Decoding Strategies

Week 9: From Probabilities to Text

November 2025

Learning Goals & Plan for Today

Learning Goals

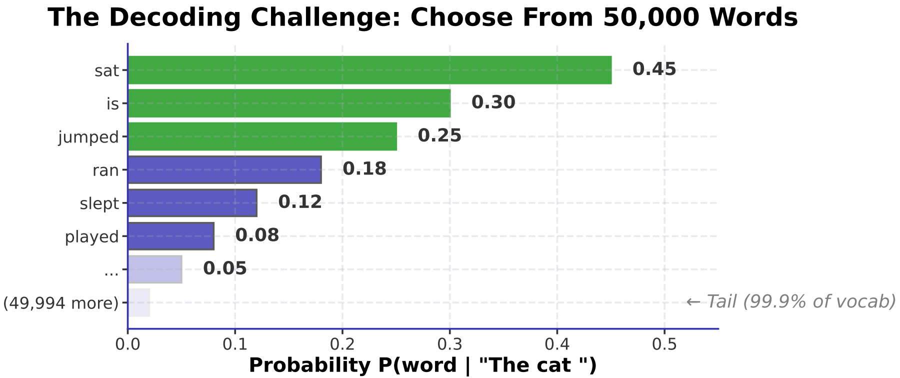
1. Discover why predicting one word at a time creates text quality problems
2. Learn how different decoding strategies solve these problems
3. Practice selecting and tuning methods for different use cases

Plan for Today

1. The challenge: Word predictions → Complete text
2. The toolbox: 6 strategies for text generation
3. Hands-on: Compare methods in practice

Notebook available: `week09_decoding_lab.ipynb`

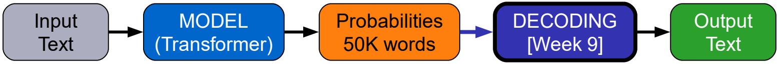
The Decoding Challenge: Choosing From 50,000 Words



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

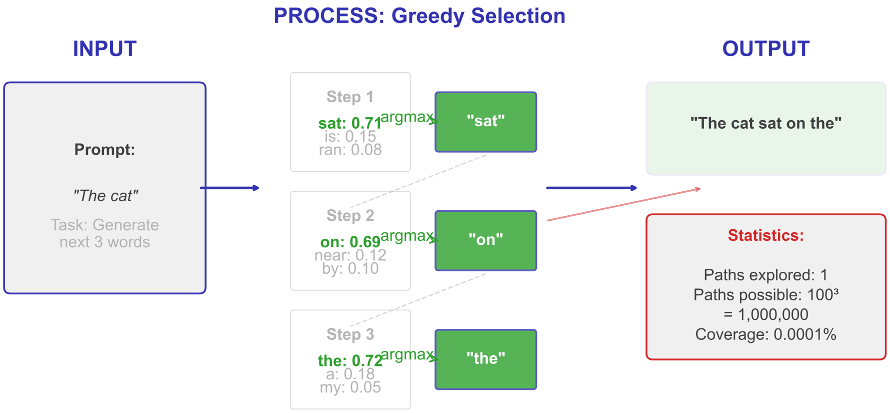


Our Journey:

1. We trained models (Weeks 3-7: RNN → Transformers → 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 (Too Narrow)



PROCESS: Greedy Selection

INPUT

Prompt:

"The cat"

Task: Generate next 3 words

Step 1

sat: 0.71 → argmax → "sat"

is: 0.15

ran: 0.08

Step 2

on: 0.69 → argmax → "on"

near: 0.12

by: 0.10

Step 3

the: 0.72 → argmax → "the"

a: 0.18

my: 0.05

OUTPUT

"The cat sat on the"

Statistics:

