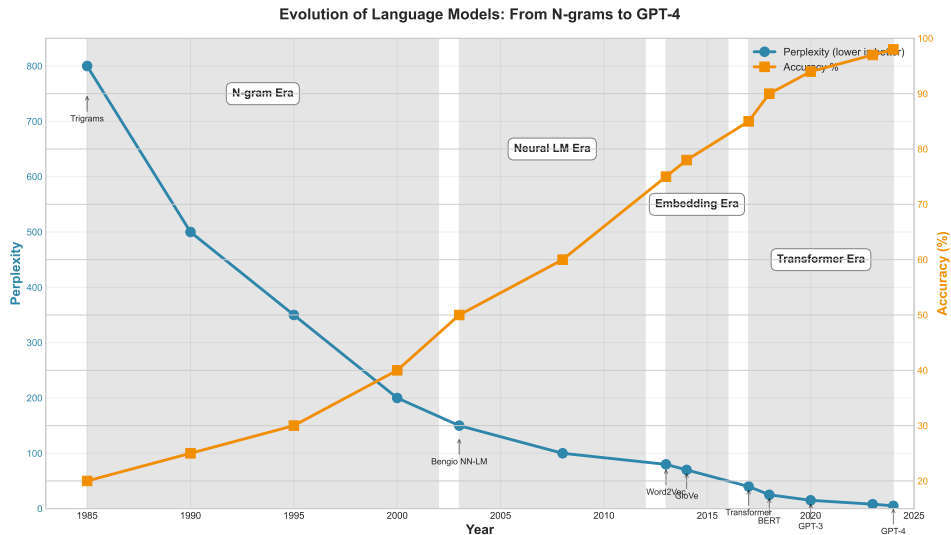## Natural Language Processing Course
Week 2: Neural Language Models and Word Embeddings

Restructured with 4-Part Format

2024

Evolution of Language Models: From N-grams to GPT-4

Four Major Eras in Next-Word Prediction:

N-grams Era (1980s-2000s): Count and Predict

How it predicted the next word:

Vocabulary:
- Fixed word list (10k-100k words)
- Out-of-vocabulary (OOV) $\rightarrow$ <UNK>
- Simple tokenization (spaces, punctuation)

Context:
- Fixed window (typically 2-5 words)
- "The cat sat" $\rightarrow$ predict next word
- No long-range dependencies

Strengths: Simple, interpretable, no training needed
Limitations: Sparsity, no semantics, fixed context

Method:
- Count n-gram frequencies
- Markov assumption
- Smoothing techniques (Laplace, Kneser-Ney)

Prediction Formula:

$$P(w_n|w_{n-2}, w_{n-1}) = \frac{C(w_{n-2}, w_{n-1}, w_n)}{C(w_{n-2}, w_{n-1})}$$

Example: P(mat—cat, sat) = 45/50 = 0.9

Week 2: Neural Language Models - Overview

Part 1: Introduction & Motivation
- Interactive word association
- The semantic understanding problem
- Real-world impact and applications
- Historical journey to Word2Vec

Part 2: Core Concepts
- Distributional hypothesis
- From discrete to continuous
- Word2Vec architecture
- Implementation deep dive

Part 3: Challenges & Solutions
- Training at scale
- Evaluation methodologies
- Fundamental limitations
- Advanced techniques

Part 4: Applications & Future
- Hands-on applications
- Modern evolution (BERT, GPT)
- Industry state-of-the-art
- Looking forward

Goal: Master how computers learn word meaning through context

Part 1

Introduction and Motivation

Why Computers Need to Understand Word Meaning

When you see this word, what comes to mind?

OCEAN

When you see this word, what comes to mind?

OCEAN

water
35% of you

sea
25% of you

beach
20% of you

waves
20% of you

You naturally understand semantic relationships!

But until 2003, computers saw:

- ocean = ID 7849
- water = ID 2341
- No connection whatsoever!

The Semantic Gap: Computers vs Humans

How Humans See Words:

- cat $\approx$ kitten (similar animals)
- Paris $\leftrightarrow$ France (location relation)
- running $\sim$ ran (same verb, different tense)
- doctor $\leftrightarrow$ hospital (association)

Rich semantic network with relationships, similarities, and associations

How Computers Saw Words (Pre-2003):

- cat = 1247
- kitten = 8923
- Paris = 4567
- France = 2109

Arbitrary IDs with no notion of meaning or relationships

The Challenge: Bridge this semantic gap!

Real System Failures Without Semantic Understanding

Early Google Search (2000):
- Search: "car" → Missed: "automobile", "vehicle"
- Search: "running shoes" → Missed: "jogging sneakers"

Machine Translation Disasters:
- "The spirit is willing but the flesh is weak"
- → Russian → English:
- "The vodka is good but the meat is rotten"

Customer Service Chatbots (2005):
- Customer: "I want to return my purchase"
- Bot: "I don't understand. Did you mean 'buy'?"
- → Couldn't link "return" with "refund", "exchange"

Economic Impact: Billions lost due to poor search and translation

Where Word Embeddings Power Your Life (2024)

Entertainment:

- **Spotify:** 256-dim song embeddings
- **Netflix:** Show similarity vectors
- **TikTok:** Video understanding
- **YouTube:** Related videos
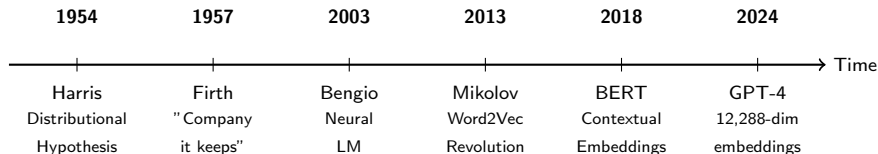
Productivity:

- **Gmail:** Smart compose (BERT)
- **Grammarly:** Context awareness
- **Notion AI:** Semantic search
- **Slack:** Message threading

Commerce:

- **Amazon:** Product similarity
- **Google Ads:** Ad matching
- **Airbnb:** Listing embeddings
- **Uber:** Location understanding

Market Size:

- Embedding API Market: $2.7B by 2025
- OpenAI Embeddings: 1M+ developers
- Vector Database Market: $4.3B by 2028

Every AI application today relies on word embeddings!

