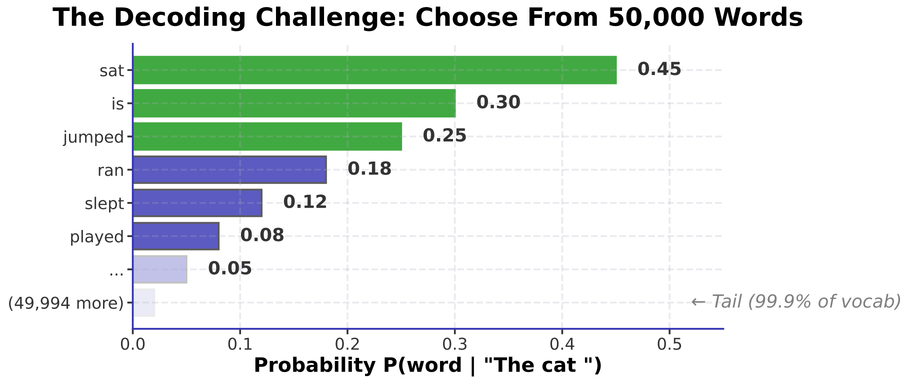
Decoding Strategies

Week 9: From Probabilities to Text

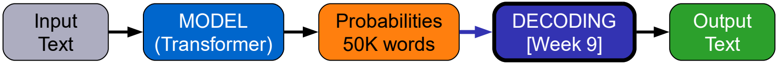
November 2025



The Question: Given these probabilities for "The cat __", which word should we pick?

At each step, model outputs probability distribution over entire vocabulary - how do we choose?

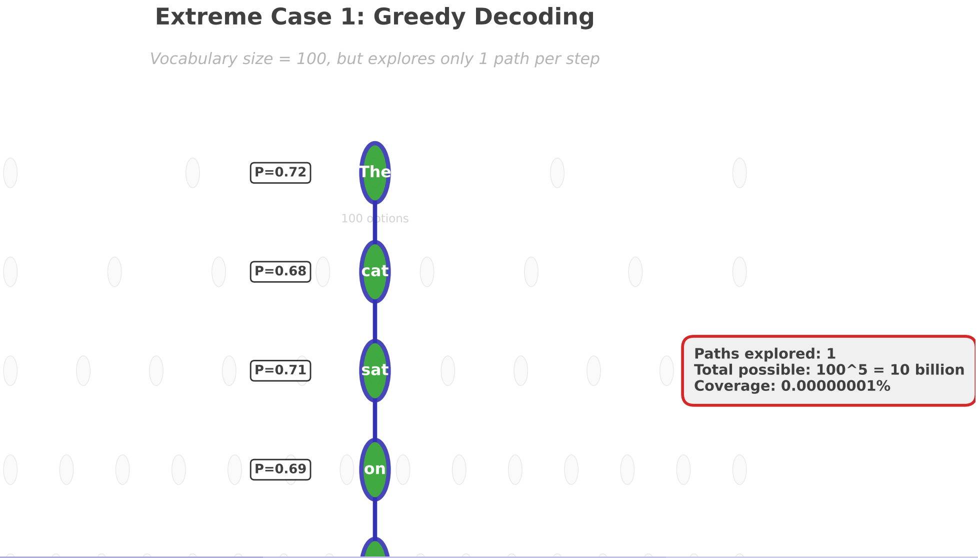
Context: How We Got Here



Our Journey:

1. We trained models (Weeks 3-7: RNN $\rightarrow$ Transformers $\rightarrow$ BERT/GPT)
2. They learned to predict: $P(\text{word}|\text{context})$
3. They output probability distributions over 50,000+ words
4. **Today**: How do we convert these probabilities into actual text?

Models predict probabilities. Decoding converts probabilities to text.


Extreme Case 1: Greedy Decoding
Vocabulary size = 100, but explores only 1 path per step
P=0.72
The
100 options
P=0.68
cat
P=0.71
sat
P=0.69
on
Paths explored: 1
Total possible: 100^5 = 10 billion
Coverage: 0.00000001%

What If We Explored More Paths?

Greedy chose: “The cat sat” (P=0.68)

But it ignored these alternatives:

“The cat walked”	P=0.12	(might lead to better text)
“The cat jumped”	P=0.08	(more interesting)
“The cat slept”	P=0.06	(different story)
“The cat ran”	P=0.04	(action-oriented)

Question: What if we kept ALL 100 words at each step?

Think: $100 \times 100 \times 100 \times 100 \times 100 = ?$

What If We Explored More Paths?

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But it ignored these alternatives:

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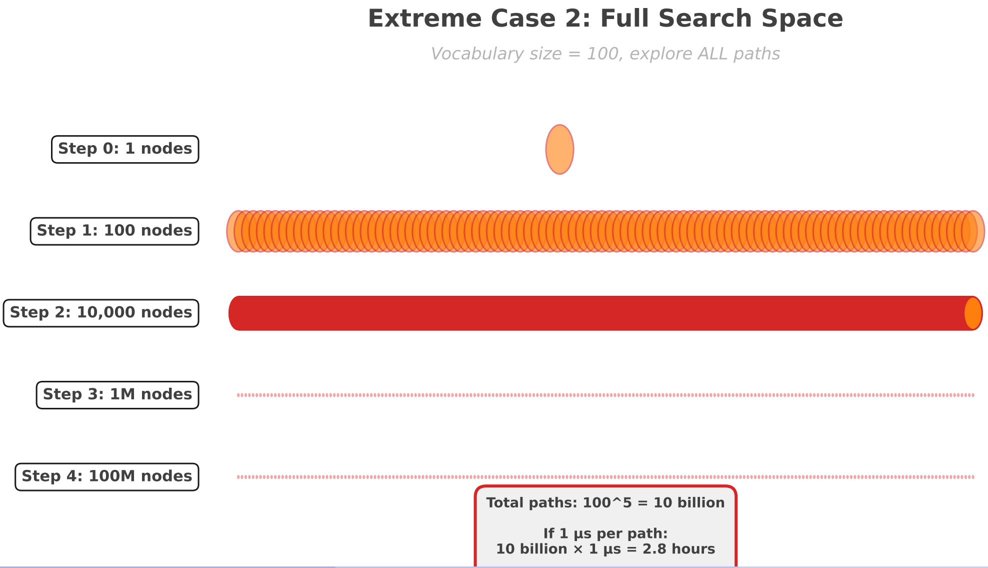
Question: What if we kept ALL 100 words at each step?