Paths explored: 1

Paths possible: 100^3

= 1,000,000

Coverage: 0.0001%

Extreme 1: Too narrow - misses 99.9999999% of search space

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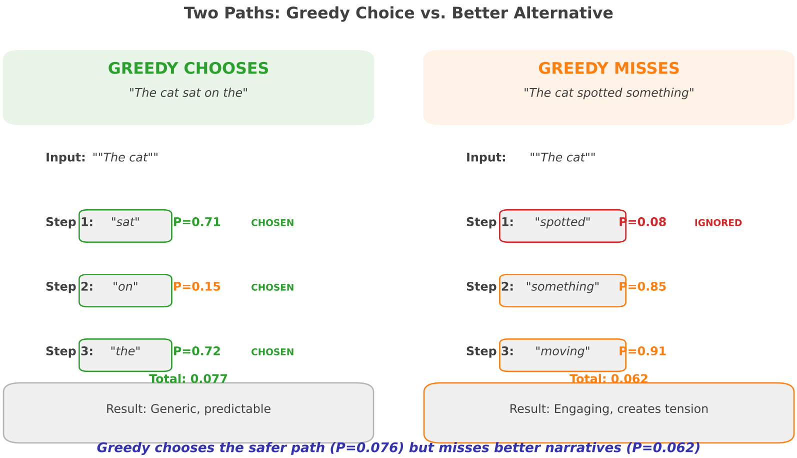
Question: What if we kept ALL 100 words at each step?

Think: 100 × 100 × 100 × 100 × 100 = ?

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

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

Greedy's Fatal Flaw: Missing Better Paths



Two Paths: Greedy Choice vs. Better Alternative

GREEDY CHOOSES

"The cat sat on the"

Input: *""The cat""*

Step 1: *"sat"* **P=0.71** **CHOSEN**

Step 2: *"on"* **P=0.15** **CHOSEN**

Step 3: *"the"* **P=0.72** **CHOSEN**

Total: 0.077

Result: Generic, predictable

GREEDY MISSES

"The cat spotted something"

Input: *""The cat""*

Step 1: *"spotted"* **P=0.08** **IGNORED**

Step 2: *"something"* **P=0.85**

Step 3: *"moving"* **P=0.91**

Total: 0.062

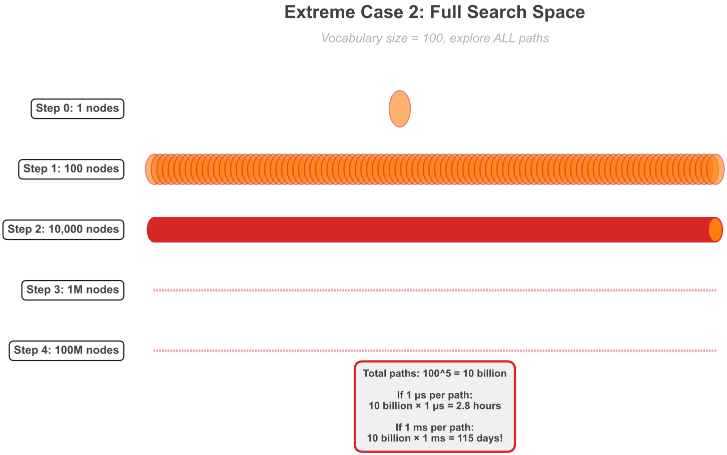
Result: Engaging, creates tension

Greedy chooses the safer path (P=0.076) but misses better narratives (P=0.062)

The Problem: High first-step probability $\neq$ Best complete sentence

Greedy commits early, missing narratively richer paths despite lower initial probability

Extreme Case 2: Full Search Space (Too Broad)



Extreme Case 2: Full Search Space

Vocabulary size = 100, explore ALL paths

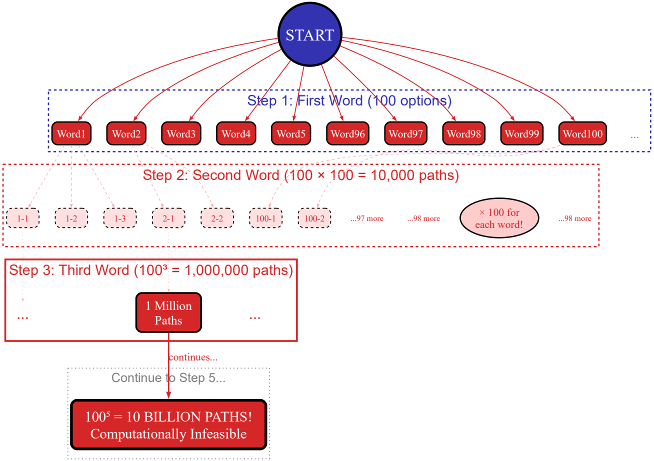
Total paths: 100^5 = 10 billion

If 1 μs per path:
10 billion × 1 μs = 2.8 hours

If 1 ms per path:
10 billion × 1 ms = 115 days!