The Journey to Understanding: Timeline

1954	1957	2003	2013	2018	2024

→ Time

Harris	Firth	Bengio	Mikolov	BERT	GPT-4
Distributional	"Company	Neural	Word2Vec	Contextual	12,288-dim
Hypothesis	it keeps"	LM	Revolution	Embeddings	embeddings

Key Breakthroughs:

- **1954-1957:** Theoretical foundation - words defined by context
- **2003:** First neural language model with continuous representations
- **2013:** Word2Vec makes embeddings practical and scalable
- **2018:** Contextualized embeddings (same word, different contexts)
- **2024:** Massive embeddings powering GPT-4, Claude, Gemini

The demo that shocked the NLP world:[1]

$$\text{king - man + woman =}$$

---
[1] Mikolov et al. (2013). "Linguistic regularities in continuous space word representations"

The demo that shocked the NLP world:[1]

$$\text{king - man + woman = queen}$$

Why this was revolutionary:

- Computer discovered gender relationships automatically
- No one programmed these rules
- Learned purely from reading text
- Worked across many relationship types

More examples that work:

- Paris - France + Italy = Rome
- sushi - Japan + Mexico = tacos
- Einstein - scientist + artist = Picasso

- bigger - big + small = smaller
- walking - walk + swim = swimming
- CEO - company + country = president

---

[1]Mikolov et al. (2013). "Linguistic regularities in continuous space word representations"

Part 1 Summary: Why This Matters

Key Insights:

1. **The Problem:** Computers treating words as meaningless IDs
2. **The Impact:** Billions in losses, poor user experiences
3. **The Solution:** Learn meaning from context (distributional hypothesis)
4. **The Breakthrough:** Word2Vec made it practical (2013)

What's Next:

- Part 2: How do we actually create these word vectors?
- Understanding the mathematics and algorithms
- Building Word2Vec from scratch

Remember: Every modern AI system (ChatGPT, Claude, Gemini) started here!

Part 2

Core Concepts

How Computers Learn Word Meaning from Context

The Distributional Hypothesis: Foundation

Core Principle (Firth, 1957):

> "You shall know a word by the company it keeps"

Example: What is a "zorb"?

- The <u>zorb</u> ate the cheese
- I saw a <u>zorb</u> in my garden
- The <u>zorb</u> ran under the couch
- My cat chased the <u>zorb</u>

The Distributional Hypothesis: Foundation

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- My cat chased the <u>zorb</u>

You probably guessed: zorb = mouse (or similar small animal)

Mathematical Formulation:

- Words with similar distributions have similar meanings
- similarity$(w_1, w_2) \propto P(\text{context}|w_1) \cdot P(\text{context}|w_2)$
- Context defines meaning!

Mystery word = [BLANK]. What is it?

1. The [BLANK] was delicious
2. I ordered [BLANK] with extra cheese
3. The [BLANK] delivery arrived in 30 minutes
4. We shared a large [BLANK] at the party
5. My favorite [BLANK] topping is pepperoni

Mystery word = [BLANK]. What is it?

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3. The [BLANK] delivery arrived in 30 minutes
4. We shared a large [BLANK] at the party
5. My favorite [BLANK] topping is pepperoni

Answer: pizza

This is exactly how Word2Vec learns:

- Sees millions of sentences
- Learns what words appear in similar contexts
- Groups them close together in vector space
- No dictionary needed!

From Discrete IDs to Continuous Vectors

One-Hot Encoding (Old Way):
- Vocabulary size: 50,000 words
- cat = [0,0,1,0,0,...,0] (50K dimensions!)
- dog = [0,0,0,1,0,...,0]

Problems:
- No similarity: cat · dog = 0
- Huge vectors: 50K dimensions
- Sparse: 49,999 zeros
- No learning: Fixed representation

Dense Embeddings (Word2Vec):
- Typical size: 100-300 dimensions
- cat = [0.2, -0.4, 0.7, ..., 0.1]
- dog = [0.3, -0.3, 0.6, ..., 0.2]

Benefits:
- Similarity: cat · dog = 0.89
- Compact: 100-300 dims
- Dense: All values meaningful
- Learnable: Updated during training

Key: Every dimension captures some semantic property

The Goldilocks Zone: Why 100-300 Dimensions?

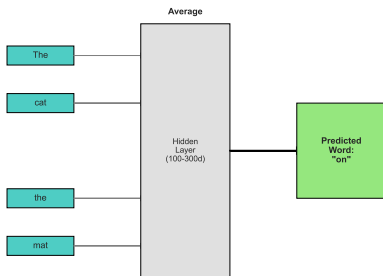Embedding Dimensions vs Performance Trade-off
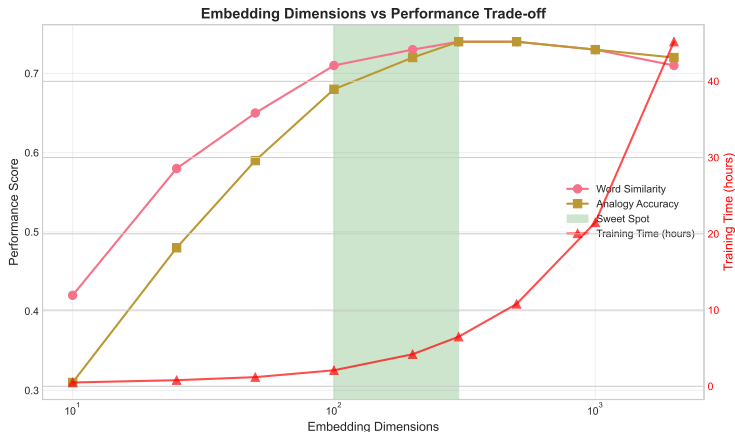
Empirical Findings:

- **¡ 50 dims:** Too compressed, loses nuances
- **100-300 dims:** Sweet spot for most tasks
- **¿ 500 dims:** Diminishing returns, overfitting risk

