **Step 1** (Sequence is Cauchy). Define $v_k := T^k(v_0)$ (applying T iteratively). For $k \geq 1$:

$$\|v_{k+1} - v_k\| = \|T(v_k) - T(v_{k-1})\| \leq \gamma \|v_k - v_{k-1}\|.$$

Iterating this inequality:

$$\|v_{k+1} - v_k\| \leq \gamma^k \|v_1 - v_0\|.$$

For $n > m$, by the triangle inequality:

$$\|v_n - v_m\| \leq \sum_{k=m}^{n-1} \|v_{k+1} - v_k\| \quad (1)$$

$$\leq \sum_{k=m}^{n-1} \gamma^k \|v_1 - v_0\| \quad (2)$$

$$= \gamma^m \frac{1 - \gamma^{n-m}}{1 - \gamma} \|v_1 - v_0\| \quad (3)$$

$$\leq \frac{\gamma^m}{1 - \gamma} \|v_1 - v_0\|. \quad (4)$$

Since $\gamma < 1$, $\gamma^m \rightarrow 0$ as $m \rightarrow \infty$, so (v_k) is a Cauchy sequence.

Step 2 (Completeness implies convergence). Since V is complete, there exists $v^* \in V$ such that $v_k \rightarrow v^*$.

Step 3 (Limit is a fixed point). Since T is a contraction, it is continuous. Thus:

$$T(v^*) = T\left(\lim_{k \rightarrow \infty} v_k\right) = \lim_{k \rightarrow \infty} T(v_k) = \lim_{k \rightarrow \infty} v_{k+1} = v^*.$$

So v^* is a fixed point. By uniqueness (proved above), it is the **unique** fixed point. \square (Existence and Convergence)

Proof of (3): Rate From Step 1 above, taking $m = 0$ and letting $n \rightarrow \infty$:

$$\|v^* - v_0\| \leq \sum_{k=0}^{\infty} \|v_{k+1} - v_k\| \leq \|v_1 - v_0\| \sum_{k=0}^{\infty} \gamma^k = \frac{\|v_1 - v_0\|}{1 - \gamma}.$$

For $k \geq 1$, applying the contraction property:

$$\|v_k - v^*\| = \|T(v_{k-1}) - T(v^*)\| \leq \gamma \|v_{k-1} - v^*\|.$$

Iterating:

$$\|v_k - v^*\| \leq \gamma^k \|v_0 - v^*\| \leq \frac{\gamma^k}{1 - \gamma} \|v_1 - v_0\|,$$

which is EQ-3.15. \square (Rate)

Remark 3.6.2 (The key mechanisms). This proof deploys several fundamental techniques:

1. **Telescoping series:** Write $\|v_n - v_m\| \leq \sum_{k=m}^{n-1} \|v_{k+1} - v_k\|$ to control differences
2. **Geometric series:** Bound $\sum_{k=m}^{\infty} \gamma^k = \gamma^m / (1 - \gamma)$ using $\gamma < 1$
3. **Completeness:** Cauchy sequences converge—this is **essential** and fails in incomplete spaces (e.g., rationals \mathbb{Q})
4. **Continuity from contraction:** Contractions are uniformly continuous, so limits pass through T

These techniques will reappear in convergence proofs for TD-learning (Chapters 8, 12) and stochastic approximation (later chapters).

Example 3.6.3 (Failure without completeness). Define $T : \mathbb{Q} \rightarrow \mathbb{Q}$ by $T(x) = (x + 2/x)/2$ —Newton-Raphson iteration for finding $\sqrt{2}$. Near $x = 1.5$, this map is a contraction: $|T(x) - T(y)| < 0.5|x - y|$ for $x, y \in [1, 2] \cap \mathbb{Q}$. Starting from $x_0 = 3/2 \in \mathbb{Q}$, the sequence $x_{k+1} = T(x_k)$ remains in \mathbb{Q} and converges... but to $\sqrt{2} \notin \mathbb{Q}$. The fixed point exists in \mathbb{R} but not in the incomplete space \mathbb{Q} . This is why completeness is essential

for [THM-3.6.2-Banach]—and why we need $B_b(\mathcal{S})$ to be a Banach space for value iteration to converge to a *valid* value function.

