Decoding Strategies

Week 9: From Prediction to Generation

NLP Course 2025

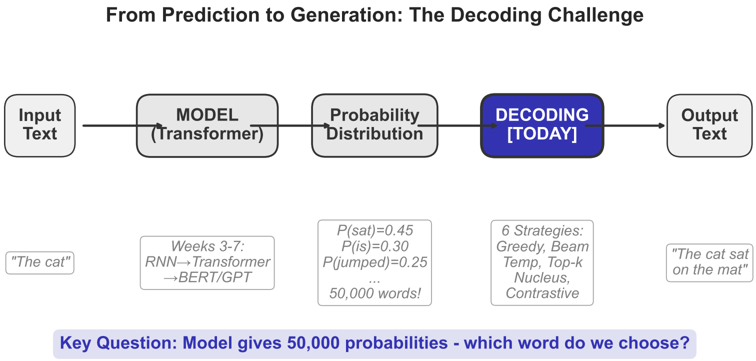
Enhanced with Contrastive Search (2025)

November 9, 2025

Two-Tier BSc Discovery

Main: 25 slides — Appendix: 19 slides

How We Got Here: The Prediction Story



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.

Today's Challenge: From Probabilities to Text

The Setup: Model gives us probabilities for next word

Example: "The cat __"

$$P(\text{sat}) = 0.45, \quad P(\text{is}) = 0.30, \quad P(\text{jumped}) = 0.25, \quad \ldots \quad (50{,}000 \text{ words})$$

Naive Approach 1: Pick highest
→ **Greedy Decoding**

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

Problem: Repetitive, boring

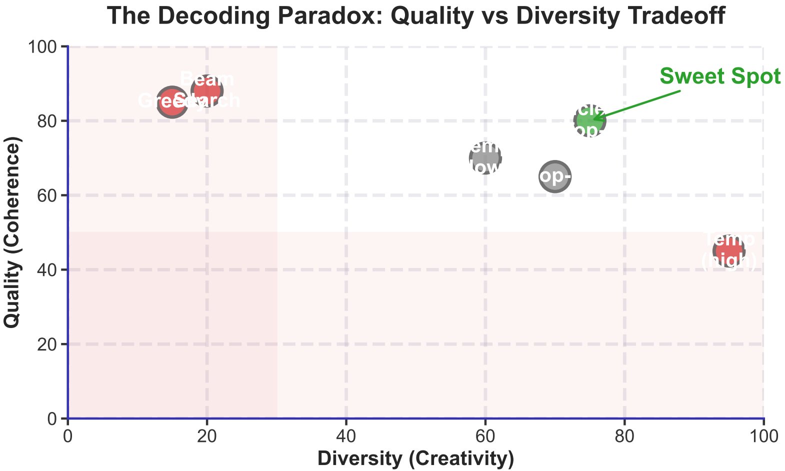
Naive Approach 2: Pick random
→ **Pure Sampling**

Result:
"The purple flying mathematics..."

Problem: Nonsense, incoherent

Core Challenge: Need text that is *coherent* AND *creative*

Today: 6 strategies to solve this - from simple to sophisticated



Discovery Question: Why is best text boring and creative text nonsense?

The central challenge: How to balance coherence with creativity

Three Decoding Families

Deterministic

Methods:

- Greedy
- Beam search

Traits:

- Same output
- High quality
- No creativity

Stochastic

Methods:

- Temperature
- Top-k
- Nucleus

Traits:

- Random
- Creative
- Variable quality

Balanced

Methods:

- Contrastive
- Hybrid

Traits:

- Best of both
- No repetition
- Modern std

Different tasks need different strategies - no single best method

6 methods total: Each optimizes different quality-diversity tradeoff

Greedy Decoding: The Baseline

How It Works:

1. Compute probabilities
2. Pick highest probability
3. Add to sequence
4. Repeat until done

Example:

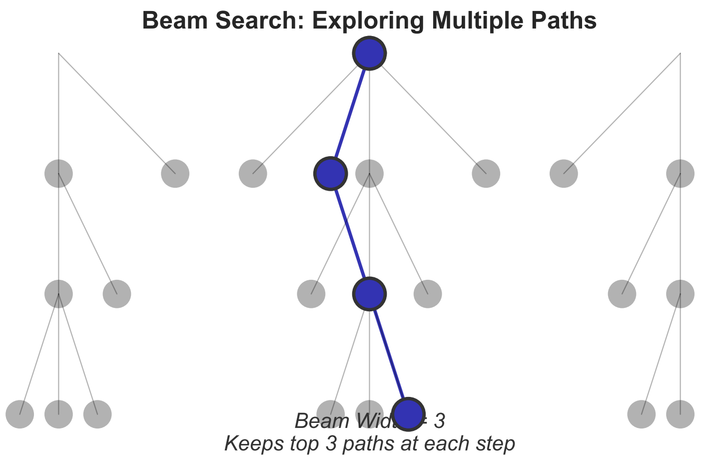
$P(\text{cat}) = 0.45 \leftarrow$ Pick!
$P(\text{dog}) = 0.30$
$P(\text{bird}) = 0.25$

When to Use:

- Code generation
- Short responses
- Speed critical
- Reproducibility

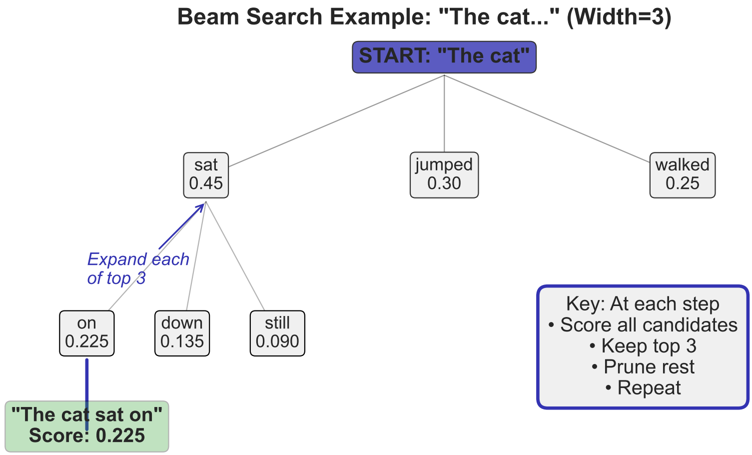
Problem: Degeneration
"The city is a city in a city..."
Model gets stuck in loops

Simplest but prone to repetition



Key Insight: Keep top-k hypotheses at each step to find better sequences

Beam width = 3-5 typical. Balance greedy (1) vs exhaustive (∞)



Worked example: "The cat..." with width=3 shows pruning in action

Beam Search: Detail

Algorithm:

1. Start: Keep top-k tokens
2. Expand: All continuations
3. Score: Multiply probs
4. Prune: Keep top-k sequences
5. Repeat until END

Scoring:

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

With length normalization:

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

Best For:

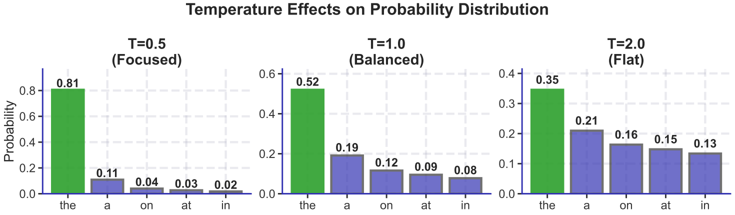
- Machine translation
- Summarization
- Question answering
- "Correct" answer tasks

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

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

Beam search: workhorse for deterministic tasks

Temperature Sampling: Control Randomness



Key Insight: Temperature reshapes probability distribution

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

Temperature Calculation: Step-by-Step

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

Step 1: Scale by T=0.5 (MORE PEAKED)
Scaled = [2.0/0.5, 1.0/0.5, 0.5/0.5, 0.2/0.5]
= [4.0, 2.0, 1.0, 0.4]
Softmax → [0.73, 0.18, 0.07, 0.02]
→ 73% on "cat" (VERY FOCUSED)

Step 2: Scale by T=1.0 (UNCHANGED)
Scaled = [2.0, 1.0, 0.5, 0.2]
Softmax → [0.53, 0.19, 0.12, 0.10]
→ **53% on "cat" (BALANCED)**