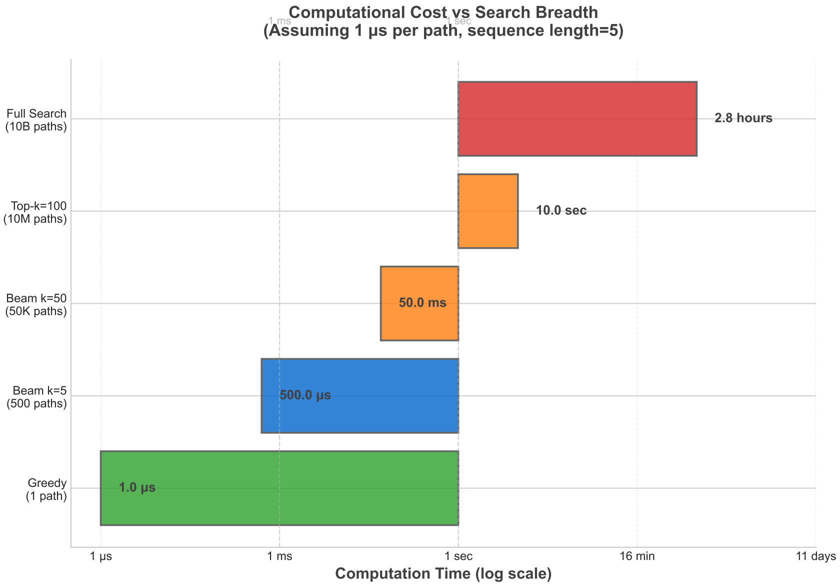
Think: $100 \times 100 \times 100 \times 100 \times 100 = ?$

Answer: 10 billion paths! Let's see what happens...

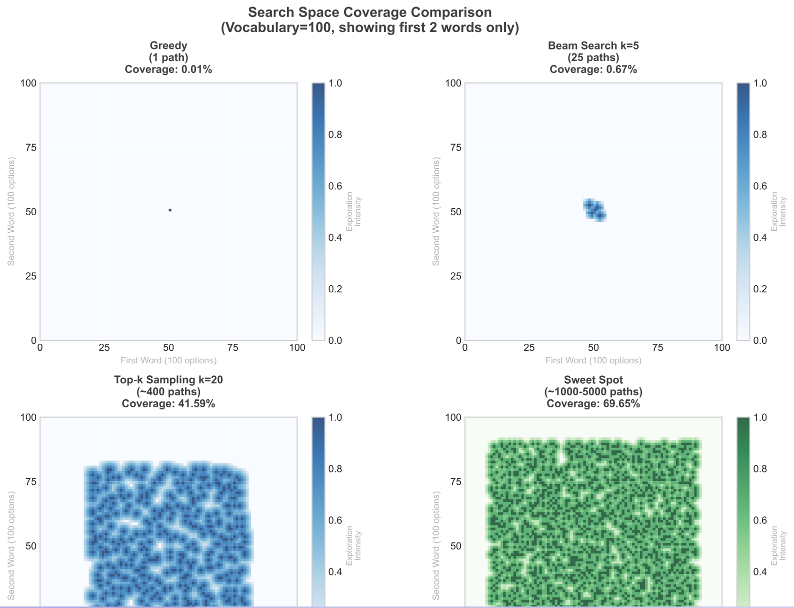
From 1 path to ALL paths - what could go wrong?


Extreme Case 2: Full Search Space
Vocabulary size = 100, explore ALL paths
Step 0: 1 nodes
Step 1: 100 nodes
Step 2: 10,000 nodes
Step 3: 1M nodes
Step 4: 100M nodes
Total paths: 100^5 = 10 billion
If 1 μs per path:
10 billion × 1 μs = 2.8 hours

The Computational Reality



Finding the Sweet Spot



Method 1: Greedy Decoding

Core Mechanism:

$$w_t = \underset{w \in V}{\operatorname{argmax}}\, P(w \mid w_1, \ldots, w_{t-1})$$

At each step, pick the single word with highest probability

Characteristics:

- Deterministic (same input $\rightarrow$ same output)
- Fast: O(1) per step
- No exploration

Method 1 of 6: Greedy = always pick argmax

Method 2: Beam Search

Core Mechanism:
Maintain k hypotheses ("beams") at each step
Expand each hypothesis, keep top-k by cumulative probability

Characteristics:

- Explores k paths simultaneously (typically k=3-5)
- Trade exploration vs computation
- Still deterministic for fixed k

Method 2 of 6: Beam = keep top-k paths

Core Mechanism:

$$P_T(w_i) = \frac{\exp(z_i/T)}{\sum_j \exp(z_j/T)}$$

Reshape probability distribution with temperature T, then sample

Characteristics:

- T ¡ 1: More focused (sharper distribution)
- T ¿ 1: More random (flatter distribution)
- Stochastic: different output each time

Method 3 of 6: Temperature = control randomness

Method 4: Top-k Sampling

Core Mechanism:

1. Sort words by probability
2. Keep only top k words (e.g., k=50)
3. Renormalize and sample from these k

Characteristics:

- Filters out low-probability “junk” words
- Fixed cutoff (always k words)
- Can combine with temperature

Method 4 of 6: Top-k = filter then sample

Method 5: Nucleus (Top-p) Sampling

Core Mechanism:

1. Sort words by probability
2. Keep minimum set where cumulative probability $\geq$ p
3. Sample from this set

Characteristics:

- Adaptive: number of words varies
- Focuses on “nucleus” of probability mass (typically p=0.9)
- Adjusts to distribution shape

Method 5 of 6: Nucleus = adaptive probability mass

Method 6: Contrastive Search

Core Mechanism:
Choose word that maximizes:

$$\text{score} = (1 - \alpha) \cdot \text{model probability} - \alpha \cdot \text{similarity to previous}$$

Penalize words similar to already-generated text

Characteristics:

- Explicitly avoids repetition
- Balances coherence and diversity
- Deterministic with hyperparameter α

Method 6 of 6: Contrastive = penalize repetition

Checkpoint Quiz 1: Match the Method

Methods:

1. Greedy
2. Beam Search
3. Temperature
4. Top-k
5. Nucleus
6. Contrastive

Match to Mechanisms:

A. Sample from reshaped distribution

B. Keep top-k paths at each step

C. Always pick argmax

D. Filter to k words, then sample

E. Penalize similarity to previous

F. Adaptive probability mass cutoff

Checkpoint Quiz 1: Match the Method

Methods:

1. Greedy
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Match to Mechanisms:

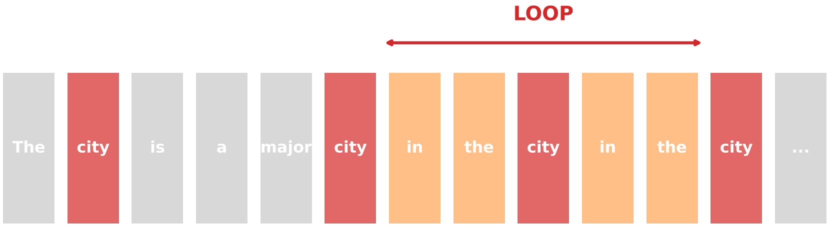
A. Sample from reshaped distribution
B. Keep top-k paths at each step
C. Always pick argmax
D. Filter to k words, then sample
E. Penalize similarity to previous
F. Adaptive probability mass cutoff

Answers: 1→C, 2→B, 3→A, 4→D, 5→F, 6→E

Now you know the toolbox - let's see WHY each tool exists!