Word2Vec: Two Architectures
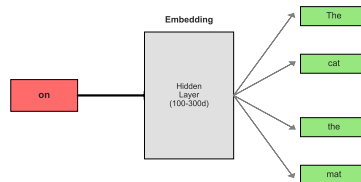
CBOW (Continuous Bag of Words):

CBOW Architecture: Predict Center from Context

Skip-gram:

Skip-gram Architecture: Predict Context from Center

- Predict center from context
- Input: [the, cat, on, mat]
- Output: sat
- Faster to train
- Better for frequent words

- Predict context from center
- Input: sat
- Output: [the, cat, on, mat]
- Slower but more accurate
- Better for rare words

Skip-gram Training: Step by Step

Sentence: "The quick brown fox jumps"

Window size = 2 (look 2 words left and right)

Step	Center Word	Context to Predict
1	quick	[the, brown]
2	brown	[the, quick, fox, jumps]
3	fox	[quick, brown, jumps]

Training Process:

1. Take center word embedding
2. Try to predict context words
3. Measure prediction error
4. Update embeddings to reduce error
5. Repeat millions of times

Result: Words appearing in similar contexts get similar embeddings

Implementing Word2Vec in PyTorch

```python
import torch
import torch.nn as nn
import torch.nn.functional as F

class Word2Vec(nn.Module):
    def __init__(self, vocab_size, embed_dim=100):
        super().__init__()
        # Two embedding matrices
        self.center_embeddings = nn.Embedding(
            vocab_size, embed_dim
        )
        self.context_embeddings = nn.Embedding(
            vocab_size, embed_dim
        )

    def forward(self, center, context, neg_samples):
        # Get embeddings
        center_emb = self.center_embeddings(center)
        context_emb = self.context_embeddings(context)
        neg_emb = self.context_embeddings(neg_samples)

        # Positive samples (should be similar)
        pos_score = torch.sum(
            center_emb * context_emb, dim=1
        )
        pos_loss = F.logsigmoid(pos_score)

        # Negative samples (should be different)
        neg_score = torch.bmm(
            neg_emb, center_emb.unsqueeze(2)
        ).squeeze()
        neg_loss = F.logsigmoid(-neg_score).sum(1)

        return -(pos_loss + neg_loss).mean()
```

Key Components:

- **Two matrices:** Center and context embeddings
- **Positive samples:** Real context words
- **Negative samples:** Random words (not in context)

Training Trick:

- Full softmax over 50K words is expensive
- Solution: Negative sampling
- Only update a few random words
- 5-20 negative samples typical

Loss Function:

- Maximize similarity with real context
- Minimize similarity with random words

Training Word2Vec: The Complete Loop

```python
def train_word2vec(corpus, vocab_size, embed_dim=100, epochs=5, window=2):
    model = Word2Vec(vocab_size, embed_dim)
    optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

    for epoch in range(epochs):
        total_loss = 0
        for sentence in corpus:
            # Generate training samples from sentence
            for i, center_word in enumerate(sentence):
                # Get context words within window
                context_words = []
                for j in range(max(0, i-window), min(len(sentence), i+window+1)):
                    if i != j:
                        context_words.append(sentence[j])

                # Get negative samples (5 random words not in context)
                neg_samples = get_negative_samples(vocab_size, 5, avoid=context_words)

                # Forward pass
                loss = model(center_word, context_words, neg_samples)

                # Backward pass
                optimizer.zero_grad()
                loss.backward()
                optimizer.step()

                total_loss += loss.item()

        print(f"Epoch {epoch}: Loss = {total_loss:.4f}")

    return model.center_embeddings.weight.data  # Final embeddings
```

Result: After training on millions of sentences, similar words cluster together!

Word Embeddings Automatically Cluster by Meaning
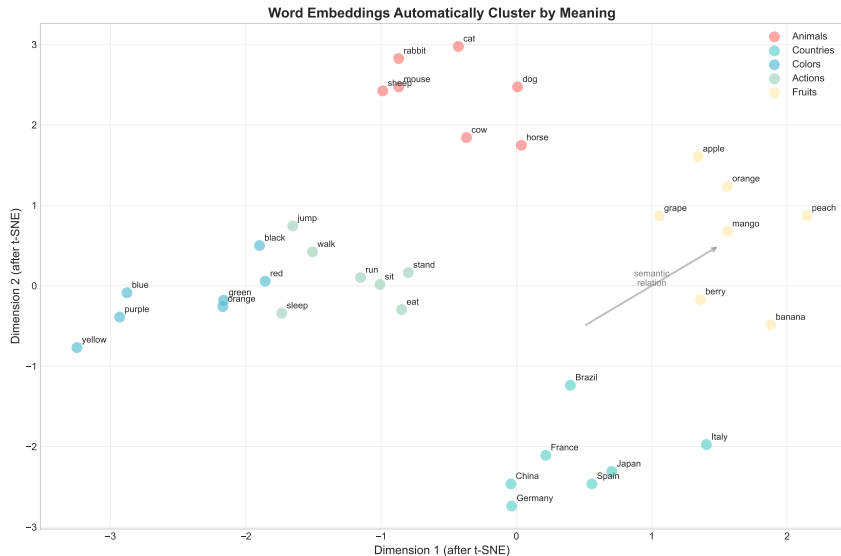
Mathematical Intuition: Why Dot Product = Similarity

The Skip-gram Objective:

$$\max \sum_{t=1}^{T} \sum_{-c \leq j \leq c, j \neq 0} \log P(w_{t+j}|w_t)$$

Where probability is defined as:

$$P(w_O|w_I) = \frac{\exp(v_{w_O}^T v_{w_I})}{\sum_{w=1}^{W} \exp(v_w^T v_{w_I})}$$

Key Insight:

- Dot product $v_{w_O}^T v_{w_I}$ measures similarity
- Higher dot product $\rightarrow$ higher probability of co-occurrence
- Training maximizes dot product for words that appear together
- Result: Similar words have high dot product (cosine similarity)

Geometry emerges from statistics: Similar contexts $\rightarrow$ Similar vectors

Part 2 Summary: Core Concepts Mastered

What We Learned:

1. **Distributional Hypothesis:** Context defines meaning
2. **Dense Vectors:** 100-300 dimensions capture semantics
3. **Skip-gram Model:** Predict context from center word
4. **Training Process:** Maximize co-occurrence probability
5. **Implementation:** Two embedding matrices + negative sampling

Key Takeaways:

- Word meaning emerges from statistical patterns
- No linguistic knowledge required
- Scalable to millions of words
- Foundation for all modern NLP

Next: Part 3 - Challenges and Solutions

- How to train on billions of words efficiently?
- How to evaluate embedding quality?
- What are the limitations?