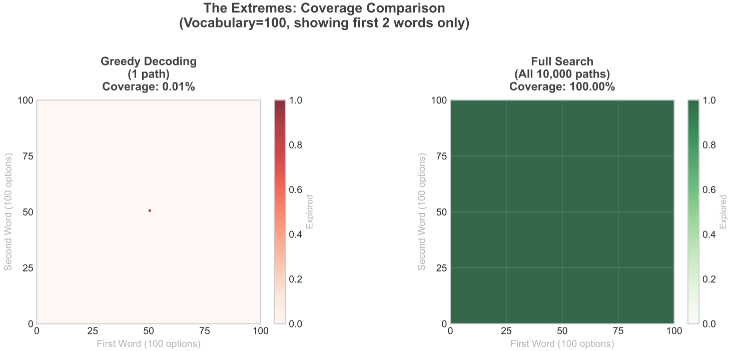
Extreme 2: Too broad - exponential explosion makes this impossible

Full Exploration: From One Path to Billions



The Problem: How do we explore more than 1 but less than 10 billion paths?

The Extremes: Why Neither Works



Greedy (0.01% coverage):

- Too narrow - misses better paths
- Fast but low quality
- Prone to repetition loops

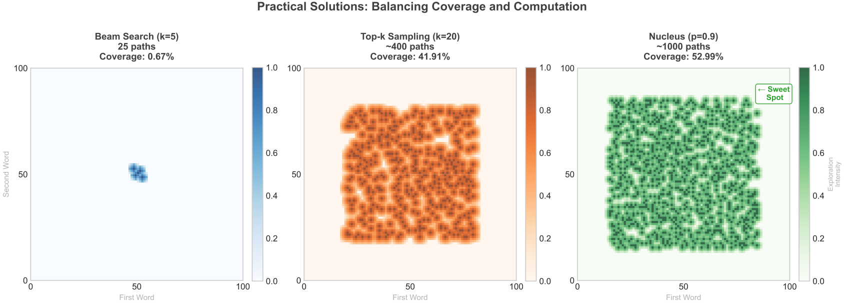
Full Search (100% coverage):

- Too broad - computationally infeasible
- Perfect in theory, impossible in practice
- Would take days/years to complete

Key Insight: We need methods that explore 1-5% of space intelligently

Neither extreme is practical - the solution lies in between

The Sweet Spot: Balanced Exploration



The Solution: 1-5% Coverage

- **Not too narrow**: Explores enough paths to find good sequences
- **Not too broad**: Computationally feasible (seconds, not days)
- **Strategic exploration**: Focus on promising regions of search space

Coming Next: Learn 6 specific methods that achieve this balance

The sweet spot: Methods that intelligently explore 1-5% of the search space

Method 1: Greedy Decoding

Core Mechanism:

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

At each step, pick the single word with highest probability

Characteristics:

- Deterministic (same input → same output)
- Fast: O(1) per step
- No exploration

Method 1 of 6: Greedy = always pick argmax

Method 2: Beam Search

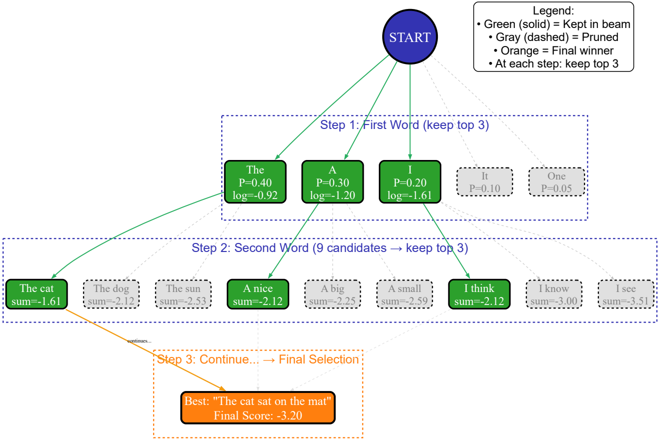
Core Mechanism:
Maintain k hypotheses ("beams") at each step
Expand each hypothesis, keep top-k by cumulative probability

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

Beam Search: Step-by-Step Example



START

Legend:
- Green (solid) = Kept in beam
- Gray (dashed) = Pruned
- Orange = Final winner
- At each step: keep top 3

Step 1: First Word (keep top 3)

The
P=0.40
log=-0.92

A
P=0.30
log=-1.20

I
P=0.20
log=-1.61

It
P=0.10

One
P=0.05

Step 2: Second Word (9 candidates → keep top 3)

The cat
sum=-1.61

The dog
sum=-2.12

The sun
sum=-2.53

A nice
sum=-2.12

A big
sum=-2.25

A small
sum=-2.59

I think
sum=-2.12

I know
sum=-3.00

I see
sum=-3.51

continues...