Remark 3.6.3 (The $1/(1-\gamma)$ factor). The bound EQ-3.15 shows the convergence rate depends on $1/(1-\gamma)$. When $\gamma \rightarrow 1$ (nearly undiscounted), convergence slows dramatically—this explains why high- γ RL (e.g., $\gamma = 0.99$) requires many iterations. The factor γ^k gives **exponential convergence**: doubling k squares the error.

4.7 3.7 Bellman Operator is a Contraction

We now prove the central result: the Bellman optimality operator \mathcal{T} is a γ -contraction on $(B_b(\mathcal{S}), \|\cdot\|_\infty)$.

Remark 3.7.0 (Self-mapping property). Before proving contraction, we verify that \mathcal{T} maps bounded measurable functions to bounded measurable functions. Under our standing assumptions—bounded rewards $|r(s, a)| \leq R_{\max}$ and discount $\gamma < 1$ ([DEF-3.4.1])—if $\|V\|_\infty < \infty$, then:

$$\|\mathcal{T}V\|_\infty = \sup_{s \in \mathcal{S}} \left| \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] \right| \leq R_{\max} + \gamma \|V\|_\infty < \infty.$$

This establishes boundedness. Measurability of $s \mapsto (\mathcal{T}V)(s)$ is immediate in the finite-action case (where the supremum is a maximum over finitely many measurable functions) and holds under standard topological hypotheses; see 2.8.2 and Chapter 2, §2.8.2 (in particular [THM-2.8.3]).

Theorem 3.7.1 (Bellman Operator Contraction)

The Bellman optimality operator $\mathcal{T} : B_b(\mathcal{S}) \rightarrow B_b(\mathcal{S})$ defined by:

$$(\mathcal{T}V)(s) = \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right]$$

is a γ -contraction with respect to $\|\cdot\|_\infty$:

$$\|\mathcal{T}V - \mathcal{T}W\|_\infty \leq \gamma \|V - W\|_\infty \quad \text{for all } V, W \in B_b(\mathcal{S}). \quad (3.16)$$

Proof. **Step 1** (Non-expansiveness of sup). For any real-valued functions f, g on \mathcal{A} ,

$$\left| \sup_{a \in \mathcal{A}} f(a) - \sup_{a \in \mathcal{A}} g(a) \right| \leq \sup_{a \in \mathcal{A}} |f(a) - g(a)|.$$

Indeed, $f(a) \leq g(a) + |f(a) - g(a)| \leq \sup_{a'} g(a') + \sup_{a'} |f(a') - g(a')|$ for all a , so taking \sup_a yields $\sup_a f(a) \leq \sup_a g(a) + \sup_a |f(a) - g(a)|$. Swapping f, g gives the reverse inequality, and combining yields the claim.

Step 2 (Pointwise contraction). Fix $s \in \mathcal{S}$ and define, for each $a \in \mathcal{A}$,

$$F_V(a) := r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a), \quad F_W(a) := r(s, a) + \gamma \int_{\mathcal{S}} W(s') P(ds' | s, a).$$

Then $(\mathcal{T}V)(s) = \sup_a F_V(a)$ and $(\mathcal{T}W)(s) = \sup_a F_W(a)$. By Step 1,

$$|(\mathcal{T}V)(s) - (\mathcal{T}W)(s)| \leq \sup_{a \in \mathcal{A}} |F_V(a) - F_W(a)| = \gamma \sup_{a \in \mathcal{A}} \left| \int_{\mathcal{S}} (V - W)(s') P(ds' | s, a) \right|.$$

Since $P(\cdot | s, a)$ is a probability measure and $V - W$ is bounded,

$$\left| \int_{\mathcal{S}} (V - W)(s') P(ds' | s, a) \right| \leq \int_{\mathcal{S}} |V(s') - W(s')| P(ds' | s, a) \leq \|V - W\|_\infty.$$

Therefore $|(\mathcal{T}V)(s) - (\mathcal{T}W)(s)| \leq \gamma \|V - W\|_\infty$ for all s .

Step 3 (Supremum over states). Taking $\sup_{s \in \mathcal{S}}$ yields $\|\mathcal{T}V - \mathcal{T}W\|_\infty \leq \gamma \|V - W\|_\infty$, which is (3.16). \square

Remark 3.7.1 (The sup-stability mechanism). The proof exploits the **non-expansiveness of sup**: taking a supremum is a 1-Lipschitz operation. Formally, for any functions f, g ,

$$|\sup_a f(a) - \sup_a g(a)| \leq \sup_a |f(a) - g(a)|.$$

This is a fundamental technique in dynamic programming theory, appearing in proofs of policy improvement theorems and error propagation bounds.