Part 3

Challenges and Solutions

Scaling, Evaluation, and Limitations

Softmax: From Scores to Probabilities

Example: Next word prediction after "The cat sat on the..."

Step 1: Neural Network Scores

Word	Score
mat	2.1
floor	1.8
chair	0.3
table	0.1
sky	-1.2

Step 2: Apply Exponential

Word	exp(score)
mat	8.17
floor	6.05
chair	1.35
table	1.11
sky	0.30
Sum	**16.98**

Step 3: Normalize (Divide by Sum)

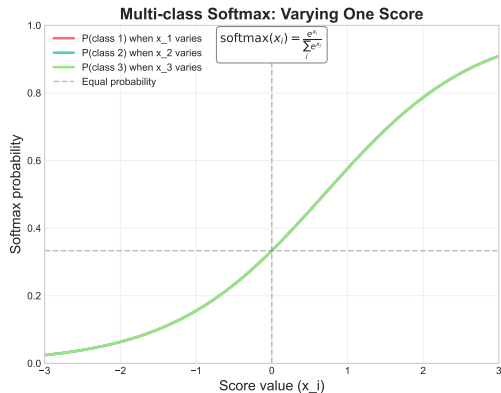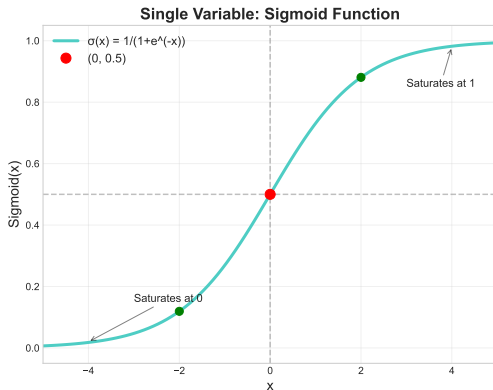| Word	Probability
mat	0.481
floor	0.356
chair	0.079
table	0.065
sky	0.018
Sum	**1.000**

Softmax Formula:
$$P(w_i) = \frac{e^{s_i}}{\sum_j e^{s_j}}$$

Result: "mat" has 48.1% probability!

Softmax Function: Mathematical Behavior

Softmax Function Behavior

Single Variable: Sigmoid Function

Multi-class Softmax: Varying One Score
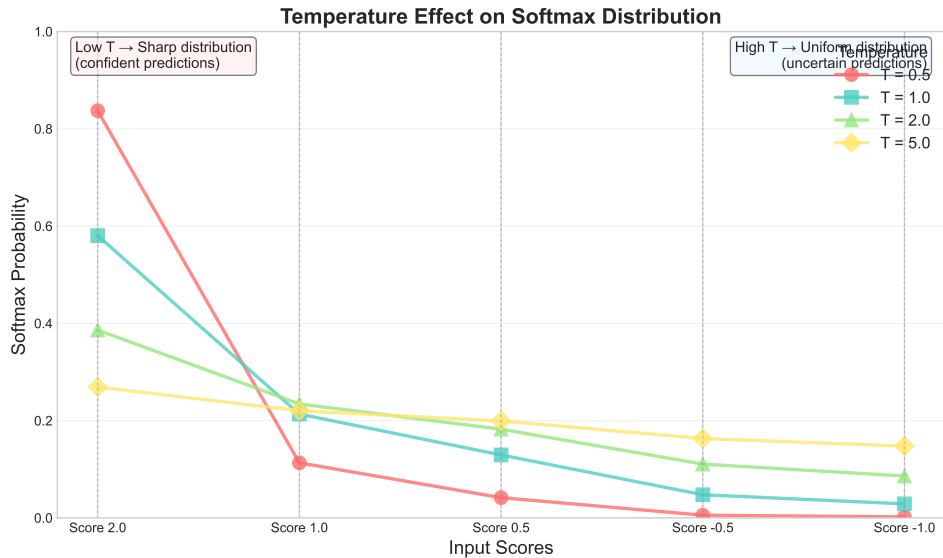
$$\text{softmax}(x_i) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

Key Properties:

- **Single variable:** Reduces to sigmoid function
- **Multi-class:** Competition between classes - increasing one score decreases others' probabilities
- **Saturation:** Extreme values lead to near 0 or 1 probabilities

Temperature Effect on Softmax Distribution

Challenge 1: Computational Complexity

The Softmax Bottleneck:
Original formulation requires normalizing over entire vocabulary:

$$P(w_O|w_I) = \frac{\exp(v_{w_O}^T v_{w_I})}{\sum_{w=1}^{W} \exp(v_w^T v_{w_I})}$$

Problem:
- Vocabulary size W = 50,000+ words
- Must compute 50,000 dot products per training step
- Billions of training steps needed
- Computationally infeasible!

Solutions:

1. **Hierarchical Softmax:**
   - Binary tree of words
   - $O(\log W)$ instead of $O(W)$
   - Path through tree to each word

2. **Negative Sampling:**
   - Only update k random words
   - Typically k = 5-20
   - Dramatic speedup
   - Better performance!

Solution: Negative Sampling Explained

Instead of: Predicting the right word from 50,000 options
We ask: Is this word the right context word? (Binary classification)

Center	Word	Label
cat	sits (real context)	1
cat	on (real context)	1
cat	elephant (random)	0
cat	democracy (random)	0
cat	quantum (random)	0

Sampling Strategy:

- Sample negative words by frequency: $P(w) \propto f(w)^{3/4}$
- The 3/4 power reduces dominance of very common words
- Gives rare words more chance to be negative samples

Result: 1000x speedup with better quality embeddings!