Step 3: Continue... → Final Selection

Best: "The cat sat on the mat"
Final Score: -3.20

Worked example shows why beam search finds better sequences than greedy

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

Method 3: Temperature Sampling

Core Mechanism:

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

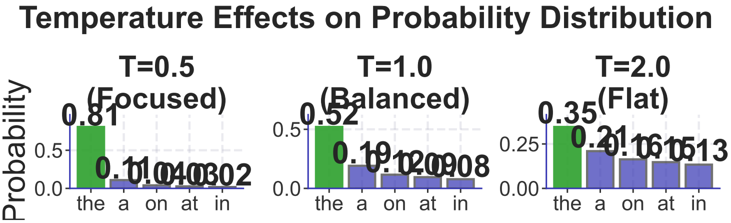
Reshape probability distribution with temperature T, then sample

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

Temperature Sampling: Control Randomness



Key Insight: Temperature reshapes probability distribution

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

Temperature: Worked Example

Original probabilities: "The cat __"

- sat: P = 0.40
- is: P = 0.30
- jumped: P = 0.20
- walked: P = 0.10

After temperature T = 0.5 (more focused):

- sat: P = 0.52 (increased)
- is: P = 0.28
- jumped: P = 0.15
- walked: P = 0.05 (decreased)

After temperature T = 2.0 (more random):

- sat: P = 0.30 (decreased)
- is: P = 0.28
- jumped: P = 0.24
- walked: P = 0.18 (increased)

Lower T sharpens distribution, higher T flattens it

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

Top-k Sampling: Filter the Tail

How it works:

1. Sort all 50,000 words by probability (descending)
2. Keep only the top k words (e.g., k = 50)
3. Discard the remaining 49,950 low-probability words
4. Renormalize probabilities to sum to 1.0
5. Sample from the filtered k words

Result:

- Prevents unlikely/nonsensical words
- Fixed vocabulary size (always k words)
- Combines well with temperature

Prevents sampling from long tail of unlikely words

Top-k: Worked Example

Top-k Example: k=3

1. Original Probabilities:

cat: 0.45
dog: 0.18
bird: 0.15
horse: 0.10
mouse: 0.08
...: 0.04

2. Keep Top-3:

cat: 0.45
dog: 0.18
bird: 0.15
(discard rest)

3. Renormalize:

Sum = 0.45 + 0.18 + 0.15 = 0.78
cat: 0.45/0.78 = 0.58
dog: 0.18/0.78 = 0.23
bird: 0.15/0.78 = 0.19

Result: Sample from {cat: 58%, dog: 23%, bird: 19%}

Prevents sampling from long tail ("mouse" eliminated)

Concrete numbers show k=50 filtering process

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

Nucleus (Top-p) Sampling: Dynamic Cutoff

Process (p = 0.9 example):

1. Sort words by probability: sat (0.40), is (0.30), jumped (0.20), ...
2. Add cumulative probabilities: 0.40, 0.70, 0.90, ...
3. Stop when cumulative $\geq$ p (here: 3 words reach 0.90)
4. Sample from these words only

Adaptive behavior:

- Peaked distribution: fewer words needed (e.g., 3 words)
- Flat distribution: more words needed (e.g., 100 words)
- Same p value, different vocabulary sizes

Nucleus adapts to distribution shape - not fixed like top-k

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

The Degeneration Problem

The Degeneration Problem: Model Repetition

Real Output from Greedy Decoding:

"The city of New York is a major city in the United States. The city is known for its diverse culture and the city has many tourist attractions. The city is also home to the city's financial district..."

Problem: "the city" appears 6 times in 4 sentences!