Quiz 1: Can you match each method to its mechanism?

Greedy Decoding Gets Stuck



Output: "The city is a major city in the city in the city..."

Greedy's Problem: Trapped in loops, can't escape
Why Beam Helps: Explores k=3-5 paths, avoids greedy trap

Problem 1 of 6: Greedy decoding creates loops → Beam search explores alternatives

High Temperature Creates Nonsense

The	**glorp**	is	very	**blorptastic**	
She	likes	to	eat	**qwerty**	food
I	went	to	the	**flurb**	yesterday
The	weather	is	**zxqp**	today	

Generated words not in vocabulary!

Greedy & Beam's Problem: Same input → same output always
Why Temperature Helps: Sampling introduces randomness, enables creativity

Problem 2 of 6: Deterministic methods lack variation → Temperature adds controlled randomness

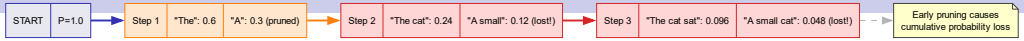
Zero Creativity: Always Same Output

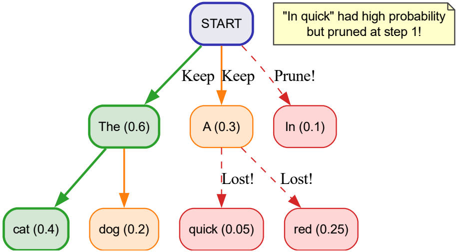
Asked 100 times → Always: "The weather is nice today."

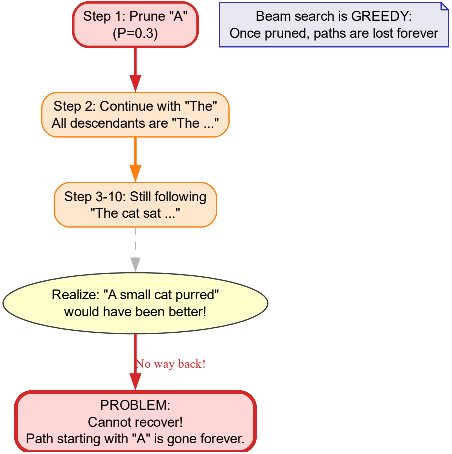
Temperature's Problem: Pure sampling includes low-quality words
Why Top-k Helps: Filter to k=50 best words, then sample

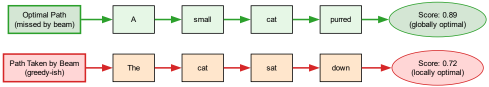
Problem 3 of 6: Can't balance quality & creativity → Top-k filters unlikely words

Beam Search Limitation: Missing Better Paths





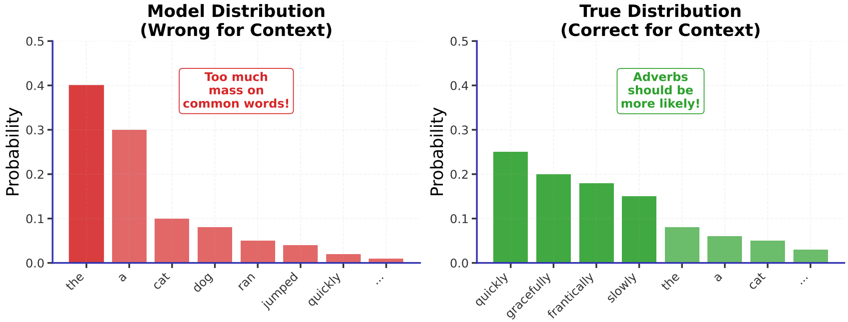




Problem 4 of 6: Even beam search prunes early, cannot recover optimal path - 4 perspectives

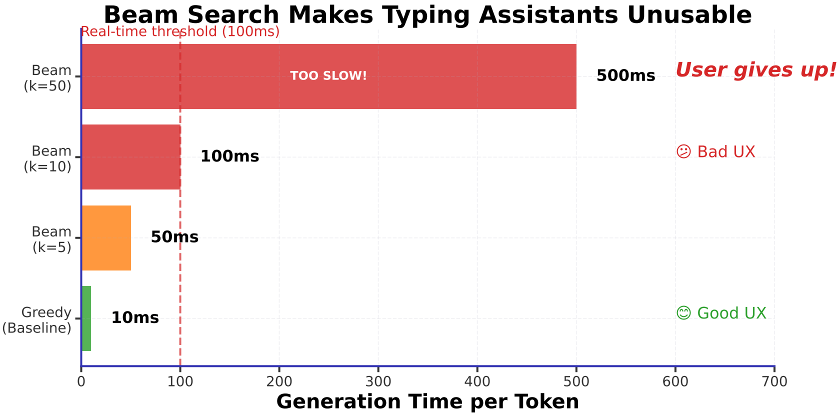
Why Nucleus? Problem: Distribution Tail Contains Junk

Context: "The cat ran ___"



Top-k's Problem: Fixed k doesn't adapt to distribution shape
Why Nucleus Helps: Adaptive cutoff at p=0.9 probability mass

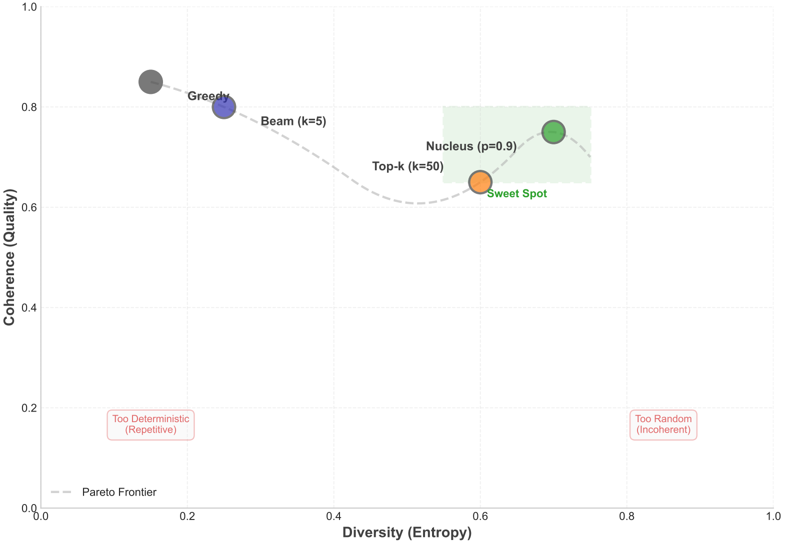
Problem 5 of 6: Tail contains junk → Nucleus adapts to distribution



All Methods' Problem: Can still produce generic, repetitive text
Why Contrastive Helps: Explicitly penalizes similarity to previous tokens

Problem 6 of 6: Generic text persists → Contrastive reduces repetition

The Quality-Diversity Tradeoff



Solution 1 → Beam Search: Explore Multiple Paths

Problem 1 Recap:
Greedy decoding: Trapped in loops
Always picks highest probability
Misses better sequences