Challenge 2: How Do We Evaluate Embeddings?

The Problem: How do we know if our embeddings are "good"?

Intrinsic Evaluation:

- **Word Similarity:**
    - Dataset: WordSim-353
    - Human ratings vs cosine similarity
    - Correlation: 0.6-0.7 typical
- **Word Analogies:**
    - king - man + woman = ?
    - Google analogy dataset
    - Accuracy: 60-75% typical

Modern Approach (2024):

- Skip intrinsic evaluation
- Directly evaluate on downstream tasks
- Use pre-trained embeddings as starting point

Extrinsic Evaluation:

- **Downstream Tasks:**
    - Sentiment analysis
    - Named entity recognition
    - Machine translation
- **Key Finding:**
    - Good intrinsic $\neq$ Good extrinsic
    - Task-specific fine-tuning helps
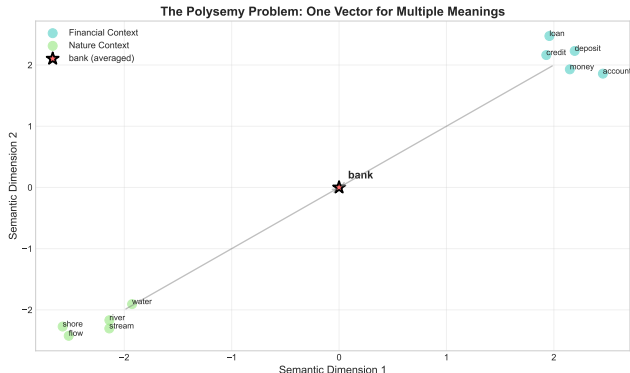
One Vector Per Word... But Words Have Multiple Meanings!

Example: "bank"
- "I deposited money at the bank" (financial institution)
- "We sat by the river bank" (edge of river)

Word2Vec gives one vector that averages both meanings:

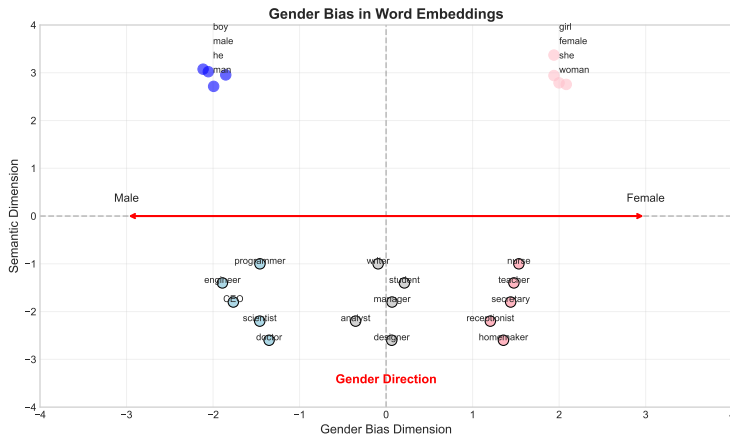The Polysemy Problem: One Vector for Multiple Meanings

Embeddings Learn Societal Biases from Text:

Problematic Analogies Found:
- man : computer programmer :: woman : homemaker
- man : doctor :: woman : nurse

Gender Bias in Word Embeddings

Advanced Techniques: Beyond Basic Word2Vec

FastText (2016):
- Uses character n-grams
- "where" = "wh", "whe", "her", "ere", "re"
- Handles unseen words
- Better for morphologically rich languages

GloVe (2014):
- Global matrix factorization
- Combines count-based and predictive
- Often better for word analogies

ELMo (2018):
- Contextualized embeddings
- Different vector per context
- Bi-directional LSTM
- Solves polysemy problem

Modern (2024):
- BERT/GPT embeddings
- Learned during pre-training
- Task-specific fine-tuning
- 768-12,288 dimensions

Word2Vec pioneered the field, but modern methods build on its foundation

Part 3 Summary: Challenges Addressed

Challenges We Explored:

1. **Computational:** Softmax over 50K words $\rightarrow$ Negative sampling
2. **Evaluation:** Intrinsic vs extrinsic metrics
3. **Polysemy:** One vector per word limitation
4. **Bias:** Embeddings reflect societal biases

Solutions and Evolution:

- Negative sampling: 1000x speedup
- Task-specific evaluation
- Contextualized embeddings (BERT/GPT)
- Debiasing techniques

Next: Part 4 - Applications and Future

- Build real applications with embeddings
- See modern systems in action
- Understand the path forward

Part 4

Applications and Future

From Word2Vec to Modern AI Systems

Build It: Semantic Search Engine

Let's build a search engine that understands meaning!

Traditional Search:

- Query: "car"
- Finds: Only documents with "car"
- Misses: "automobile", "vehicle"

Semantic Search:

- Query: "car"
- Finds: "car", "automobile", "vehicle", "BMW"
- Understands synonyms and related concepts

Implementation Steps:

1. Load pre-trained Word2Vec embeddings
2. Convert documents to vectors (average word embeddings)
3. Convert query to vector
4. Find documents with highest cosine similarity
5. Return ranked results

This is the foundation of Google Search, Elastic Search, and more!

Semantic Search Implementation

```python
import numpy as np
from sklearn.metrics.pairwise import cosine_similarity

class SemanticSearch:
    def __init__(self, word2vec_model):
        self.w2v = word2vec_model
        self.documents = []
        self.doc_vectors = []

    def add_document(self, doc):
        """Add document to search index"""
        self.documents.append(doc)
        # Convert document to vector (average of word vectors)
        words = doc.lower().split()
        vectors = [self.w2v[word] for word in words if word in self.w2v]
        doc_vector = np.mean(vectors, axis=0) if vectors else np.zeros(100)
        self.doc_vectors.append(doc_vector)

    def search(self, query, top_k=5):
        """Find most similar documents to query"""
        # Convert query to vector
        words = query.lower().split()
        vectors = [self.w2v[word] for word in words if word in self.w2v]
        query_vector = np.mean(vectors, axis=0) if vectors else np.zeros(100)

        # Calculate similarities
        similarities = cosine_similarity([query_vector], self.doc_vectors)[0]

        # Return top k results
        top_indices = np.argsort(similarities)[::-1][:top_k]
        return [(self.documents[i], similarities[i]) for i in top_indices]
```