Why? Always picking argmax → same patterns repeated

Solution: Penalize tokens similar to recent context (Contrastive Search)

Discovery Question: Why do models repeat themselves?

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

Contrastive Search: Penalize Repetition

The scoring function:

$$\text{score}(w) = (1-\alpha) \cdot P(w \mid \text{context}) - \alpha \cdot \max_{w' \in \text{past}} \text{sim}(w, w')$$

Two components:

- Model probability: how likely is this word?
- Similarity penalty: how similar to words we already used?
- α balances the two (typically 0.6)

Effect:

- High-probability words that repeat context get penalized
- Forces model to use semantically different words
- Prevents “the cat sat on the cat on the cat...”

Explicitly prevents degeneration in long text generation

Contrastive vs Nucleus: Direct Comparison

Same Prompt, Different Methods

Prompt: "The future of artificial intelligence is"

"...is pro
many ind
significa
educat

"...is rapidly evolving, bringing unprecedented opportunities across sectors ranging from medicine to climate science, while raising important ethical questions."

+ Diverse
+ Creative
+ No repetition

Contrastive Search explicitly penalizes copying recent context

Contrastive adds explicit similarity penalty that Nucleus lacks

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

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E. Penalize similarity to previous

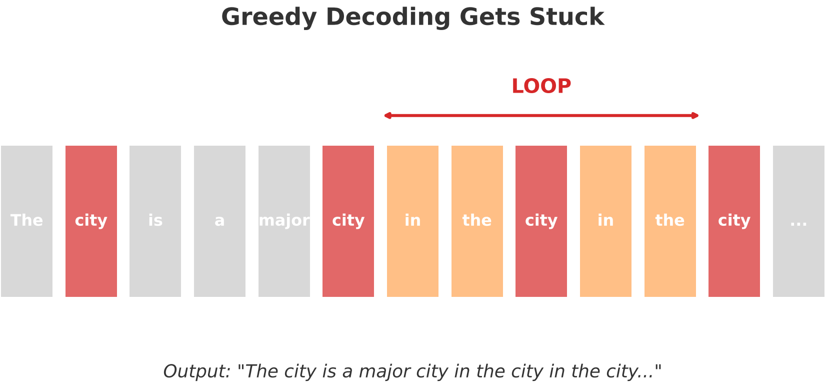
F. Adaptive probability mass cutoff

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?

Why Beam Search? Problem: Repetition Loops

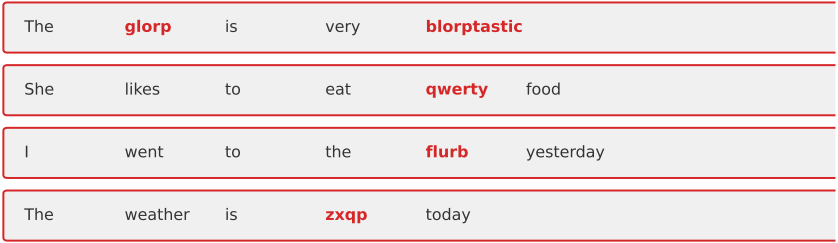

Greedy Decoding Gets Stuck
LOOP
The
city
is
a
major
city
in
the
city
in
the
city
...
Output: "The city is a major city in the city in the city..."

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

Why Temperature? Problem: No Diversity

High Temperature Creates Nonsense



The **glorp** is very **blorptastic**

She likes to eat **qwerty** food

I went to the **flurb** yesterday

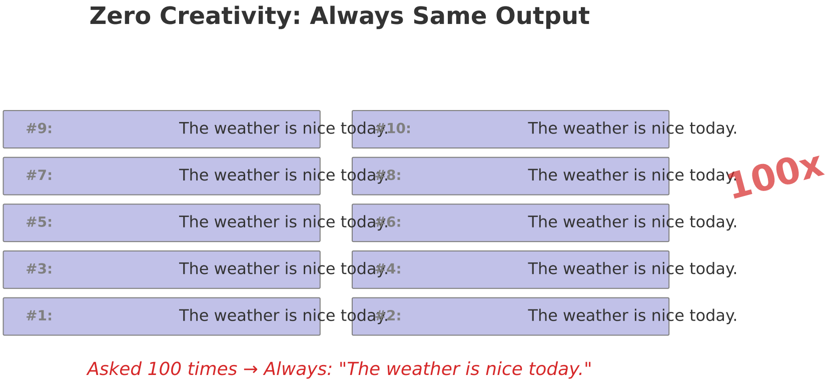
The weather is **zxqp** today

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

Why Top-k? Problem: Too Boring or Too Crazy



Zero Creativity: Always Same Output

#9: The weather is nice today.

