Decoding Strategies

Week 9: From Prediction to Generation

NLP Course 2025

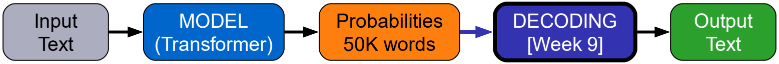
Enhanced with Contrastive Search (2025)

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 → 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.

Today's Challenge: From Probabilities to Text

The Setup: Model gives us probabilities for next word

Example: "The cat __"

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

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:

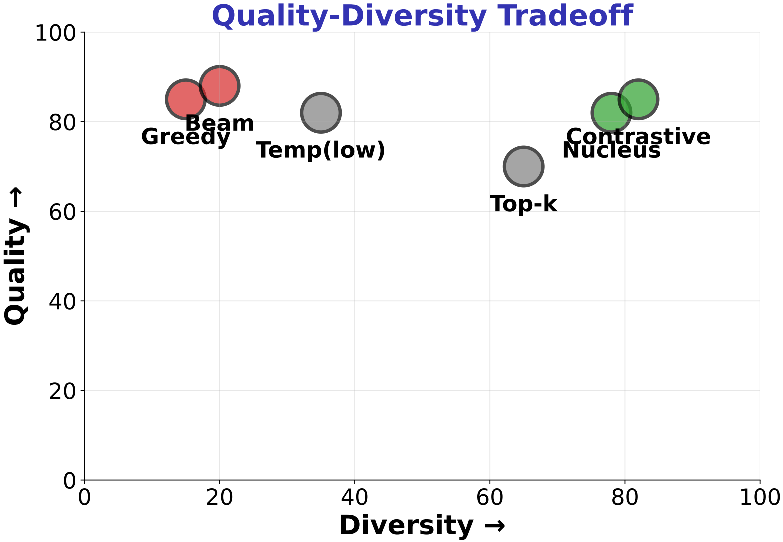
"The purple flying mathematics..."

Problem: Nonsense, incoherent

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

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

The Quality-Diversity Tradeoff



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

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

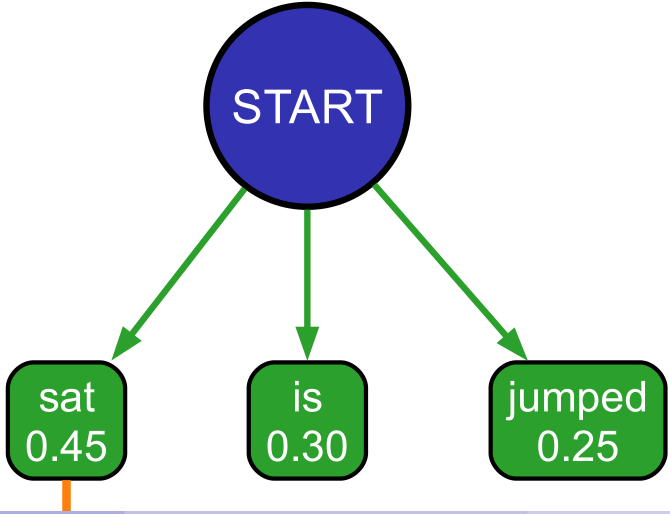
Problem: Degeneration
"The city is a city in a city..."
Model gets stuck in loops

Simplest but prone to repetition

Beam Search: Explore Multiple Paths

../figures/beam_search_visual_bsc.pdf

Beam Search: Step-by-Step Example



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:

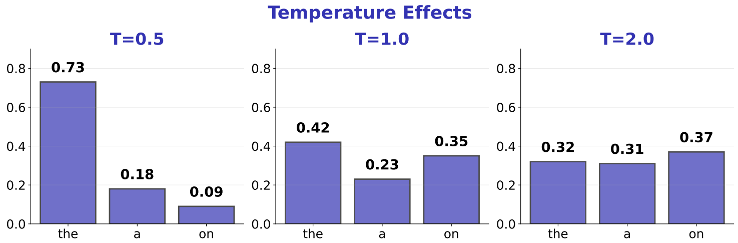
- Machine translation
- Summarization
- Question answering
- “Correct” answer tasks