Real-World Applications (2024)

Content Recommendation:
- Netflix: Show embeddings
- Spotify: Song2Vec
- YouTube: Video embeddings
- Amazon: Product2Vec

Language Understanding:
- ChatGPT: Token embeddings
- Google Translate: Multilingual embeddings
- Grammarly: Context understanding
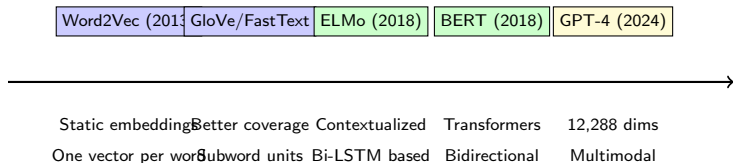
Search and Retrieval:
- Google: Semantic search
- Bing: Neural matching
- Enterprise search: Document similarity

Novel Applications:
- Code2Vec: Programming embeddings
- Molecule2Vec: Drug discovery
- Graph2Vec: Social networks

Any data with context can use embedding techniques!

Evolution: From Word2Vec to GPT

| Word2Vec (2013) | GloVe/FastText | ELMo (2018) | BERT (2018) | GPT-4 (2024) |

| Static embeddings | Better coverage | Contextualized | Transformers | 12,288 dims |
| One vector per word | Subword units | Bi-LSTM based | Bidirectional | Multimodal |

Key Progression:

- Static $\rightarrow$ Contextualized
- Words $\rightarrow$ Subwords $\rightarrow$ Tokens
- 300 dims $\rightarrow$ 12,288 dims
- Single task $\rightarrow$ Multi-task $\rightarrow$ General intelligence

Future Directions: What's Next?

Current Research (2024):
- **Efficient Embeddings:** Maintain quality at 64 dimensions
- **Multimodal:** Text + Image + Audio in same space
- **Dynamic:** Embeddings that update with new information
- **Personalized:** User-specific embedding spaces

Challenges Being Solved:
- **Long Context:** Embed entire books (1M+ tokens)
- **Cross-lingual:** Universal embeddings for all languages
- **Interpretability:** Understanding what each dimension means
- **Continual Learning:** Updating without forgetting

Connection to Next Week:
- Week 3: RNNs - Processing sequences with embeddings
- Embeddings are the input to all modern NLP models
- Foundation we'll build on for rest of course

Week 2 Summary: Words Have Meaning!

Journey We Took:
1. Started with words as meaningless IDs
2. Learned the distributional hypothesis
3. Built Word2Vec from scratch
4. Tackled challenges (scale, bias, polysemy)
5. Applied to real problems

Key Takeaways:
- **Core Insight:** Similar contexts → Similar meanings
- **Technical:** Skip-gram + negative sampling = efficient training
- **Practical:** Embeddings power all modern AI
- **Evolution:** Static → Contextualized → Multimodal

Your Homework:
- Build semantic search engine (notebook provided)
- Explore biases in pre-trained embeddings
- Try word arithmetic with different models

> **Remember:** Every ChatGPT response starts with embeddings!

Neural LM Era (2003-2013): Learning Representations

Bengio's breakthrough: Learn while predicting

Vocabulary:

- Larger fixed vocabulary (50k)
- Learned word embeddings (30-100 dim)
- Still word-level tokenization

Context:

- Fixed window with hidden states
- Concatenate embedding vectors
- Some semantic understanding

Key Innovations:

- **Distributed representations**
- **End-to-end learning**
- **Generalization beyond seen n-grams**

Architecture (Bengio 2003):

1. Input: Previous n-1 words
2. Lookup: Word $\rightarrow$ Embedding vector
3. Concatenate: $[e_{w_{t-2}}, e_{w_{t-1}}]$
4. Hidden layer: $h = \tanh(H \cdot x + b)$
5. Output: $y = \text{softmax}(W \cdot h)$

Training:

- Minimize cross-entropy loss
- Backpropagation through time
- Learn embeddings $+$ weights jointly

Computational Cost:

- Training: Days to weeks
- Inference: $O(|V| \cdot H)$ per word

Impact: 30-50% perplexity reduction vs n-grams $+$ Similar words get similar embeddings!

Embedding Era (2013-2017): Semantic Understanding

Word2Vec/GloVe: Meaning before prediction

Vocabulary:
- Large vocabularies (100k-1M)
- Rich 100-300 dim embeddings
- Subword models (FastText)

Context:
- Window-based but semantic
- Skip-gram: predict context from center
- CBOW: predict center from context

Method:
- Separate embedding training
- Negative sampling for efficiency
- Cosine similarity for prediction

Next-word prediction:

$$P(w_{next}|context) \propto \exp(v_{context}^T \cdot v_{w_{next}})$$

Find: $\operatorname{argmax}_w \cos(v_w, v_{context})$

Word Embeddings: Semantic Clustering in Vector Space

Raw Embedding Space (First 2 Dimensions) / t-SNE Projection of Embedding Space

Legend: Animals, Countries, Professions, Actions
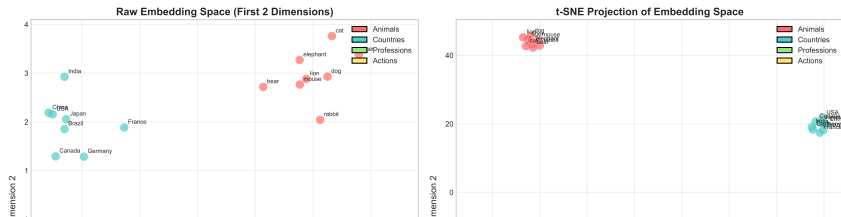
Transformer Era (2017-Present): Attention is All You Need

BERT, GPT: Context-aware predictions

Vocabulary:
- Subword tokens (30k-50k BPE/WordPiece)
- No OOV problem
- Multilingual support

Context:
- Full sequence (512-32k+ tokens)
- Bidirectional (BERT) or causal (GPT)
- Positional encodings

Method:
- Self-attention mechanism
- Multi-head attention
- Deep architectures (12-96+ layers)

Prediction:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) V$$

Context-dependent embeddings!