#10: The weather is nice today.

#7: The weather is nice today.

#8: The weather is nice today.

#5: The weather is nice today.

#6: The weather is nice today.

#3: The weather is nice today.

#4: The weather is nice today.

#1: The weather is nice today.

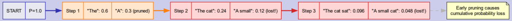
#2: The weather is nice today.

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

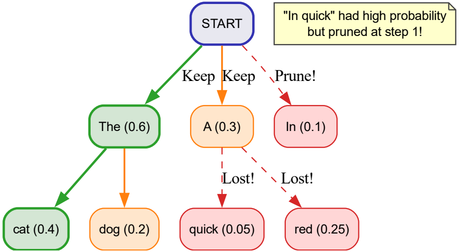
Temperature's Problem: Pure sampling includes low-quality words
Why Top-k Helps: Filter to k=50 best words, then sample

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

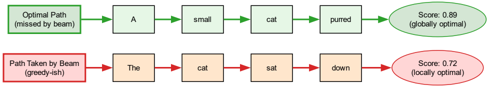
Beam Search Limitation: Missing Better Paths

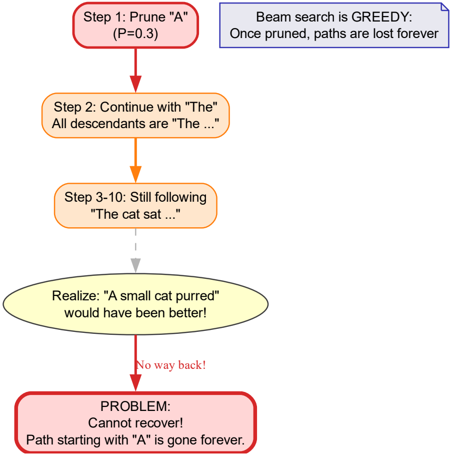


Early pruning causes cumulative probability loss



"In quick" had high probability but pruned at step 1!

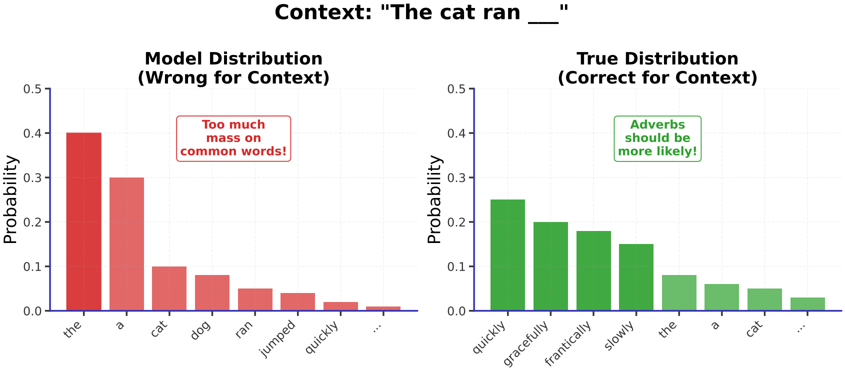



Step 1: Prune "A"
(P=0.3)
Step 2: Continue with "The"
All descendants are "The ..."
Step 3-10: Still following
"The cat sat ..."
Realize: "A small cat purred"
would have been better!
No way back!
PROBLEM:
Cannot recover!
Path starting with "A" is gone forever.