Need: Way to explore alternatives

Solution: Beam Search:
Keep top-k paths at each step
Explore k=3-5 hypotheses simultaneously
Pick best complete sequence at end

Result: Finds better sequences than greedy

How it solves Problem 1: Maintains multiple candidates, avoids greedy trap

Solution 1 of 6: Beam search for better quality

Solution 2 → Temperature: Add Controlled Randomness

Problem 2 Recap:
No diversity: Same output always
Deterministic selection
No creativity

Need: Controlled randomness

Solution: Temperature:
Reshape probability distribution
T ¡ 1: More focused
T ¿ 1: More random
Sample from adjusted distribution

Result: Different outputs each time

How it solves Problem 2: Sampling introduces stochasticity, enables diversity

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Solution 2 of 6: Temperature for creativity control

Solution 3 → Top-k: Filter Unlikely Words

Problem 3 Recap:
Can't balance quality & creativity
Pure sampling too random
Greedy too boring

Need: Filter bad words, keep good

Solution: Top-k Sampling:
Keep only top-k most likely tokens
Cut tail of distribution
Renormalize probabilities
Sample from filtered set

Result: Diverse but not nonsensical

How it solves Problem 3: Fixed cutoff prevents tail sampling while allowing creativity

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Solution 3 of 6: Top-k for controlled sampling

Solution 4 $\rightarrow$ Nucleus: Dynamic Vocabulary Cutoff

Problem 4 Recap:
Top-k has fixed cutoff
Peaked distribution: Wastes probability
Flat distribution: Still allows junk

Need: Adaptive cutoff

Solution: Nucleus (Top-p):
Choose smallest set with cumulative prob $\geq$ p
Adapts to distribution shape
Peaked $\rightarrow$ small nucleus (2-3 words)
Flat $\rightarrow$ large nucleus (50+ words)

Result: Automatic quality-diversity balance

How it solves Problem 4: Dynamic cutoff adapts to each prediction step

Solution 4 of 6: Nucleus for adaptive sampling

Solution 5 $\rightarrow$ Top-k + Temperature: Hybrid Control

Problem 5 Recap:
Temperature alone doesn't filter tail
Top-k alone doesn't control randomness
Need both filtering AND tuning

Need: Combine strategies

Solution: Hybrid Methods:
Apply temperature THEN top-k
Or: Apply nucleus THEN temperature
Leverages strengths of both
Production systems use combinations

Result: Fine-grained control over generation

How it solves Problem 5: Layered strategies handle multiple issues simultaneously

Solution 5 of 6: Hybrid methods for comprehensive control

Solution 6 $\rightarrow$ Contrastive: Explicit Degeneration Prevention

Problem 6 Recap:
Repetition even with sampling
Long generation degenerates
Context similarity causes loops

Need: Explicit repetition penalty

Solution: Contrastive Search:
Score = Probability - $\alpha\times$ Similarity
Penalize tokens similar to recent context
Balance quality with diversity
Modern standard for long text

Result: Human-like text without repetition

How it solves Problem 6: Direct similarity penalty prevents copying context

Solution 6 of 6: Contrastive for degeneration-free generation

Checkpoint Quiz 2: Which Method for Which Problem?

Match Solution to Problem:

1. Beam Search $\rightarrow$?
2. Temperature $\rightarrow$?
3. Top-k $\rightarrow$?
4. Nucleus $\rightarrow$?
5. Hybrid $\rightarrow$?
6. Contrastive $\rightarrow$?

Problems to Solve:

A. Too boring OR too crazy
B. Missing better paths
C. Wrong distribution tail
D. No diversity
E. Repetition despite diversity
F. Dynamic vocabulary needed

Checkpoint Quiz 2: Which Method for Which Problem?

Match Solution to Problem:

1. Beam Search → ?
2. Temperature → ?
3. Top-k → ?
4. Nucleus → ?
5. Hybrid → ?
6. Contrastive → ?

Problems to Solve:

A. Too boring OR too crazy
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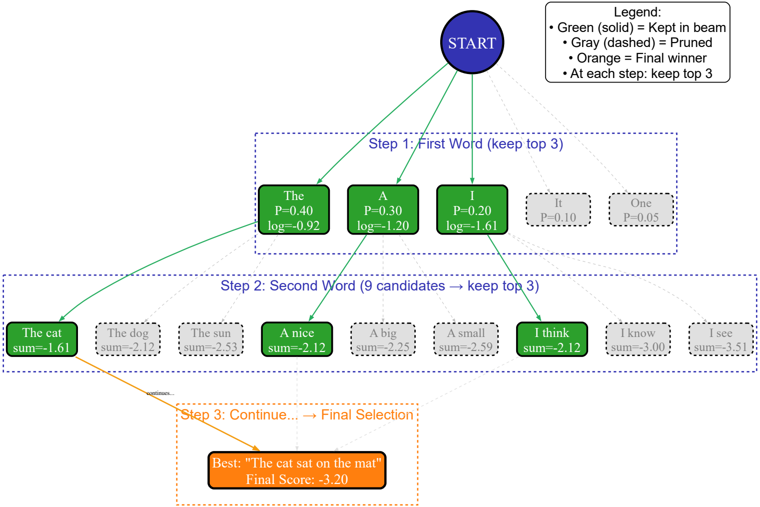
Answers: 1→B, 2→D, 3→A, 4→F, 5→C, 6→E

Each method targets a specific failure mode!

Quiz 2: Understanding the method-problem mapping

Beam Search: Step-by-Step Example



Beam Search: Algorithm & Settings

Algorithm:

1. Start: Keep top-k tokens
2. Expand: Generate continuations for each
3. Score: Multiply probabilities
4. Prune: Keep top-k sequences
5. Repeat until END token

Scoring:

$$\text{score}(y_1 \ldots y_t) = \prod_{i=1}^{t} P(y_i | y_{<i})$$

With length normalization:

$$\text{score} = \frac{1}{t} \sum_{i=1}^{t} \log P(y_i | y_{<i})$$

Best For:

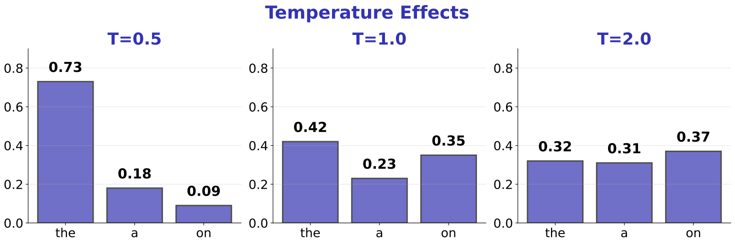
- Machine translation
- Summarization
- Question answering
- Tasks with "correct" answer

Parameters:
Width = 3-5 (translation)
Width = 10 (diverse outputs)

Tradeoffs:
+ Better quality than greedy
+ Diverse hypotheses
- Still deterministic
- 4-5× slower than greedy