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: Worked Example

../figures/temperature_calculation_bsc.pdf

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

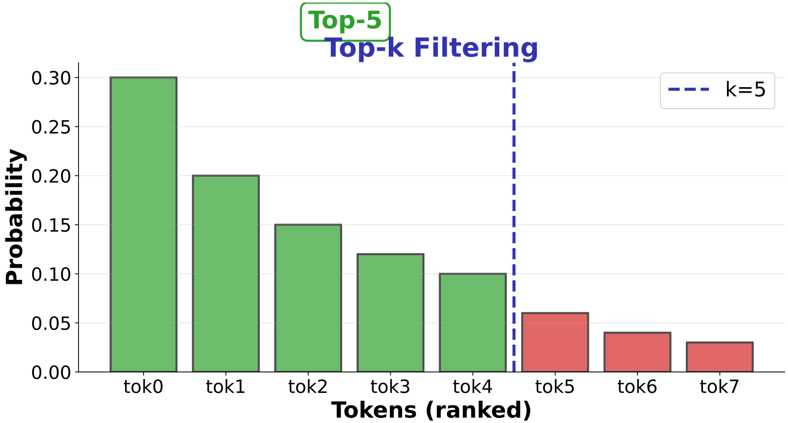
Practical Settings:

- $\mathbf{T = 0.1\text{-}0.3}$: Factual Q&A
- $\mathbf{T = 0.7}$: Chatbots
- $\mathbf{T = 0.9\text{-}1.2}$: Creative
- $\mathbf{T = 1.5+}$: 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)

../figures/topk_example_bsc.pdf

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]

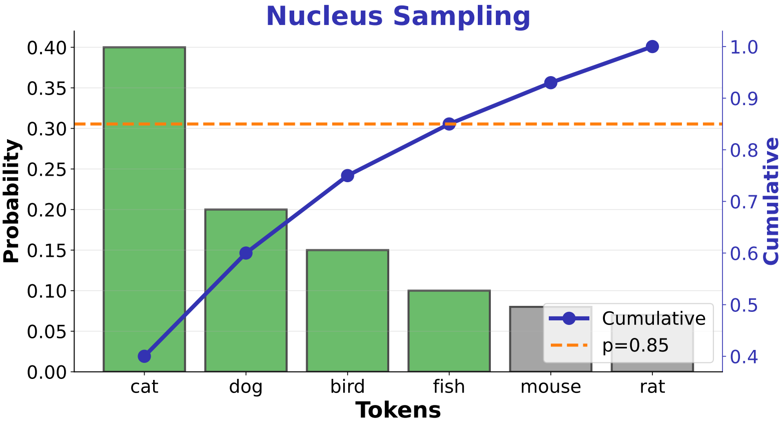
Typical Values:
k = 40-50 (balanced)
k = 10-20 (focused)
k = 100+ (very diverse)

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

Solution: Dynamic cutoff

Top-k improves over temperature but inflexible

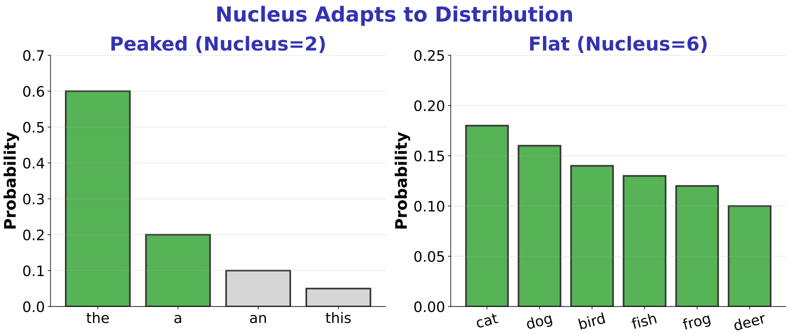
Nucleus (Top-p) Sampling: Dynamic Cutoff



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:

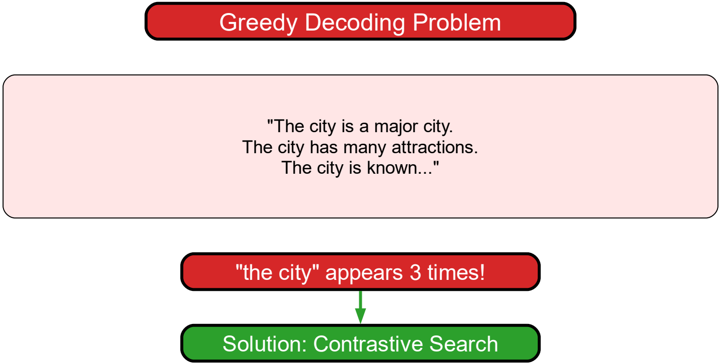
- p = 0.85-0.90: Dialogue
- p = 0.90-0.95: Creative
- p = 0.95-0.99: Very diverse