Beam search is GREEDY: Once pruned, paths are lost forever

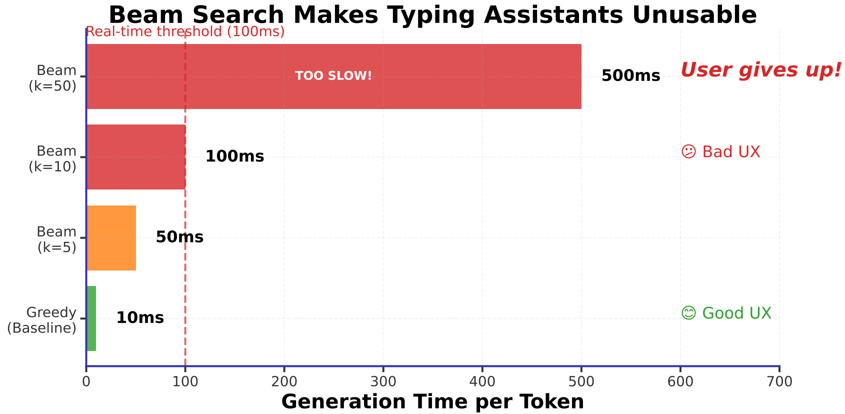
Problem 4 of 6: Even beam search prunes early, cannot recover optimal path - 4 perspectives

Why Nucleus? Problem: Distribution Tail Contains Junk



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

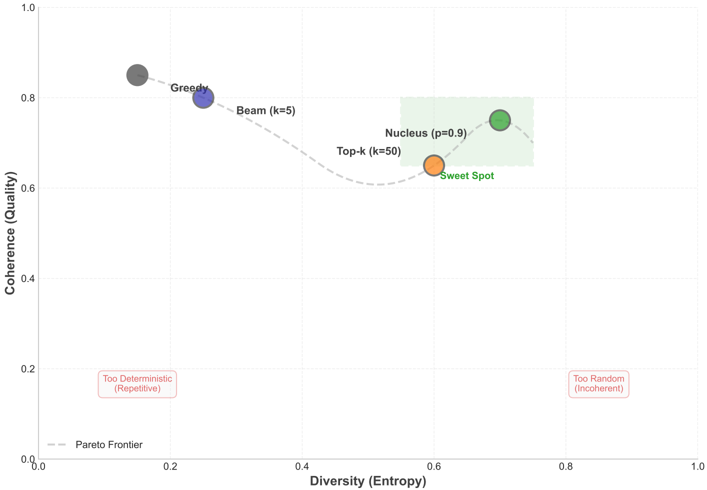
Problem 5 of 6: Tail contains junk → Nucleus adapts to distribution



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



Key Insight: We saw problems and their solutions. Each method balances quality vs diversity.

All 6 problems relate to balancing coherence with creativity

Checkpoint Quiz 2: Which Method for Which Problem?

Match Solution to Problem:

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

Problems to Solve:

A. Too boring OR too crazy

B. Repetition loops

C. No diversity

D. Fixed k doesn't adapt

E. Generic repetitive text

Checkpoint Quiz 2: Which Method for Which Problem?

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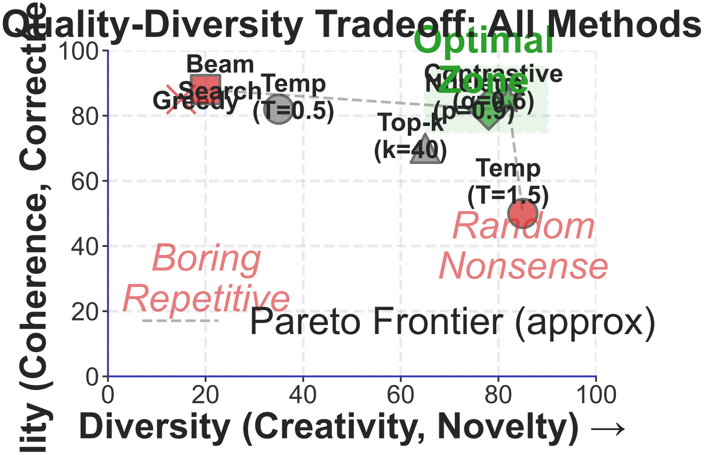
D. Fixed k doesn't adapt