Remark 3.7.2 (Norm specificity). The contraction (3.16) holds specifically in the **sup-norm** $\|\cdot\|_\infty$. The Bellman operator is generally **not** a contraction in L^1 or L^2 norms—the proof crucially uses

$$\int_{\mathcal{S}} |V(s') - W(s')| P(ds' | s, a) \leq \|V - W\|_\infty,$$

which fails for other L^p norms. This norm choice has practical implications: error bounds in RL propagate through the $\|\cdot\|_\infty$ norm, meaning worst-case state errors matter most.

Corollary 3.7.2 (Existence and Uniqueness of V^*)

There exists a unique $V^* \in B_b(\mathcal{S})$ satisfying the Bellman optimality equation $V^* = \mathcal{T}V^*$.

Proof. Immediate from Theorems 3.6.2 and 3.7.1: \mathcal{T} is a γ -contraction on the Banach space $(B_b(\mathcal{S}), \|\cdot\|_\infty)$, so it has a unique fixed point. \square

Corollary 3.7.3 (Value Iteration Convergence)

For any initial value function $V_0 \in B_b(\mathcal{S})$, the sequence:

$$V_{k+1} = \mathcal{T}V_k \tag{3.17}$$

converges to V^* with exponential rate:

$$\|V_k - V^*\|_\infty \leq \frac{\gamma^k}{1-\gamma} \|\mathcal{T}V_0 - V_0\|_\infty. \tag{3.18}$$

Proof. Immediate from Theorems 3.6.2 and 3.7.1. \square

Proposition 3.7.4 (Reward perturbation sensitivity)

Fix $(\mathcal{S}, \mathcal{A}, P, \gamma)$ and let r and $\tilde{r} = r + \Delta r$ be bounded measurable one-step reward functions. Let V_r^* and $V_{\tilde{r}}^*$ denote the unique fixed points of the corresponding Bellman optimality operators on $B_b(\mathcal{S})$. Then:

$$\|V_{\tilde{r}}^* - V_r^*\|_\infty \leq \frac{\|\Delta r\|_\infty}{1-\gamma}.$$

Proof. Let \mathcal{T}_r and $\mathcal{T}_{\tilde{r}}$ denote the two Bellman optimality operators. For any $V \in B_b(\mathcal{S})$ and any $s \in \mathcal{S}$,

$$|(\mathcal{T}_{\tilde{r}}V)(s) - (\mathcal{T}_rV)(s)| = \left| \sup_{a \in \mathcal{A}} \left[\tilde{r}(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] - \sup_{a \in \mathcal{A}} \left[r(s, a) + \gamma \int_{\mathcal{S}} V(s') P(ds' | s, a) \right] \right| \leq \sup_{a \in \mathcal{A}} |\tilde{r}(s, a) - r(s, a)|.$$

so $\|\mathcal{T}_{\tilde{r}}V - \mathcal{T}_rV\|_\infty \leq \|\Delta r\|_\infty$.

Using the fixed point identities $V_r^* = \mathcal{T}_rV_r^*$ and $V_{\tilde{r}}^* = \mathcal{T}_{\tilde{r}}V_{\tilde{r}}^*$ and the contraction of $\mathcal{T}_{\tilde{r}}$,

$$\|V_{\tilde{r}}^* - V_r^*\|_\infty = \|\mathcal{T}_{\tilde{r}}V_{\tilde{r}}^* - \mathcal{T}_rV_r^*\|_\infty \leq \|\mathcal{T}_{\tilde{r}}V_{\tilde{r}}^* - \mathcal{T}_{\tilde{r}}V_r^*\|_\infty + \|\mathcal{T}_{\tilde{r}}V_r^* - \mathcal{T}_rV_r^*\|_\infty \leq \gamma \|V_{\tilde{r}}^* - V_r^*\|_\infty + \|\Delta r\|_\infty.$$

Rearranging yields $\|V_{\tilde{r}}^* - V_r^*\|_\infty \leq \|\Delta r\|_\infty / (1 - \gamma)$. \square

Remark 3.7.5 (Practical implications). Corollary 3.7.3 guarantees that **value iteration always converges**, regardless of initialization V_0 . The rate (3.18) shows that after k iterations, the error shrinks by γ^k . For $\gamma = 0.9$, we have $\gamma^{10} \approx 0.35$; for $\gamma = 0.99$, we need $k \approx 460$ iterations to reduce error by a factor of 100. This explains why high-discount RL is computationally expensive.