Beam search is the workhorse for deterministic tasks

Temperature Sampling: Control Randomness



Key Insight: Temperature reshapes probability distribution

T $<$ 1: more focused. T $=$ 1: unchanged. T $>$ 1: more random

Temperature: Step-by-Step Calculation

Given: Logits = [2.0, 1.0, 0.5, 0.2]
Tokens = ["cat", "dog", "bird", "fish"]

T=0.5: [4.0, 2.0, 1.0, 0.4] → [0.73, 0.18, 0.07, 0.02]

→ 73% on "cat" (FOCUSED)

T=1.0: [2.0, 1.0, 0.5, 0.2] → [0.42, 0.23, 0.16, 0.13]

→ 42% on "cat" (BALANCED)

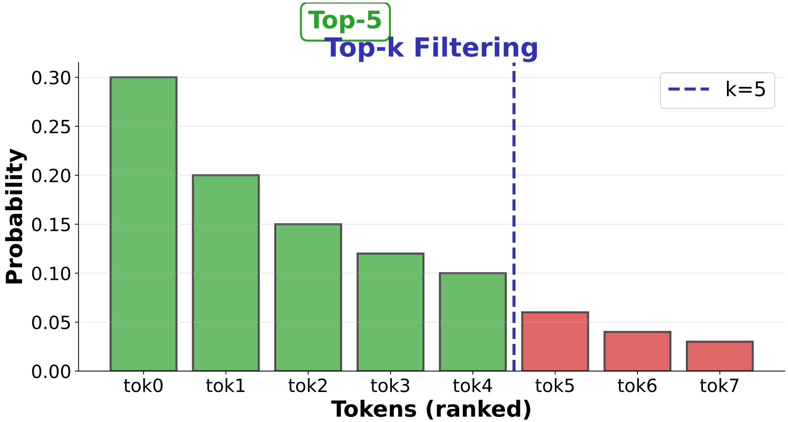
T=2.0: [1.0, 0.5, 0.25, 0.1] → [0.32, 0.26, 0.23, 0.19]

→ 32% on "cat" (FLAT)

Lower T = more peaked | Higher T = more flat

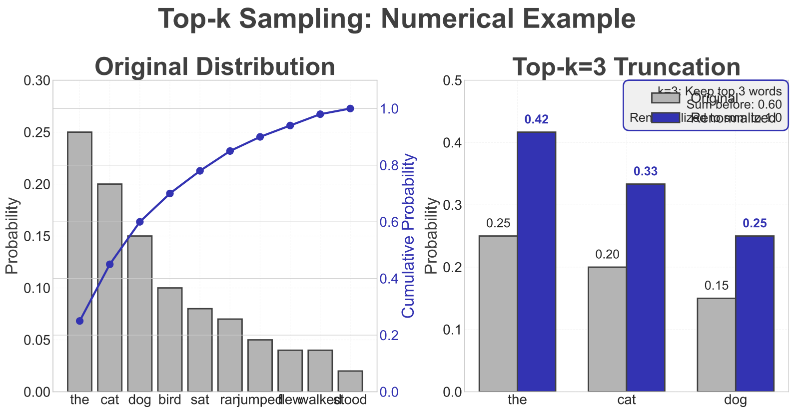
Concrete numbers show how temperature scaling works

Top-k Sampling: Filter the Tail

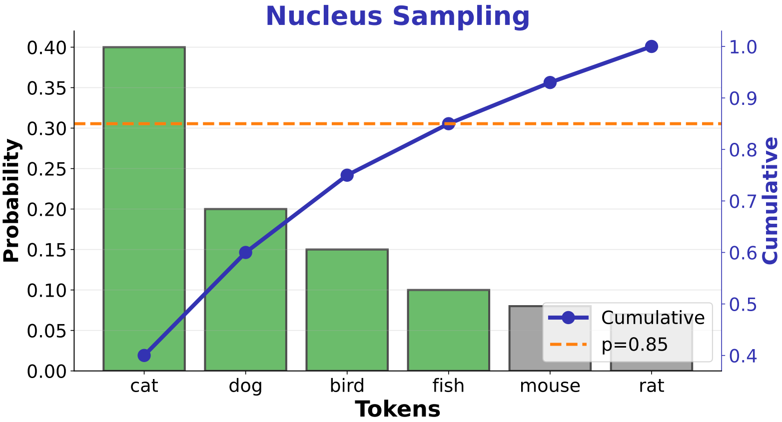


Key Insight: Only sample from top-k most likely tokens

Prevents sampling from long tail of unlikely words



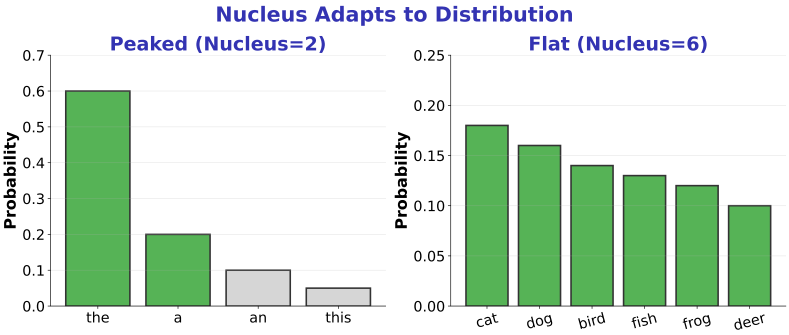
Concrete numbers show k=50 filtering process



Key Insight: Adapt vocabulary size to distribution shape

Nucleus size grows/shrinks based on probability spread

Nucleus: How Distribution Shape Matters



Same p value gives different vocabulary sizes for peaked vs flat distributions

The Degeneration Problem

Greedy Decoding Problem

"The city is a major city.
The city has many attractions.
The city is known..."

"the city" appears 3 times!

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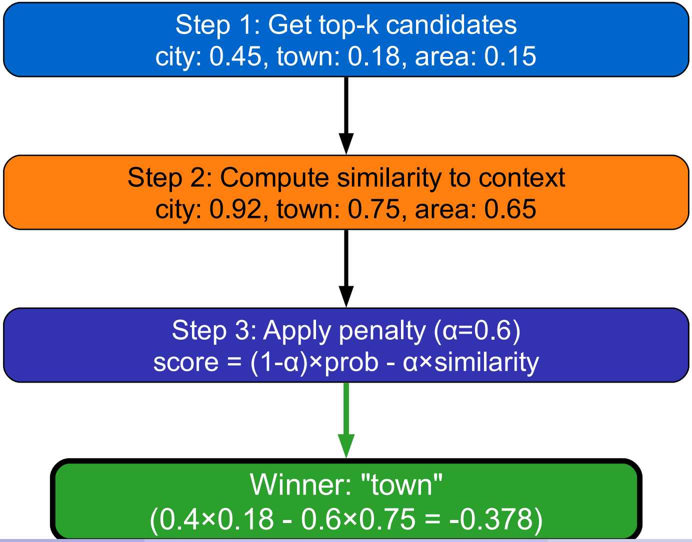
Solution: Contrastive Search

Discovery Question: Why do models repeat themselves?