Step 3: Scale by T=2.0 (FLATTER)
Scaled = [1.0, 0.5, 0.25, 0.1]
Softmax → [0.38, 0.23, 0.17, 0.15]
→ 38% on "cat" (MUCH FLATTER)

General Formula:

$$p_i = \frac{\exp(\text{logit}_i/T)}{\sum_j \exp(\text{logit}_j/T)}$$

Lower T → More confident (peaky)
Higher T → More random (flat)

Concrete numbers show how temperature scaling works

Temperature: Detail

How It Works:
Given logits $z_1, \ldots, z_V$

Scale by temperature T:

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

Sample from p

Effect:
$T \to 0$: argmax
$T = 1$: standard softmax
$T \to \infty$: uniform

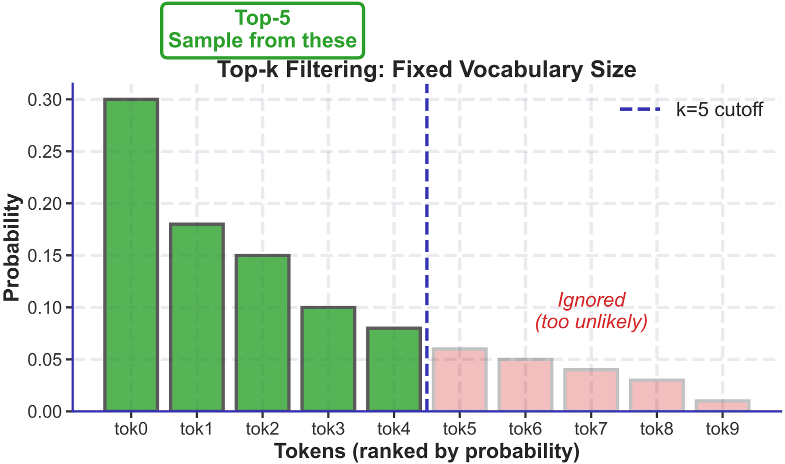
Practical Settings:

- **T = 0.1-0.3**: Factual Q&A
- **T = 0.7**: Chatbots
- **T = 0.9-1.2**: Creative
- **T = 1.5+**: Experimental

\+ Simple to implement
\+ Continuous control
\- No quality guarantee
\- Can be nonsense

Temperature: simplest randomness control

Top-k Sampling: Filter the Tail



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

Prevents sampling from long tail of unlikely words

Top-k: Worked Example (k=3)

Top-k Example: k=3

1. Original Probabilities:

cat: 0.45
dog: 0.18
bird: 0.15
fish: 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)

Filtering + renormalization prevents tail sampling

Top-k: Detail

Algorithm:

1. Compute $P(w_i)$ for all
2. Sort by probability
3. Keep only top-k
4. Renormalize
5. Sample from p'

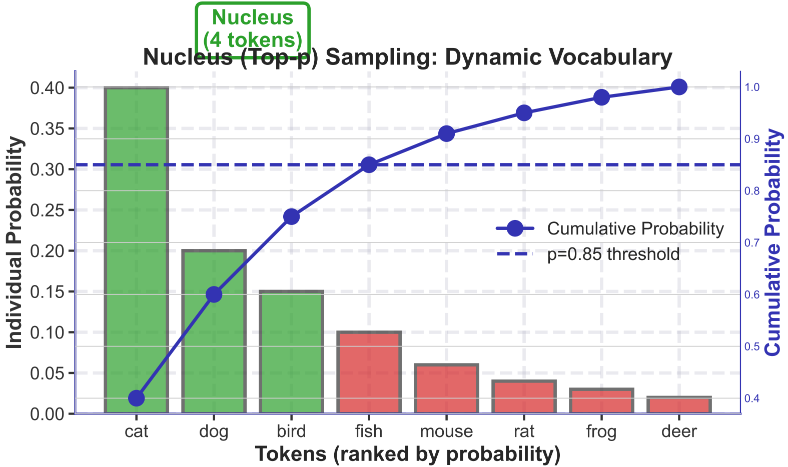
Example (k=3):
Original: [0.45, 0.18, 0.15, ...]
Keep: [0.45, 0.18, 0.15]
Renorm: [0.58, 0.23, 0.19]