Remark 3.7.6 (OPE preview — Direct Method). Off-policy evaluation (Chapter 9) can be performed via a **model-based Direct Method**: estimate (\hat{P}, \hat{r}) and apply the policy Bellman operator repeatedly under the model to obtain

$$\widehat{V}^\pi := \lim_{k \rightarrow \infty} (\mathcal{T}_{\hat{P}, \hat{r}}^\pi)^k V_0, \quad (3.22)$$

for any bounded V_0 . The contraction property (with $\gamma < 1$ and bounded \hat{r}) guarantees existence and uniqueness of \widehat{V}^π . Chapter 9 develops full off-policy evaluation (IPS, DR, FQE), comparing the Direct Method previewed here to importance-weighted estimators.

Remark 3.7.7 (The deadly triad — when contraction fails). The contraction property 3.7.1 guarantees convergence for **exact**, **tabular** value iteration. However, three ingredients common in deep RL can break this guarantee:

1. **Function approximation**: Representing V or Q via neural networks restricts us to a function class \mathcal{F} . The composed operator $\Pi_{\mathcal{F}} \circ \mathcal{T}$ (project-then-Bellman) is generally **not** a contraction.
2. **Bootstrapping**: TD methods update toward $r + \gamma V(s')$, using the current estimate V . Combined with function approximation, this can cause divergence.
3. **Off-policy learning**: Learning about one policy while following another introduces distribution mismatch.

The combination—function approximation + bootstrapping + off-policy—is Sutton’s **deadly triad** ((Sutton and Barto 2018, sec. 11.3)). Classical counterexamples (e.g., Baird’s) demonstrate that the resulting learning dynamics can diverge even with linear function approximation. Chapter 7 introduces target networks and experience replay as partial mitigations. The fundamental tension, however, remains unresolved in theory—deep RL succeeds empirically despite lacking the contraction guarantees we have established here. Understanding this gap between theory and practice is a central theme of Part III.

4.8 3.8 Connection to Contextual Bandits ($\gamma = 0$)

The **contextual bandit** from Chapter 1 is the special case $\gamma = 0$ (no state transitions, immediate rewards only).

Definition 3.8.1 (Bandit Bellman Operator)

For a contextual bandit with Q-function $Q : \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R}$ (the expected immediate reward from Chapter 1), the **bandit Bellman operator** is:

$$(\mathcal{T}_{\text{bandit}} V)(x) := \sup_{a \in \mathcal{A}} Q(x, a). \quad (3.19)$$

This is precisely the MDP Bellman operator (3.12) specialized to $\gamma = 0$, since in the bandit setting the one-step reward is $r(x, a) = Q(x, a)$ (and when \mathcal{A} is finite the supremum is a maximum):

$$(\mathcal{T} V)(x) = \sup_a [r(x, a) + \gamma \cdot 0] = \sup_a Q(x, a) = (\mathcal{T}_{\text{bandit}} V)(x).$$

In particular, the right-hand side does not depend on V : bandits have no bootstrapping term, because there is no next-state value to propagate.

Proposition 3.8.1 (Bandit operator fixed point in one iteration)

For bandits ($\gamma = 0$), the optimal value function is:

$$V^*(x) = \sup_{a \in \mathcal{A}} Q(x, a), \quad (3.20)$$

and value iteration converges in **one step**: $V_1 = \mathcal{T}_{\text{bandit}}V_0 = V^*$ for any V_0 .

Proof. Since $\gamma = 0$, applying the Bellman operator:

$$(\mathcal{T}_{\text{bandit}}V)(x) = \sup_a Q(x, a) = V^*(x),$$

independent of V . Thus $V_1 = V^*$ for any V_0 . \square

Remark 3.8.1 (Contrast with MDPs). For $\gamma > 0$, value iteration requires multiple steps because we must propagate value information backward through state transitions. For bandits, there are no state transitions—rewards are immediate—so the optimal value is the statewise supremum of the immediate Q -values. This is why Chapter 1 could focus on learning $Q(x, a)$ without explicitly constructing value functions.