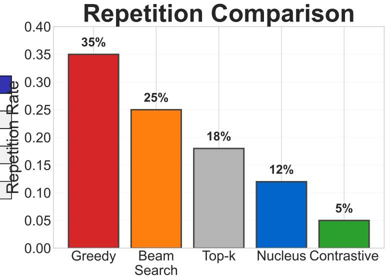
Greedy and beam search maximize probability - but high probability = repeating recent context

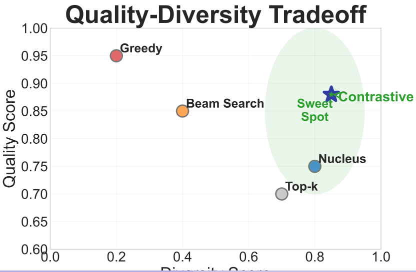

Step 1: Get top-k candidates
city: 0.45, town: 0.18, area: 0.15
Step 2: Compute similarity to context
city: 0.92, town: 0.75, area: 0.65
Step 3: Apply penalty (α=0.6)
score = (1-α)×prob - α×similarity
Winner: "town"
(0.4×0.18 - 0.6×0.75 = -0.378)

Contrastive Search vs Nucleus Sampling

Method Comparison

Aspect	Nucleus (Top-p)	Contrastive
Diversity	High	High
Repetition	Medium	Very Low
Coherence	Good	Excellent
Speed	Fast O(V log V)	Slower O(k×T²)
Parameters	p, temperature	α, k, penalty
Best for	General use	Long generation





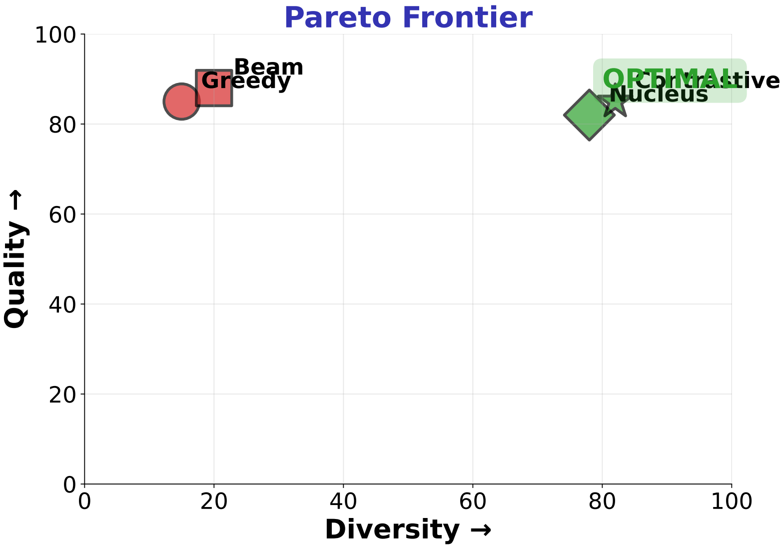
Context: "The weather today is"

Nucleus Sampling:

- beautiful and sunny with clear skies
- perfect for a walk in the park

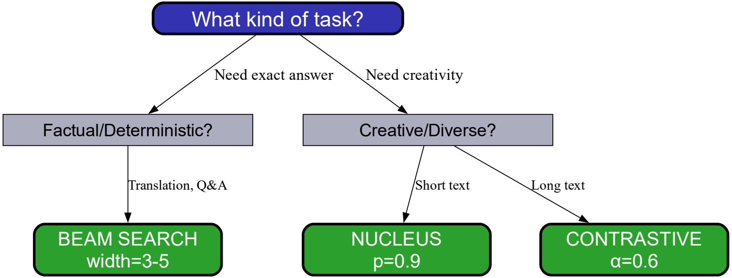
Contrastive Search:

- beautiful with clear blue skies
- perfect for outdoor activities today



Pareto Frontier: No method dominates all others

Choosing the Right Method: Decision Tree



Start with task requirements, follow tree to recommended method

Task-Specific Recommendations

Task	Method	Parameters
Translation	Beam	w=3-5
Factual QA	Greedy	T=0.3
Code	Greedy	T=0
Dialogue	Nucleus	p=0.9
Creative	Nucleus	p=0.95
Long Stories	Contrastive	α=0.6

Comprehensive mapping from 8 common tasks to optimal decoding strategies

Checkpoint Quiz 3: Choose the Right Method

Given these tasks, which method would you use?

1. **Medical report summary**
   - Needs: Accuracy, no hallucination
2. **Creative story writing**
   - Needs: Diversity, creativity
3. **Code generation**
   - Needs: Correctness, explore options
4. **Customer service chat**
   - Needs: Natural, varied responses
5. **Legal document**
   - Needs: Precise, formal
6. **Long blog post**
   - Needs: Coherent, no repetition

Checkpoint Quiz 3: Choose the Right Method

Given these tasks, which method would you use?

1. **Medical report summary**
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   - Needs: Coherent, no repetition

Answers:

1. Greedy/Low temp (T=0.1-0.3) 2. Nucleus (p=0.95, T=1.0) 3. Beam Search (k=3-5)
4. Nucleus (p=0.9, T=0.7) 5. Greedy (T=0) 6. Contrastive (=0.6)

Quiz 3: Real-world task selection is crucial for quality

Key Takeaways

1. **6 Problems** $\rightarrow$ **6 Solutions**: Each method solves specific failure mode
2. **Deterministic** (Greedy, Beam): High quality, no diversity - factual tasks
3. **Stochastic** (Temperature, Top-k, Nucleus): Diverse but variable quality
4. **Balanced** (Contrastive): Explicit degeneration prevention
5. **Task matters**: Translation $\rightarrow$ Beam — Dialogue $\rightarrow$ Nucleus — Stories $\rightarrow$ Contrastive
6. **Tradeoffs**: Speed vs Quality, Diversity vs Coherence

Modern Standard: Nucleus (top-p=0.9) + Temperature (T=0.7) for most applications

Next: Lab - Implement all 6 methods, measure quality-diversity tradeoffs

Decoding strategy matters as much as model architecture

From Probabilities to Text: The Complete Journey

What We Learned:

- Models give us probability distributions (Week 3-7)
- Converting to text has 6 fundamental challenges
- Each decoding method addresses specific problems
- No universal best - choose based on task requirements
- Production systems use hybrid methods (Nucleus + Temperature)

Complete pipeline from model training to text generation

Technical Appendix

25 slides: Complete mathematical treatment

A1-A5: Beam Search Mathematics
A6-A10: Sampling Mathematics
A11-A14: Contrastive Search & Degeneration
A15-A19: Advanced Topics & Production
A20-A25: The 6 Problems - Technical Analysis (NEW)