Typical Values:
k = 40-50 (balanced)
k = 10-20 (focused)
k = 100+ (very diverse)

Limitation:
Fixed cutoff regardless of distribution!
Peaked: Wastes mass
Flat: Too many bad tokens

Solution: Dynamic cutoff

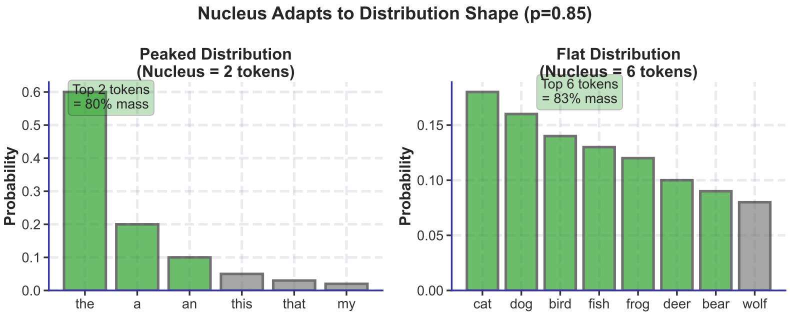
Top-k improves over temperature but inflexible



Key Insight: Adapt vocabulary size to distribution shape

Nucleus size grows/shrinks based on probability spread

Nucleus: How Distribution Shape Matters



Same p value → different vocabulary for peaked vs flat

Nucleus (Top-p): Detail

Algorithm:

1. Sort tokens by $P(w_i)$
2. Compute cumulative sum
3. Find smallest set where cum $\geq p$
4. Sample from nucleus

Example (p=0.85):
Cumsum: [0.40, 0.60, 0.75, 0.85]
Nucleus: First 4 tokens

Recommended:

- p = 0.85-0.90: Dialogue
- p = 0.90-0.95: Creative
- p = 0.95-0.99: Very diverse

Why Better:
Peaked → small nucleus
Flat → large nucleus
Adapts automatically!

Current Standard
ChatGPT, Claude, GPT-4

Nucleus: modern standard for high-quality generation

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 $\rightarrow$ same patterns repeated

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

Discovery: Why do models repeat themselves?

Greedy/beam maximize probability - but high prob = repeating recent context

Contrastive Search: How It Works

Step 1: Get top-k candidates by probability

- city: 0.45
- town: 0.18
- area: 0.15
- place: 0.12

Step 2: Compute similarity to recent context

Context: "...the city has..."

- city: 0.92 (cosine similarity)
- town: 0.75 (cosine similarity)
- area: 0.65 (cosine similarity)
- place: 0.60 (cosine similarity)

Step 3: Apply diversity penalty (α=0.6)

score = (1-α)×P(token) - α×similarity

city: 0.4×0.45 - 0.6×0.92 = -0.372
town: 0.4×0.18 - 0.6×0.75 = -0.378
area: 0.4×0.15 - 0.6×0.65 = -0.330
place: 0.4×0.12 - 0.6×0.60 = -0.312

Winner: "town" (high prob, lower similarity)

Key Insight: Balance probability (coherence) with diversity (novelty)