Remark 3.8.2 (Chapter 1 formulation). Recall from Chapter 1 the bandit optimality condition: the optimal value (1.9) is attained by the greedy policy (1.10), yielding

$$V^*(x) = \max_{a \in \mathcal{A}} Q(x, a), \quad Q(x, a) = \mathbb{E}_\omega[R(x, a, \omega)].$$

This is exactly (3.20). The bandit formulation is the $\gamma = 0$ MDP.

4.9 3.9 Computational Verification

We now implement value iteration and verify the convergence theory numerically.

4.9.1 3.9.1 Toy MDP: GridWorld Navigation

Setup: A 5×5 grid. Agent starts at $(0, 0)$, goal is $(4, 4)$. Actions: {up, down, left, right}. Rewards: +10 at goal, -1 per step (encourages shortest paths). Transitions: deterministic (move in chosen direction unless blocked by boundary).

```
from __future__ import annotations

from dataclasses import dataclass
from typing import Tuple

import numpy as np

@dataclass
class GridWorldConfig:
    size: int = 5
    gamma: float = 0.9
    goal_reward: float = 10.0

class GridWorldMDP:
    """Deterministic GridWorld used in Section 3.9.1."""

    def __init__(self, cfg: GridWorldConfig | None = None) -> None:
        self.cfg = cfg or GridWorldConfig()
        self.size = self.cfg.size
        self.gamma = self.cfg.gamma
        self.goal_reward = self.cfg.goal_reward

        self.goal = (self.size - 1, self.size - 1)
```

```

self.n_states = self.size * self.size
self.n_actions = 4 # up, down, left, right

self.P = np.zeros((self.n_states, self.n_actions, self.n_states))
self.r = np.zeros((self.n_states, self.n_actions))

for i in range(self.size):
    for j in range(self.size):
        s = self._state_index(i, j)
        if (i, j) == self.goal:
            for a in range(self.n_actions):
                self.P[s, a, s] = 1.0
                self.r[s, a] = self.goal_reward
            continue
        for a in range(self.n_actions):
            i_next, j_next = self._next_state(i, j, a)
            s_next = self._state_index(i_next, j_next)
            self.P[s, a, s_next] = 1.0
            self.r[s, a] = -1.0

def _state_index(self, i: int, j: int) -> int:
    return i * self.size + j

def _next_state(self, i: int, j: int, action: int) -> Tuple[int, int]:
    if action == 0: # up
        return max(i - 1, 0), j
    if action == 1: # down
        return min(i + 1, self.size - 1), j
    if action == 2: # left
        return i, max(j - 1, 0)
    return i, min(j + 1, self.size - 1) # right

def bellman_operator(self, values: np.ndarray) -> np.ndarray:
    q_values = self.r + self.gamma * np.einsum("ijk,k->ij", self.P, values)
    return np.max(q_values, axis=1)

def value_iteration(
    self,
    V_init: np.ndarray | None = None,
    *,
    max_iter: int = 256,
    tol: float = 1e-10,
) -> Tuple[np.ndarray, list[float]]:
    values = np.zeros(self.n_states) if V_init is None else V_init.copy()
    errors: list[float] = []
    for _ in range(max_iter):
        updated = self.bellman_operator(values)
        error = float(np.max(np.abs(updated - values)))
        errors.append(error)
        values = updated
        if error < tol:
            break
    return values, errors

```

```

def run_gridworld_convergence_check() -> None:
    mdp = GridWorldMDP()
    V_star, errors = mdp.value_iteration()

    start_state = mdp._state_index(0, 0)
    goal_state = mdp._state_index(*mdp.goal)
    expected_goal = mdp.goal_reward / (1.0 - mdp.gamma)

    print("iters", len(errors), "final_err", f"{errors[-1]:.3e}")
    print("V_start", f"{V_star[start_state]:.6f}")
    print("V_goal", f"{V_star[goal_state]:.6f}", "expected_goal", f"{expected_goal:.6f}")

    V_init = np.zeros(mdp.n_states)
    initial_gap = float(np.max(np.abs(mdp.bellman_operator(V_init) - V_init)))
    print("initial_gap", f"{initial_gap:.6f}")

    print("k ||V_{k+1}-V_k||_inf bound_from_EQ_3_18 bound_ok")
    for k, err in enumerate(errors[:10]):
        bound = (mdp.gamma**k / (1.0 - mdp.gamma)) * initial_gap
        bound_ok = err <= bound + 1e-9
        print(f"{k:2d} {err:18.10f} {bound:16.10f} {bound_ok}")

    ratios = [
        errors[k] / errors[k - 1]
        for k in range(1, min(len(errors), 25))
        if errors[k - 1] > 1e-12
    ]
    tail = ratios[-8:]
    print("tail_ratios", " ".join(f"{r:.4f}" for r in tail))

    grid = V_star.reshape((mdp.size, mdp.size))
    print("grid")
    for i in range(mdp.size):
        print(" ".join(f"{grid[i, j]:7.2f}" for j in range(mdp.size)))