Revolutionary Features:
- "King" has different embeddings in "King of England" vs "King bed"
- Can handle: "The ___ that I saw yesterday was ___" (long-range)
- Zero-shot learning capabilities

Comparing Prediction Approaches: Same Task, Different Methods

Task: Predict next word after "The cat sat on the ___"

Era	How it Works	Top Predictions	Why?
N-grams	Count "cat sat on the X" in corpus	mat (0.6), floor (0.2), chair (0.1)	Pure statistics
Neural LM	Learned patterns from embeddings	mat (0.4), floor (0.3), carpet (0.2)	Semantic similarity
Word2Vec	Find words similar to context vector	mat (0.35), rug (0.25), surface (0.20)	Geometric proximity
GPT-4	Attention over entire context	mat (0.3), [depends on prior context]	Full understanding

Key Evolution:

- **N-grams:** What words followed this sequence before?
- **Neural/Embeddings:** What words are semantically appropriate?
- **Transformers:** What makes sense given everything?

Appendix A: Skip-gram Objective Derivation

Full Mathematical Formulation:
Given a sequence of words $w_1, w_2, ..., w_T$, maximize:

$$\mathcal{L} = \frac{1}{T} \sum_{t=1}^{T} \sum_{-c \le j \le c, j \ne 0} \log P(w_{t+j}|w_t)$$

Where:

$$P(w_O|w_I) = \frac{\exp(v_{w_O}'^T v_{w_I})}{\sum_{w=1}^{W} \exp(v_w'^T v_{w_I})}$$

Gradient with respect to center word:

$$\frac{\partial \log P(w_O|w_I)}{\partial v_{w_I}} = v_{w_O}' - \sum_{w=1}^{W} P(w|w_I) \cdot v_w'$$

Interpretation:

- First term: Move toward actual context word
- Second term: Move away from expected context (all words weighted by probability)
- Result: Embeddings organize by co-occurrence patterns

Appendix A: Negative Sampling Mathematics

Original objective (expensive):

$$\log P(w_O|w_I) = \log \frac{\exp(v_{w_O}^{'T} v_{w_I})}{\sum_{w=1}^{W} \exp(v_w^{'T} v_{w_I})}$$

Negative sampling objective (efficient):

$$\log \sigma(v_{w_O}^{'T} v_{w_I}) + \sum_{i=1}^{k} \mathbb{E}_{w_i \sim P_n(w)}[\log \sigma(-v_{w_i}^{'T} v_{w_I})]$$

Where:

- $\sigma(x) = \frac{1}{1+e^{-x}}$ (sigmoid function)
- $k =$ number of negative samples (typically 5-20)
- $P_n(w) \propto f(w)^{3/4}$ (noise distribution)

Why it works:

- Transforms problem to binary classification
- Distinguishing real from noise is sufficient
- Dramatically reduces computation: O(k) instead of O(W)

Concrete Example: Computing P(cat—context)

Given: "The <u>cat</u> sat on the mat" with window=1

Simplified vocabulary: {the, cat, sat, on, mat} = {0, 1, 2, 3, 4}

Embeddings (2D for visualization):

Word	v (input)	v' (output)
the	[0.5, 0.3]	[0.4, 0.6]
cat	[0.8, 0.2]	[0.7, 0.4]
sat	[0.3, 0.7]	[0.5, 0.8]
on	[0.4, 0.5]	[0.3, 0.6]
mat	[0.6, 0.4]	[0.8, 0.3]

Calculate P(sat—cat):

$$v_{cat}^T \cdot v'_{sat} = [0.8, 0.2] \cdot [0.5, 0.8] = 0.4 + 0.16 = 0.56 \tag{1}$$

$$\exp(0.56) = 1.75 \tag{2}$$

$$Z = \sum_w \exp(v_{cat}^T \cdot v'_w) = 1.73 + 1.75 + 1.61 + 1.87 + 1.94 = 8.9 \tag{3}$$

$$P(sat|cat) = \frac{1.75}{8.9} = 0.197 \approx 19.7\% \tag{4}$$

Concrete Example: Gradient Update

One gradient step for center word "cat":

Initial: $v_{cat} = [0.8, 0.2]$, learning rate $\alpha = 0.1$

Gradient components:

- Positive: Pull toward "sat" (actual context)
- Negative: Push away from expected distribution

Calculation:

$$\nabla = v'_{sat} - \sum_w P(w|cat) \cdot v'_w \tag{5}$$

$$= [0.5, 0.8] - (0.194 \cdot [0.4, 0.6] + 0.197 \cdot [0.5, 0.8] + ...) \tag{6}$$

$$= [0.5, 0.8] - [0.48, 0.62] \tag{7}$$

$$= [0.02, 0.18] \tag{8}$$

Update:

$$v_{cat}^{new} = v_{cat} + \alpha \cdot \nabla = [0.8, 0.2] + 0.1 \cdot [0.02, 0.18] = [0.802, 0.218]$$

Result: "cat" moves slightly closer to "sat" in embedding space!

Concrete Example: Negative Sampling Calculation

Training instance: Center="cat", Positive="sat", Negatives={the, mat}

Loss calculation step-by-step:

1. Positive pair (cat, sat):

$$\text{score}_{pos} = v_{cat}^T \cdot v'_{sat} = 0.56 \tag{9}$$

$$\text{loss}_{pos} = -\log \sigma(0.56) = -\log(0.636) = 0.452 \tag{10}$$

2. Negative pairs:

$$\text{score}_{neg1} = v_{cat}^T \cdot v'_{the} = 0.52 \tag{11}$$

$$\text{loss}_{neg1} = -\log \sigma(-0.52) = -\log(0.373) = 0.987 \tag{12}$$

$$\text{score}_{neg2} = v_{cat}^T \cdot v'_{mat} = 0.70 \tag{13}$$

$$\text{loss}_{neg2} = -\log \sigma(-0.70) = -\log(0.332) = 1.103 \tag{14}$$

3. Total loss:

$$\text{Loss} = \text{loss}_{pos} + \text{loss}_{neg1} + \text{loss}_{neg2} = 0.452 + 0.987 + 1.103 = 2.542$$

Much faster: Only 3 calculations instead of 5,000!