E. Generic repetitive text

Answers: 1→B, 2→C, 3→A, 4→D, 5→E

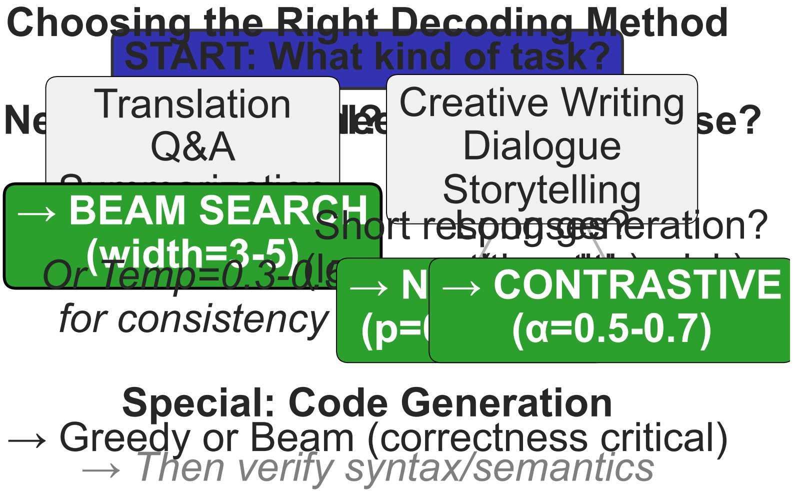
Each method targets a specific failure mode!

Quiz 2: Understanding the method-problem mapping



Pareto Frontier: No method dominates all others

Choose based on task: deterministic tasks (left), creative tasks (right)



Choosing the Right Decoding Method

START: What kind of task?

Ne… se?

Translation
Q&A
Summarization

→ BEAM SEARCH (width=3-5)

Or Temp=0.3-0.5
for consistency

Creative Writing
Dialogue
Storytelling

Short response?

Long generation?

→ N…
(p=…

→ CONTRASTIVE
(α=0.5-0.7)

Special: Code Generation

→ Greedy or Beam (correctness critical)

→ Then verify syntax/semantics

Start with task requirements, follow tree to recommended method

Task-Specific Recommendations (2025)

Task-Specific Decoding Recommendations (2025)

Deterministic Tasks

Creative Tasks

Task	Recommended	Parameter	Why?
Machine Translation	Beam Search	width=3-5	Deterministic, quality critical
Factual Q&A	Greedy / Low Temp	T=0.1-0.3	Single correct answer needed
Summarization	Beam Search	width=4	Balance coverage + conciseness
Code Generation	Greedy	T=0	Syntax errors costly
Creative Writing	Nucleus / Contrastiv	p=0.9, α=0.6	Diverse but coherent
Dialogue Systems	Nucleus	p=0.85-0.95	Natural variation needed
Story Generation	Contrastive	α=0.5-0.7	Avoid repetition in long text
Long-form Articles	Contrastive	α=0.6, p=0.9	Degeneration prevention

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**
   - 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

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 (α=0.6)

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

Key Takeaways

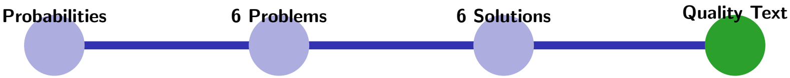
1. **6 Problems** → **6 Solutions**: Each method solves specific failure mode
2. **Deterministic** (Greedy, Beam): High quality, no diversity - factual tasks
3. **Stochastic** (Temperature, Top-k, Nucleus): Diverse but variable quality
4. **Balanced** (Contrastive): Explicit degeneration prevention
5.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

A1: Beam Search Formulation

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

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 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:

$T \to 0$: $p_i \to \begin{cases} 1 & \text{if } i = \operatorname{argmax} z \\ 0 & \text{otherwise} \end{cases}$ (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

A8: Top-k Mathematics

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 → context → 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)

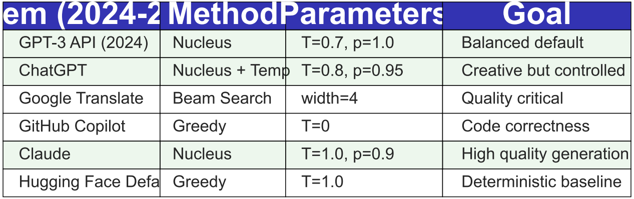
Key Insight: Contrastive's T^2 term makes it expensive for long sequences

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 Decoding Settings (Real Systems 2024-2025)



em (2024-2	Method	Parameters	Goal
GPT-3 API (2024)	Nucleus	T=0.7, p=1.0	Balanced default
ChatGPT	Nucleus + Temp	T=0.8, p=0.95	Creative but controlled
Google Translate	Beam Search	width=4	Quality critical
GitHub Copilot	Greedy	T=0	Code correctness
Claude	Nucleus	T=1.0, p=0.9	High quality generation
Hugging Face Defa	Greedy	T=1.0	Deterministic baseline

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× 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