```

run_gridworld_convergence_check()

Output:

```

iters 242 final_err 9.386e-11
V_start 37.351393
V_goal 100.000000 expected_goal 100.000000
initial_gap 10.000000
k ||V_{k+1}-V_k||_inf bound_from_EQ_3_18 bound_ok
 0      10.0000000000  100.0000000000  True
 1      9.0000000000   90.0000000000  True
 2      8.1000000000   81.0000000000  True
 3      7.2900000000   72.9000000000  True
 4      6.5610000000   65.6100000000  True
 5      5.9049000000   59.0490000000  True
 6      5.3144100000   53.1441000000  True
 7      4.7829690000   47.8296900000  True
 8      4.3046721000   43.0467210000  True

```

```

9          3.8742048900    38.7420489000  True
tail_ratios 0.9000 0.9000 0.9000 0.9000 0.9000 0.9000 0.9000 0.9000
grid
 37.35  42.61  48.46  54.95  62.17
 42.61  48.46  54.95  62.17  70.19
 48.46  54.95  62.17  70.19  79.10
 54.95  62.17  70.19  79.10  89.00
 62.17  70.19  79.10  89.00  100.00

```

Code ↔ Lab (Contraction Verification)

We verify 3.7.3 and the rate bound (3.18) using the value-iteration listing above. The repository also includes a regression test that mirrors this computation: `tests/ch03/test_value_iteration.py`. - Run: `.venv/bin/pytest -q tests/ch03/test_value_iteration.py`

4.9.2 3.9.2 Analysis

The numerical experiment confirms:

1. **Convergence:** value iteration converges within the configured iteration budget, with final update size below the tolerance.
2. **Rate bound check:** the printed quantity $\|V_{k+1} - V_k\|_\infty$ remains below the right-hand side of (3.18) in the displayed iterations, providing a numerical sanity check on the contraction-based rate.
3. **Exponential decay:** consecutive error ratios are essentially constant at $\gamma = 0.9$, matching the contraction mechanism.
4. **Goal-state semantics:** since the goal is absorbing with per-step reward `goal_reward`, we obtain $V^*(\text{goal}) = \text{goal_reward}/(1 - \gamma)$.

Key observations:

- The theoretical bound is **tight**: observed errors track γ^k behavior closely
- Higher γ (closer to 1) implies slower convergence: for $\gamma = 0.99$, convergence requires on the order of hundreds of iterations in this GridWorld.
- Value iteration is **robust**: it converges for any initialization V_0 (here $V_0 \equiv 0$)

4.10 3.10 RL Bridges: Previewing Multi-Episode Dynamics

In Chapter 11 we extend the within-session MDP of this chapter to an inter-session (multi-episode) MDP. Chapter 1's contextual bandit formalism and the discounted MDP formalism of this chapter both treat a single session in isolation. In practice, many objectives are inter-session: actions taken today influence the probability of future sessions and the distribution of future states.

The multi-episode formulation introduces three concrete changes:

1. Inter-session state transitions: the state includes variables such as satisfaction, recency, and loyalty tier, and these evolve across sessions as functions of engagement signals (clicks, purchases) and exogenous factors (seasonality).
2. Retention (hazard) modeling: a probabilistic mechanism decides whether another session occurs, based on the current inter-session state.
3. Long-term value across sessions: the return sums rewards over sessions, not only within a single session.

The operator-theoretic content does not change: once inter-session dynamics are part of the transition kernel, Bellman operators remain contractions under discounting, and value iteration remains a fixed-point method. Conceptually, this clarifies reward design. Chapter 1's reward (1.2) includes $\delta \cdot \text{CLICKS}$ as a proxy for long-run value; in Chapter 11 we encode engagement into the state dynamics through retention, so long-run effects are represented without relying on a separate proxy term.