α=0: Pure greedy | α=0.6: Balanced | α=1.0: Maximum diversity

Key Insight: Balance probability with diversity penalty

Explicitly avoid copying recent context - prevents degeneration

Contrastive vs Nucleus: Comparison

Same Prompt, Different Methods

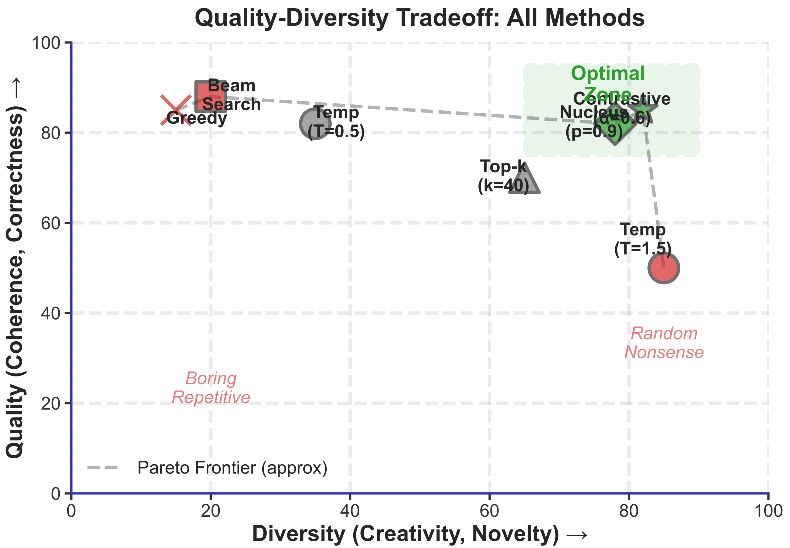
Prompt: "The future of artificial intelligence is"

Nucleus (p=0.9)	**Contrastive (α=0.6)**
"...is promising and will transform many industries. We expect to see significant advances in healthcare, education, and research in the coming years."	"...is rapidly evolving, bringing unprecedented opportunities across sectors ranging from medicine to climate science, while raising important ethical questions."
+ Diverse + Creative - Some repetition	**+ Diverse** **+ Creative** **+ No repetition**

Contrastive Search explicitly penalizes copying recent context

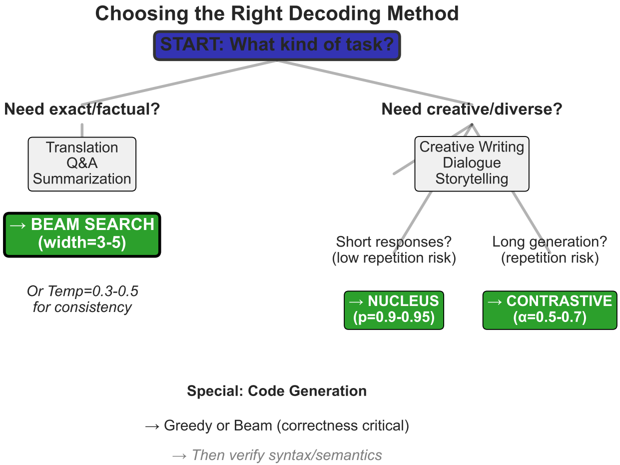
Contrastive prevents repetition better for long generation

All Methods on Quality-Diversity Space



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 (2025)

Task-Specific Decoding Recommendations (2025)

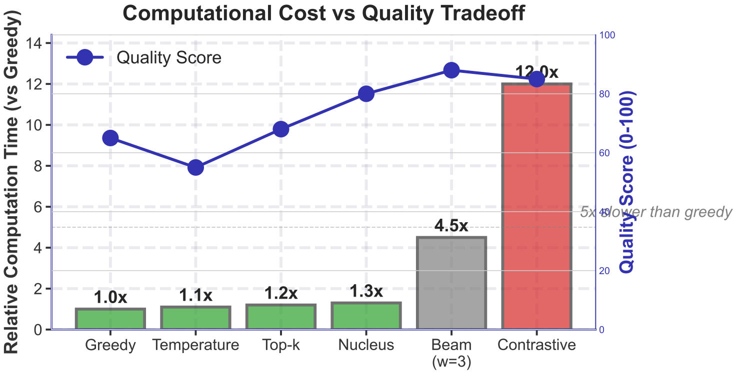
Deterministic Tasks

Creative Tasks

Task	Recommended Method	Parameters	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 / Contrastive	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: 8 tasks → optimal strategies

Computational Costs Matter



Insight: Contrastive gives best quality-diversity but 12x slower. Nucleus is best balanced choice.