Objective: Find sequence $y^* = \text{argmax}\, P(y|x)$

Decomposition:

$$P(y|x) = \prod_{t=1}^{T} P(y_t|y_{<t}, x)$$

Log-probability (more stable):

$$\log P(y|x) = \sum_{t=1}^{T} \log P(y_t|y_{<t}, x)$$

Beam Search Approximation:
Instead of exploring all V^T sequences, maintain top-k hypotheses at each step

Complexity:
Time: $O(k \cdot V \cdot T)$ where k = beam width, V = vocabulary, T = length
Space: $O(k \cdot T)$ to store hypotheses

Beam search is tractable approximation to exact search

A2: Length Normalization

Problem: Longer sequences have lower probabilities (more terms multiplied)

$$P(y_1, y_2, y_3, y_4) = \underbrace{0.5}_{y_1} \times \underbrace{0.5}_{y_2} \times \underbrace{0.5}_{y_3} \times \underbrace{0.5}_{y_4} = 0.0625$$

$$P(y_1, y_2) = 0.5 \times 0.5 = 0.25 > 0.0625$$

Bias toward shorter sequences!

Solution: Length normalization

$$\text{score}(y) = \frac{1}{|y|^\alpha} \log P(y)$$

where $\alpha \in [0.5, 1.0]$ (typically 0.6-0.7)

Effect:
Without: Beam search heavily biases toward short outputs
With: Fair comparison across different lengths

Length normalization is essential for beam search quality

A3: Beam Search Variants

Diverse Beam Search:
Partition beams into groups
Penalize within-group similarity
Result: More diverse hypotheses

Constrained Beam Search:
Force certain tokens to appear
Useful for: Keywords, entities
Applications: Controllable generation

Stochastic Beam Search:
Sample beams instead of argmax
Combines beam + sampling
More diverse than standard beam

Block n-gram Beam:
Penalize n-gram repetition
Prevents "the city is a city" loops
Common in summarization

Many beam search variants exist for specific requirements

A4: Beam Search Stopping Criteria

When to stop expanding beams?

Method 1: Fixed length
Stop at T_{max} tokens (simple but rigid)

Method 2: END token
Stop when beam generates special token (most common)

Method 3: Score threshold
Stop when best score cannot improve enough

$$\frac{\text{best\_incomplete}}{\text{best\_complete}} < \text{threshold}$$

Method 4: Timeout
Computational budget exceeded (production systems)

Choice of stopping criterion affects output length distribution

A5: Beam Search Limitations

Fundamental Issues:

1. **Exposure bias**: Trained with teacher forcing, tested with own outputs
2. **Label bias**: Cannot compare sequences of different prefixes fairly
3. **Repetition**: Still can loop ("the city is a major city")
4. **Bland outputs**: Maximizes probability, not interestingness
5. **Search errors**: May miss better sequences outside beam

When Beam Search Fails:
Open-ended generation (dialogue, stories)
Long-form text (repetition accumulates)
Creative tasks (probability $\neq$ quality)

$\rightarrow$ Need sampling-based methods

Beam search optimizes wrong objective for creative tasks

A6: Sampling as Inference

Goal: Sample $y \sim P(y|x)$ instead of $\text{argmax}\, P(y|x)$

Ancestral Sampling:
For $t = 1$ to T:
    Compute $P(y_t|y_{<t}, x)$
    Sample $y_t \sim P(\cdot|y_{<t}, x)$

Properties:
Stochastic: Different output each time
Explores full distribution (in expectation)
Can generate low-probability sequences

Variants:
Temperature: Reshape distribution before sampling
Top-k: Truncate distribution before sampling
Nucleus: Dynamic truncation before sampling

Sampling enables diversity but loses quality guarantees

A7: Temperature Mathematics

Softmax with Temperature:

$$p_i(T) = \frac{\exp(z_i/T)}{\sum_{j=1}^{V} \exp(z_j/T)}$$

Limiting Cases:

$T \to 0$: $p_i \to \begin{cases} 1 & \text{if } i = \arg\max z \\ 0 & \text{otherwise} \end{cases}$ (greedy)

$T \to \infty$: $p_i \to 1/V$ (uniform)

Entropy Analysis:

Entropy $H(p) = -\sum p_i \log p_i$ measures randomness
H increases monotonically with T
Low T ($<$0.5): $H \approx 0$ (deterministic)
High T ($>$2.0): $H \approx \log V$ (maximum entropy)

Temperature provides continuous control over distribution entropy

Formal Definition:
Let σ = permutation sorting probabilities descending

$$V_k = \{w_{\sigma(1)}, w_{\sigma(2)}, \ldots, w_{\sigma(k)}\}$$

Truncated distribution:

$$p'(w) = \begin{cases} \frac{p(w)}{\sum_{w' \in V_k} p(w')} & \text{if } w \in V_k \\ 0 & \text{otherwise} \end{cases}$$

Information Loss:
Original entropy: $H(p) = -\sum_{i=1}^{V} p_i \log p_i$
After top-k: $H(p') = -\sum_{i=1}^{k} p'_i \log p'_i < H(p)$
Loss $\approx \sum_{i=k+1}^{V} p_i \log(1/p_i)$ (tail information)

Top-k sacrifices tail probability mass for sampling quality

A9: Nucleus (Top-p) Mathematics

Formal Definition:

$$V_p = \min \left\{ V' \subseteq V : \sum_{w \in V'} p(w) \geq p \right\}$$

Smallest set with cumulative mass $\geq p$

Dynamic Vocabulary Size:

$$|V_p| = \min\{k : \sum_{i=1}^{k} p_{\sigma(i)} \geq p\}$$

Adapts to distribution shape:
Peaked: Small $|V_p|$ (2-5 tokens)
Flat: Large $|V_p|$ (50+ tokens)

Why Nucleus > Top-k:
Top-k: Fixed k regardless of $p(w)$ distribution
Nucleus: Adapts k to achieve consistent probability mass

Nucleus automatically adjusts vocabulary to distribution characteristics

A10: Sampling Quality Metrics

Quality Metrics:
Perplexity: $\exp(-\frac{1}{T}\sum \log p(y_t))$
Lower = better

BLEU (translation):
N-gram overlap with reference
0-100 scale

Human evaluation:
Fluency (1-5)
Relevance (1-5)

Diversity Metrics:
Distinct-n: $\frac{\text{unique n-grams}}{\text{total n-grams}}$
Higher = more diverse

Self-BLEU:
BLEU of output vs other outputs
Lower = more diverse

Repetition Rate:
$\frac{\text{repeated n-grams}}{\text{total n-grams}}$
Lower = less repetitive

Need both quality AND diversity metrics to evaluate decoding

A11: The Degeneration Problem (Formal)

Definition: Model-generated text with unnatural repetitions

Why It Happens:

1. Model trained on natural text (low repetition)
2. But generation maximizes $P(y_t|y_{<t})$
3. Recent context $y_{<t}$ influences P
4. Creates positive feedback: high prob word $\rightarrow$ context $\rightarrow$ same high prob word