Code ↔ Reward (MOD-zoosim.dynamics.reward)

Chapter 1's single-step reward (1.2) maps to configuration and aggregation code:

- Weights and defaults: `zoosim/core/config.py:195` (`RewardConfig`)
- Engagement weight guardrail (`delta`/
`alpha` bound): `zoosim/dynamics/reward.py:56` These safeguards keep δ small and bounded in the MVP regime while we develop multi-episode value in Chapter 11.

Code	\leftrightarrow	Simulator	(MOD-zoosim.multi_episode.session_env, MOD-zoosim.multi_episode.retention)	MOD-
------	-------------------	-----------	---	------

Multi-episode transitions and retention are implemented in the simulator:

- Inter-session MDP wrapper: `zoosim/multi_episode/session_env.py:79` (`MultiSessionEnv.step`)
- Retention probability (logistic hazard): `zoosim/multi_episode/retention.py:22` (`return_probability`)
- Retention config: `zoosim/core/config.py:208` (`RetentionConfig`), `zoosim/core/config.py:216` (`base_rate`), `zoosim/core/config.py:217` (`click_weight`), `zoosim/core/config.py:218` (`satisfaction_weight`) In this regime, engagement enters via state transitions, aligning with the long-run objective previewed by (1.2') and Chapter 11.

4.11 3.11 Summary: What We Have Built

This chapter established the operator-theoretic foundations of reinforcement learning:

Stochastic processes (Section 3.2–3.3):

- Filtrations (\mathcal{F}_t) model information accumulation over time
- Stopping times τ capture random termination (session abandonment, purchase events)
- Adapted processes ensure causality (policies depend on history, not future)

Markov Decision Processes (Section 3.4):

- Formal tuple $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ with standard Borel assumptions
- Value functions $V^\pi(s)$, $Q^\pi(s, a)$ as expected cumulative rewards
- Bellman equations (3.7) and (3.10) as recursive characterizations

Contraction theory (Section 3.6–3.7):

- Banach fixed-point theorem 3.6.2 guarantees existence, uniqueness, and exponential convergence
- Bellman operator \mathcal{T} is a γ -contraction in sup-norm 3.7.1
- Value iteration $V_{k+1} = \mathcal{T}V_k$ converges at rate γ^k 3.7.3
- Caveat: Contraction fails with function approximation (deadly triad, Remark 3.7.7)

Connection to bandits (Section 3.8):

- Contextual bandits are the $\gamma = 0$ special case (no state transitions)
- Chapter 1's formulation ([EQ-1.8], (1.9), and [EQ-1.10]) is recovered exactly

Numerical verification (Section 3.9):

- GridWorld experiment confirms theoretical convergence rate (3.18)
- Exponential decay γ^k observed empirically

What comes next:

- **Chapter 4–5:** Build the simulator (`zoosim`) with catalog, users, queries, click models
- **Chapter 6:** Implement LinUCB and Thompson Sampling for discrete template bandits
- **Chapter 7:** Continuous action optimization via $Q(x, a)$ regression
- **Chapter 9:** Off-policy evaluation (OPE) using importance sampling
- **Chapter 10:** Production guardrails (CM2 floors, *Delta*
textRank@k stability) applying CMDP theory from Section 3.5
- **Chapter 11:** Multi-episode MDPs with retention dynamics

All later algorithms—TD-learning, Q-learning, policy gradients—use Bellman operators as their organizing object, but their convergence guarantees require additional assumptions and are established case-by-case in

later chapters. In Chapter 3, the contraction property yields a complete convergence story for exact dynamic programming, and the fixed-point theorem tells us what value iteration converges to.

4.12 3.12 Exercises

Exercise 3.1 (Stopping times) [15 min]

Let (S_t) be a user satisfaction process with $S_t \in [0, 1]$. Which of the following are stopping times?

- (a) $\tau_1 = \inf\{t : S_t < 0.3\}$ (first time satisfaction drops below 0.3)
- (b) $\tau_2 = \sup\{t \leq T : S_t \geq 0.8\}$ (last time satisfaction exceeds 0.8 before horizon T)
- (c) $\tau_3 = \min\{t : S_{t+1} < S_t\}$ (first time satisfaction decreases)

Justify the answers using 3.2.4.