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



Greedy Decoding Problem

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

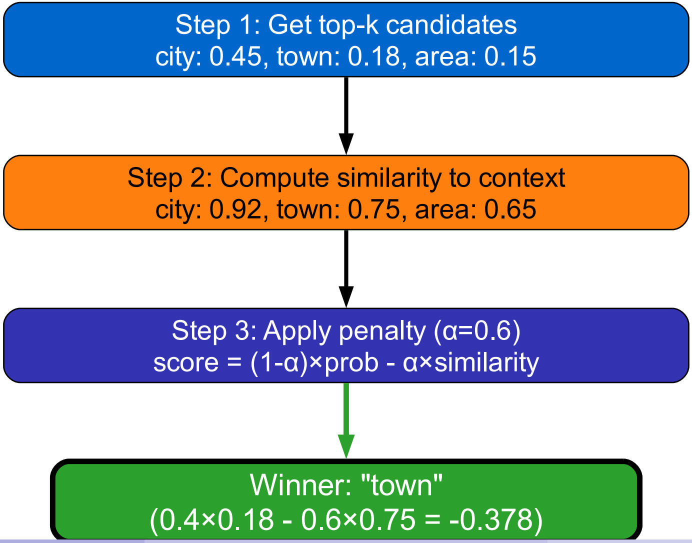
"the city" appears 3 times!

Solution: Contrastive Search

Discovery: Why do models repeat themselves?

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

Contrastive Search: Penalize Repetition (2025)



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

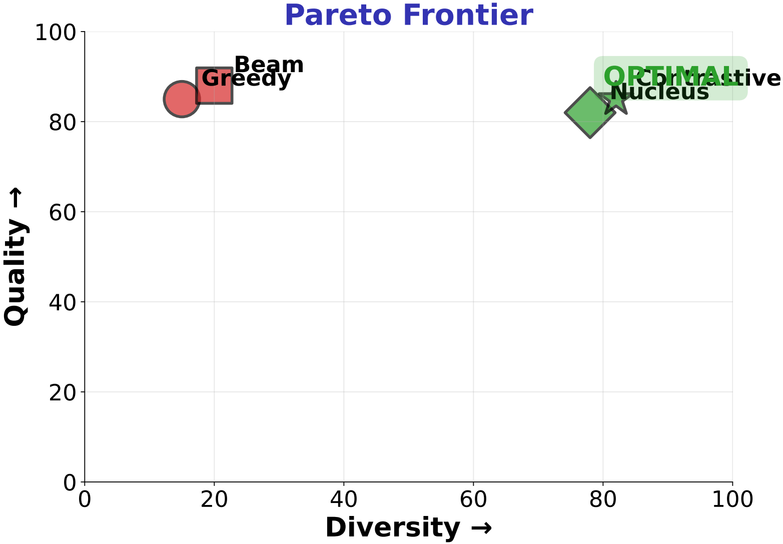
Step 3: Apply penalty (α=0.6)
score = (1-α)×prob - α×similarity

Winner: "town"
(0.4×0.18 - 0.6×0.75 = -0.378)

Contrastive vs Nucleus: Comparison

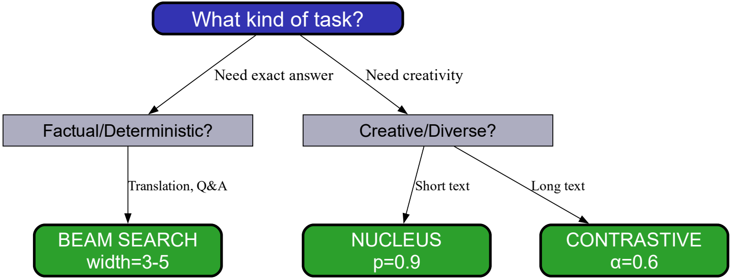
../figures/contrastive_vs_nucleus_bsc.pdf

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 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: 8 tasks → optimal strategies

Computational Costs Matter

../figures/computational_cost_comparison_bsc.pdf

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 $y^* = \operatorname{argmax} P(y|x)$

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

`../figures/length_normalization_bsc.pdf`

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 $\text{argmax}\, P(y|x)$

Ancestral Sampling:

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

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

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:
$T \to 0$: 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

A10: Quality & Diversity Metrics

../figures/quality_metrics_bsc.pdf

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 → context → 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 ≠ 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

A18: Production Settings (2024-2025)

../figures/production_settings_bsc.pdf

A19: Future Directions (2025)

Active Research:

1. Quality-diversity optimization
2. Learned decoding (RLHF, DPO)
3. Speculative decoding (4-8× 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 → learned decoding strategies

Active research area with many open questions