Quantifying Degeneration:
Repetition rate in greedy: 15-30% (depending on domain)
Repetition rate in human text: 2-5%
Gap = degeneration problem

Examples:
"*The city is a major city in the United States. The city...*"
"*I think that I think that I think...*"

Maximizing probability does not equal natural text

A12: Contrastive Search Objective

Scoring Function:

$$\text{score}(w_t) = (1-\alpha) \times \underbrace{P(w_t|y_{<t})}_{\text{model confidence}} - \alpha \times \underbrace{\max_{w_i \in y_{<t}} \text{sim}(w_t, w_i)}_{\text{context similarity}}$$

where $\alpha \in [0, 1]$ controls tradeoff

Similarity Function:

$$\text{sim}(w_i, w_j) = \frac{h_i \cdot h_j}{||h_i|| \cdot ||h_j||}$$

(cosine similarity)
using token embeddings h

Algorithm:

1. Get top-k candidates by probability
2. For each candidate, compute similarity to all tokens in $y_{<t}$
3. Apply penalty: score = prob - $\alpha \times$ max_similarity
4. Select candidate with highest score

Contrastive search explicitly penalizes copying recent context

A13: Contrastive Search Parameters

Alpha (α):
$\alpha = 0$: Pure greedy (no penalty)
$\alpha = 0.6$: Balanced (recommended)
$\alpha = 1.0$: Maximum diversity (risky)

Typical Settings:
Short text (<100 tokens): $\alpha = 0.4 - 0.5$
Medium (<500): $\alpha = 0.5 - 0.6$
Long (500+): $\alpha = 0.6 - 0.7$

Top-k for Candidates:
$k = 4$: Fast, focused
$k = 6$: Balanced (default)
$k = 10$: Diverse

Computational Cost:
For each step:

- Compute similarities: $O(k \times t)$
- t grows with generation

Total: $O(k \times T^2)$
12× slower than greedy

Hugging Face default: α=0.6, k=4

A14: Degeneration Analysis

Research Findings (2024-2025):

- Greedy decoding repetition: 18-25% (GPT-2), 12-18% (GPT-3)
- Nucleus sampling repetition: 8-12% (still above human 3-5%)
- Contrastive search repetition: 4-7% (closest to human)

Why Probability Maximization Fails:
Training objective: Next token prediction
But generation requires: Global coherence
Mismatch: Local optimum $\neq$ global quality

Solutions Hierarchy:

1. Temperature/Top-k/Nucleus: Reduce greedy's determinism
2. Contrastive: Explicit degeneration penalty
3. RLHF/DPO: Align model with human preferences (different lecture)

Contrastive search addresses fundamental limitation of likelihood-based decoding

A15: Hybrid Decoding Methods

Combining Strategies:

Nucleus + Temperature:
Apply temperature THEN nucleus

$$p_i(T) = \text{softmax}(z/T), \quad \text{then} \quad V_p \leftarrow \text{nucleus}(p_i(T))$$

Used by GPT-3 API, ChatGPT

Beam + Sampling:
Beam search with stochastic selection
Keep top-k, sample from them (not argmax)

Contrastive + Nucleus:
Nucleus for candidate generation
Contrastive scoring for selection
Best of both worlds

Hybrid methods leverage complementary strengths

A16: Constrained Decoding (2025)

Goal: Force certain tokens/patterns to appear

Lexically Constrained:
Must include keywords: {"AI", "ethics", "safety"}
Beam search variant: Track constraint satisfaction

Format Constraints:
JSON output: Force structure {"key": "value"}
Code: Force syntactic validity

NeuroLogic Decoding (2021):
Beam search + constraint satisfaction
Optimal for: Keyword-based generation

Production Use Cases:
Structured data extraction (force JSON)
Controllable summarization (force keywords)
Code generation (force syntax)

Constrained decoding enables controllable generation

A17: Computational Complexity Comparison

Method	Time per token	Total complexity	Relative speed
Greedy	$O(V)$	$O(V \times T)$	1.0× (baseline)
Temperature	$O(V)$	$O(V \times T)$	1.1× (softmax overhead)
Top-k	$O(V)$	$O(V \times T)$	1.2× (sorting)
Nucleus	$O(V \log V)$	$O(V \log V \times T)$	1.3× (sort + cumsum)
Beam (k=5)	$O(k \times V)$	$O(k \times V \times T)$	4.5× (k=5)
Contrastive	$O(k \times T)$	$O(k \times T^2)$	12× (similarity)

Key Insight: Contrastive's T^2 term makes it expensive for long sequences

Practical Impact (1000-token generation):
Greedy: 2.5 seconds
Nucleus: 3.2 seconds (best choice)
Beam: 11 seconds
Contrastive: 30 seconds (only if quality critical)

Computational cost matters for production deployment

A18: Production Settings (Real-World APIs)

Production System Settings (2025)

Default decoding parameters used by major LLM APIs and platforms

System/API	Default Method	Temperature	Top-p	Top-k	Other Parameters	Notes
GPT-4 API	Nucleus	0.7	1.0	—	frequency_penalty=0 presence_penalty=0	Can adjust all params
Claude API	Nucleus	1.0	0.999	—	max_tokens required	Temperature □ [0,1]
ChatGPT Web	Nucleus+Temp	0.7	0.95	—	Not adjustable	Optimized for chat
Gemini API	Top-k + Top-p	1.0	0.95	40	candidate_count=1	Both k and p used
Llama 2 (HF)	Configurable	1.0	0.9	50	repetition_penalty=1.0	Full control
Cohere API	Nucleus	0.75	0.999	0	frequency_penalty=0	k=0 means disabled
Mistral API	Nucleus	0.7	1.0	—	safe_mode=false	Similar to OpenAI
Together AI	Configurable	0.7	0.7	50	repetition_penalty=1.0	Multiple options

- Temperature: Lower = more deterministic, Higher = more creative
- Top-p (Nucleus): Cumulative probability threshold (typically 0.9-1.0)
- Top-k: Number of top tokens to consider (often 40-50 when used)
- Most production systems use Nucleus sampling as default
- ChatGPT and Claude optimize for conversational quality
- APIs generally allow full parameter customization

Provider Types:
Proprietary LLM
Open Source
Optimized for Chat

What ChatGPT, Claude, and other production systems actually use

A19: Future Directions & Open Problems

Active Research Areas (2025):

1. **Quality-diversity optimization**: Multi-objective search methods
2. **Learned decoding**: Train models to decode better (RLHF, DPO)
3. **Speculative decoding**: Parallel generation for speed (4-8$\times$ faster)
4. **Adaptive methods**: Choose strategy dynamically during generation
5. **Energy-based decoding**: Score sequences globally (not token-by-token)

Open Problems:
How to automatically select best T, p, k, α for new task?
How to balance fluency + factuality + creativity simultaneously?
How to decode efficiently for 100K+ token outputs?

Trend: Moving from hand-tuned parameters to learned decoding strategies

Decoding is an active research area with many open questions