Exercise 3.2 (Bellman equation verification) [15 min]

Consider a 2-state MDP with $\mathcal{S} = \{s_1, s_2\}$, $\mathcal{A} = \{a_1, a_2\}$, $\gamma = 0.9$. Transitions and rewards:

$$P(\cdot | s_1, a_1) = (0.8, 0.2), \quad r(s_1, a_1) = 5 \quad (5)$$

$$P(\cdot | s_1, a_2) = (0.2, 0.8), \quad r(s_1, a_2) = 10 \quad (6)$$

$$P(\cdot | s_2, a_1) = (0.5, 0.5), \quad r(s_2, a_1) = 2 \quad (7)$$

$$P(\cdot | s_2, a_2) = (0.3, 0.7), \quad r(s_2, a_2) = 8 \quad (8)$$

Given $V(s_1) = 50$, $V(s_2) = 60$, compute $(\mathcal{T}V)(s_1)$ and $(\mathcal{T}V)(s_2)$ using (3.12).

Exercise 3.3 (Contraction property) [20 min]

Prove that the Bellman expectation operator \mathcal{T}^π for a fixed policy π (defined in [EQ-3.9]) is a γ -contraction, using a similar argument to 3.7.1.

Exercise 3.4 (Value iteration implementation) [extended: 30 min]

Implement value iteration for the GridWorld MDP from Section 3.9.1, but with **stochastic transitions**: with probability 0.8, the agent moves in the intended direction; with probability 0.2, it moves in a random perpendicular direction. Verify that:

- (a) Value iteration still converges
- (b) The convergence rate satisfies (3.18)
- (c) The optimal policy changes (compare to deterministic case)

4.12.1 Labs

- Lab 3.1 — Contraction Ratio Tracker: execute the GridWorld contraction experiment and compare empirical ratios against the γ bound in (3.16).
- Lab 3.2 — Value Iteration Wall-Clock Profiling: sweep multiple discounts, log iteration counts, and tie the scaling back to 3.7.3 (value iteration convergence rate).

Exercise 3.5 (Bandit special case) [10 min]

Verify that for $\gamma = 0$, the Bellman operator (3.12) reduces to the bandit operator (3.19). Explain why value iteration converges in one step for bandits.

Exercise 3.6 (Discount factor exploration) [20 min]

Using the GridWorld code from Section 3.9.1, run value iteration for $\gamma \in \{0.5, 0.7, 0.9, 0.99\}$. Plot the number of iterations required for convergence (tolerance 10^{-6}) as a function of γ . Explain the relationship using (3.18).

Exercise 3.7 (RL preview: Policy evaluation) [extended: 30 min]

Implement **policy evaluation** (iterative computation of V^π for a fixed policy π using [EQ-3.8]). For the GridWorld MDP:

- (a) Define a suboptimal policy π : always go right unless at right edge (then go down)
 - (b) Compute V^π via policy evaluation: $V_{k+1} = \mathcal{T}^\pi V_k$
 - (c) Compare V^π to V^* (from value iteration)
 - (d) Verify that $V^\pi(s) \leq V^*(s)$ for all s (why must this hold?)
-

4.13 References

See `docs/references.bib` for full citations.

Key references for this chapter: - (Puterman 2014) — Definitive MDP textbook (Puterman) - (Bertsekas 2012) — Dynamic programming and optimal control (Bertsekas) - (Folland 1999) — Measure theory and functional analysis foundations - (Brezis 2011) — Banach space theory and operator methods - (Sutton and Barto 2018) — Modern RL textbook and the deadly triad discussion

4.14 3.13 Production Checklist

Production Checklist (Chapter 3)

- **Seeds:** Ensure RNGs for stochastic MDPs use fixed seeds from `SimulatorConfig.seed` for reproducibility
- **Discount factor:** Document γ choice in config files; highlight $\gamma \rightarrow 1$ convergence slowdown
- **Numerical stability:** Use double precision (`float64`) for value iteration to avoid accumulation errors
- **Cross-references:** Update Knowledge Graph (`docs/knowledge_graph/graph.yaml`) with all theorem/definition IDs
- **Tests:** Add regression tests for value iteration convergence (verify (3.18) bounds programmatically)

4.15 Exercises & Labs

Companion material for Chapter 3 lives in:

- Exercises and runnable lab prompts: `docs/book/ch03/exercises_labs.md`
- Worked solutions with printed outputs: `docs/book/ch03/ch03_lab_solutions.md`

Reproducibility checks:

- Chapter 3 regression test: `.venv/bin/pytest -q tests/ch03/test_value_iteration.py`
- Run all Chapter 3 labs: `.venv/bin/python scripts/ch03/lab_solutions.py --all`

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