Contrastive: best quality-diversity but 12× slower. **Nucleus: best balanced**

Production tradeoff: Quality vs speed vs diversity

Key Takeaways

1. **Deterministic** (Greedy, Beam): High quality, no diversity → factual tasks
2. **Temperature**: Simple randomness control → universal but crude
3. **Top-k**: Fixed vocabulary filter → prevents tail sampling
4. **Nucleus (Top-p)**: Dynamic cutoff → modern standard, adapts
5. **Contrastive (NEW)**: Degeneration prevention → long creative text
6. **Task matters**: Translation → Beam — Dialogue → Nucleus — Stories → Contrastive

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

Decoding strategy matters as much as model architecture

Technical Appendix

19 slides: Complete mathematical treatment

A1-A5: Beam Search Mathematics
A6-A10: Sampling Mathematics
A11-A14: Contrastive Search & Degeneration
A15-A19: Advanced Topics & Production

A1: Beam Search Formulation

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

Decomposition:

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

Log-probability:

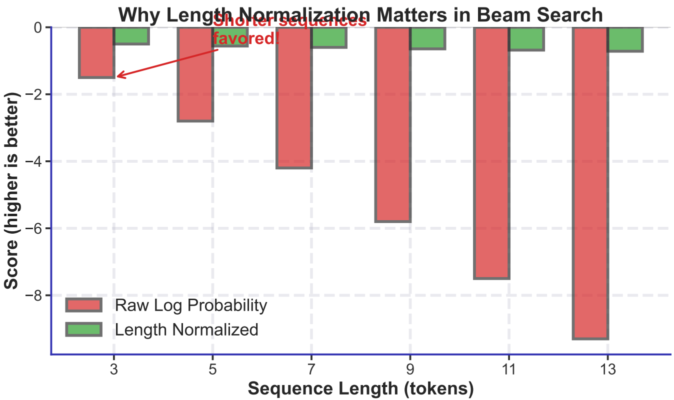
$$\log P(y|x) = \sum_{t=1}^{T} \log P(y_t|y_{<t}, x)$$

Beam Search Approximation:
Instead of V^T sequences, maintain top-k hypotheses

Complexity:
Time: $O(k \cdot V \cdot T)$
Space: $O(k \cdot T)$

Tractable approximation to exact search

A2: Length Normalization



Solution: Normalize by length

$$\text{score}(y) = \frac{1}{|y|^\alpha} \log P(y) \quad \text{where } \alpha \in [0.5, 1.0]$$

Length normalization essential for fair comparison

A3: Beam Search Variants

Diverse Beam:
Partition beams into groups
Penalize within-group similarity

Constrained Beam:
Force certain tokens
Keywords, entities

Stochastic Beam:
Sample beams (not argmax)
More diverse

Block n-gram:
Penalize n-gram repetition
"city is a city" prevention

Many variants for specific requirements

A4: Beam Search Stopping

When to stop?

1. **Fixed length**: Stop at T_{max} (simple but rigid)
2. **END token**: Special token (most common)
3. **Score threshold**: When best cannot improve
4. **Timeout**: Computational budget

Stopping criterion affects output length

A5: Beam Search Limitations

Fundamental Issues:

1. **Exposure bias**: Train with teacher forcing, test with own outputs
2. **Label bias**: Cannot compare different prefixes fairly
3. **Repetition**: Still can loop
4. **Bland outputs**: Maximizes probability $\neq$ interestingness
5. **Search errors**: May miss better sequences

When Beam Fails:
Open-ended generation, long-form text, creative tasks

$\rightarrow$ Need sampling-based methods

Beam optimizes wrong objective for creative tasks

A6: Sampling as Inference

Goal: Sample $y \sim P(y|x)$ not $\arg\max P(y|x)$

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

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

Sampling enables diversity but loses quality guarantees

Softmax with Temperature:

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

Limiting Cases:
$T \to 0$: deterministic (greedy)
$T \to \infty$: uniform ($1/V$)

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

Temperature controls distribution entropy

A8: Top-k Mathematics

Formal Definition:

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

(top k by prob)
Truncated distribution:

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

Information Loss:
$H(p') < H(p)$ (entropy decreases)
Loss $\approx$ tail information

Top-k sacrifices tail probability for quality

A9: Nucleus Mathematics

Formal Definition:

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

Smallest set with cumulative mass $\geq p$

Dynamic Size:

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

Peaked: Small $|V_p|$ (2-5)
Flat: Large $|V_p|$ (50+)