Concrete Example: Cosine Similarity Step-by-Step

Question: How similar are "king" and "queen"?

Given embeddings (3D for simplicity):

- $v_{king} = [0.6, 0.8, 0.2]$
- $v_{queen} = [0.5, 0.7, 0.4]$

Step 1: Calculate dot product

$$v_{king} \cdot v_{queen} = (0.6 \times 0.5) + (0.8 \times 0.7) + (0.2 \times 0.4) = 0.3 + 0.56 + 0.08 = 0.94$$

Step 2: Calculate magnitudes

$$||v_{king}|| = \sqrt{0.6^2 + 0.8^2 + 0.2^2} = \sqrt{0.36 + 0.64 + 0.04} = 1.02 \tag{15}$$

$$||v_{queen}|| = \sqrt{0.5^2 + 0.7^2 + 0.4^2} = \sqrt{0.25 + 0.49 + 0.16} = 0.95 \tag{16}$$

Step 3: Compute cosine similarity

$$\cos(\theta) = \frac{v_{king} \cdot v_{queen}}{||v_{king}|| \times ||v_{queen}||} = \frac{0.94}{1.02 \times 0.95} = \frac{0.94}{0.969} = 0.97$$

Interpretation: 0.97 = Very similar! (1.0 = identical, 0 = orthogonal)

Appendix A: CBOW Objective Function

Continuous Bag-of-Words (CBOW) Model:
Given context words $c = \{w_{t-m}, ..., w_{t-1}, w_{t+1}, ..., w_{t+m}\}$, predict center word w_t

Objective Function:

$$\mathcal{L} = -\frac{1}{T} \sum_{t=1}^{T} \log P(w_t|c)$$

Where:

$$P(w_t|c) = \frac{\exp(v_{w_t}^{'T} \bar{v})}{\sum_{w=1}^{W} \exp(v_w^{'T} \bar{v})}$$

And $\bar{v} = \frac{1}{2m} \sum_{-m \leq j \leq m, j \neq 0} v_{w_{t+j}}$ (average of context vectors)

Gradient with respect to output embeddings:

$$\frac{\partial \mathcal{L}}{\partial v_{w_t}'} = \bar{v} - \sum_{w=1}^{W} P(w|c) \cdot \bar{v} = \bar{v}(1 - P(w_t|c))$$

Key Insight: CBOW averages context to predict center (many-to-one)

Appendix A: GloVe Co-occurrence Matrix

Global Vectors (GloVe) Formulation:
Build co-occurrence matrix X where X_{ij} = number of times word j appears in context of word i

Objective Function:

$$J = \sum_{i,j=1}^{V} f(X_{ij})(w_i^T \tilde{w}_j + b_i + \tilde{b}_j - \log X_{ij})^2$$

Where weighting function:

$$f(x) = \begin{cases} (x/x_{max})^\alpha & \text{if } x < x_{max} \\ 1 & \text{otherwise} \end{cases}$$

Typically: $x_{max} = 100$, $\alpha = 0.75$

Key Insights:

- Combines global statistics (co-occurrence) with local context
- Directly encodes semantic relationships: $w_i^T w_j \approx \log P(j|i)$
- Training on co-occurrence ratios captures meaning

Appendix A: Subsampling Frequent Words

Problem: Frequent words like "the", "a" provide less information

Subsampling Probability:
For word w_i with frequency $f(w_i)$, discard with probability:

$$P(\text{discard } w_i) = 1 - \sqrt{\frac{t}{f(w_i)}}$$

Where t is threshold (typically 10^{-5})

Example with actual frequencies:

Word	Frequency	P(keep)	Effect
"the"	0.07	0.038	Keep 3.8%
"computer"	0.0001	1.0	Keep 100%
"neural"	0.00005	1.0	Keep 100%

Impact:

- Speeds up training by 2-10x
- Improves quality of rare word vectors
- Balances the training signal

Appendix A: t-SNE for Embedding Visualization

t-Distributed Stochastic Neighbor Embedding:
Reduce high-dimensional embeddings to 2D/3D for visualization

High-dimensional similarity (Gaussian):

$$p_{j|i} = \frac{\exp(-||x_i - x_j||^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-||x_i - x_k||^2/2\sigma_i^2)}$$

Low-dimensional similarity (Student-t):

$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k \neq l}(1 + ||y_k - y_l||^2)^{-1}}$$

Minimize KL divergence:

$$C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Gradient:

$$\frac{\partial C}{\partial y_i} = 4 \sum_j (p_{ij} - q_{ij})(y_i - y_j)(1 + ||y_i - y_j||^2)^{-1}$$

Result: Preserves local structure while revealing global patterns

Appendix C: Domain-Specific Embeddings

Medical Embeddings (BioWordVec):
- Trained on PubMed + MIMIC-III
- Captures: drug-disease relationships
- Application: Clinical decision support

Legal Embeddings (Law2Vec):
- Trained on case law + statutes
- Captures: Legal concept similarity
- Application: Legal document search

Financial Embeddings (FinBERT):
- Trained on financial news + reports
- Captures: Market sentiment
- Application: Trading signals

Code Embeddings (CodeBERT):
- Trained on GitHub repositories
- Captures: Programming patterns
- Application: Code search, bug detection

Lesson: Domain-specific training dramatically improves performance

References and Resources

Essential Papers:

- Mikolov et al. (2013). "Efficient estimation of word representations in vector space"
- Mikolov et al. (2013). "Distributed representations of words and phrases"
- Pennington et al. (2014). "GloVe: Global vectors for word representation"
- Peters et al. (2018). "Deep contextualized word representations" (ELMo)

Implementations:

- Gensim: `https://radimrehurek.com/gensim/`
- FastText: `https://fasttext.cc/`
- Hugging Face: `https://huggingface.co/`

Datasets:

- Google Analogy Test Set
- WordSim-353
- SimLex-999

Next Week: Recurrent Neural Networks - Processing sequences with embeddings