Why Nucleus > Top-k:
Top-k: Fixed k
Nucleus: Adapts to distribution

Nucleus adjusts vocabulary to distribution

How to Measure Decoding Quality

Quality Metrics

- Perplexity (lower = better)
- BLEU score (translation)
- ROUGE score (summarization)
- Human evaluation ratings
- Grammaticality score

Diversity Metrics

- Distinct-n (unique n-grams)
- Self-BLEU (lower = more diverse)
- Repetition rate
- Vocabulary richness
- Entropy of outputs

Combined Quality-Diversity Metrics

- Task success rate (does it solve the task?)
- Human preference (A/B testing)
- Pareto frontier analysis (multi-objective)

Need both quality AND diversity metrics

A11: Degeneration Problem (Formal)

Definition: Unnatural repetitions in generated text

Why It Happens:

1. Model trained on natural text (low repetition)
2. Generation maximizes $P(y_t|y_{<t})$
3. Recent context influences P
4. Feedback loop: high prob $\rightarrow$ context $\rightarrow$ same high prob

Quantifying:
Greedy repetition: 15-30%
Human text: 2-5%
Gap = degeneration

Examples: "*I think that I think that I think...*"

Maximizing probability $\neq$ natural text

A12: Contrastive Search Objective

Scoring Function:

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

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

Similarity: Cosine similarity using token embeddings

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

Algorithm:

1. Get top-k by probability
2. Compute similarity to all $y_{<t}$
3. Apply penalty: score = prob - $\alpha\times$ max_sim
4. Select highest score

Explicit penalty for copying context

A13: Contrastive Parameters

Alpha (α):
$\alpha = 0$: Pure greedy
$\alpha = 0.6$: Balanced (default)
$\alpha = 1.0$: Max diversity

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

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

Cost: $O(k \times T^2)$
12× slower than greedy
Only for quality-critical

Hugging Face default: α=0.6, k=4

A14: Degeneration Analysis (2024-2025)

Research Findings:

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

Why Probability Fails:
Training: Next token prediction
Generation: Global coherence
Mismatch: Local optimum $\neq$ global quality

Solutions Hierarchy:
1. Temp/Top-k/Nucleus: Reduce greedy determinism
2. Contrastive: Explicit penalty
3. RLHF/DPO: Align with humans (Week 10)

Contrastive addresses fundamental limitation

A15: Hybrid Methods

Combining Strategies:

Nucleus + Temperature:

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

Used by GPT-3, ChatGPT

Beam + Sampling:
Beam search + stochastic selection

Contrastive + Nucleus:
Best of both worlds

Hybrid methods leverage complementary strengths

A16: Constrained Decoding (2025)

Goal: Force tokens/patterns

Lexically Constrained:
Must include keywords
Beam variant tracks satisfaction

Format Constraints:
JSON output, code syntax

Use Cases:
Structured extraction, controllable summarization, code generation

Constrained decoding enables controllable generation

A17: Computational Complexity

Method	**Time/token**	**Total**	**Speed**
Greedy	$O(V)$	$O(VT)$	1.0×
Temperature	$O(V)$	$O(VT)$	1.1×
Top-k	$O(V)$	$O(VT)$	1.2×
Nucleus	$O(V \log V)$	$O(V \log V \cdot T)$	1.3×
Beam (k=5)	$O(kV)$	$O(kVT)$	4.5×
Contrastive	$O(kT)$	$O(kT^2)$	12×

Practical (1000 tokens):
Greedy: 2.5s — Nucleus: 3.2s — Beam: 11s — Contrastive: 30s

Computational cost matters for production

Production Decoding Settings (Real Systems 2024-2025)

System (2024-2025)	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 Default	Greedy	T=1.0	Deterministic baseline

Real settings from major production systems

A19: Future Directions (2025)

Active Research:

1. Quality-diversity optimization
2. Learned decoding (RLHF, DPO)
3. Speculative decoding (4-8$\times$ faster)
4. Adaptive methods
5. Energy-based decoding

Open Problems:
- Auto-select best parameters for new task?
- Balance fluency + factuality + creativity?
- Efficient 100K+ token decoding?

Trend: Hand-tuned $\rightarrow$ learned decoding strategies

Active research area with many open questions