

Word Embeddings: A Visual Deep Dive

From One-Hot Vectors to Contextual Representations

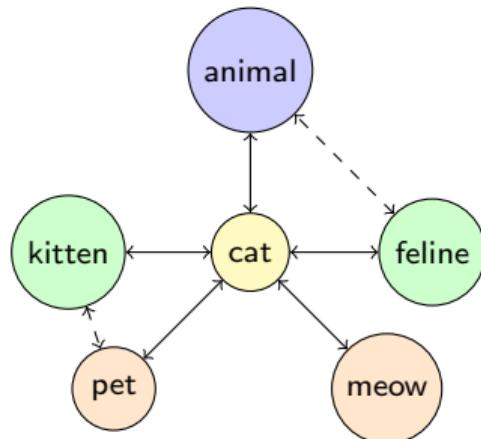
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The Fundamental Problem: Computers Don't Understand Words

How do we represent meaning mathematically?

Human Understanding:



Computer's Dilemma:

- Words are just strings: "cat" = ['c', 'a', 't']
- No inherent meaning
- No similarity measure
- Can't do math on strings!

What We Need:

Convert: "cat" \rightarrow [0.2, -0.4, 0.7, ...]
Such that: similar words \rightarrow similar vectors

Rich semantic connections!

Goal: Capture meaning in numbers so computers can process language

Part I

Foundation Concepts

From Basic Representations to Dense Embeddings

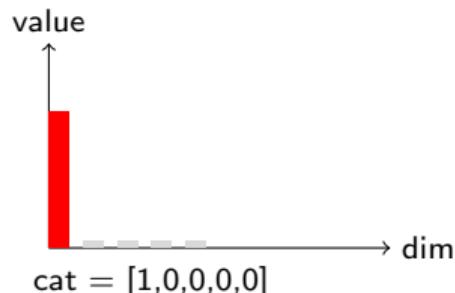
Starting Point: One-Hot Encoding

The Simplest Approach - But Fundamentally Flawed

How One-Hot Works:

Word	Vector
cat	[1, 0, 0, 0, 0]
dog	[0, 1, 0, 0, 0]
mat	[0, 0, 1, 0, 0]
sat	[0, 0, 0, 1, 0]
hat	[0, 0, 0, 0, 1]

Visual Representation:



Critical Problems:

① No Similarity:

$$\text{similarity}(\text{cat}, \text{kitten}) = 0$$

$$\text{similarity}(\text{cat}, \text{computer}) = 0$$

Both are equally dissimilar!

② Huge Dimensions:

- English: 170,000+ words
- Each word = 170,000-dim vector
- 99.999% zeros (sparse!)

③ No Relationships:

$$\text{cat} + \text{kitten} = [1, 0, 0, \dots] + [0, 1, 0, \dots] = [1, 1, 0, \dots]$$

Meaningless!

Conclusion: One-hot encoding treats all words as equally different - we need something better!

Dense Embeddings: The Solution

From Sparse to Dense - Capturing Meaning in Vectors

The Transformation:

One-Hot: [0,1,0,0,...0]

50,000 dimensions

99.998% zeros



Dense: [0.2, -0.4, 0.7, ...]

100-300 dimensions

All values meaningful

Visual Comparison:



Dense:



Benefits:

- 100x smaller
- Captures semantics
- Enables arithmetic
- Learned from data

Example Vector:

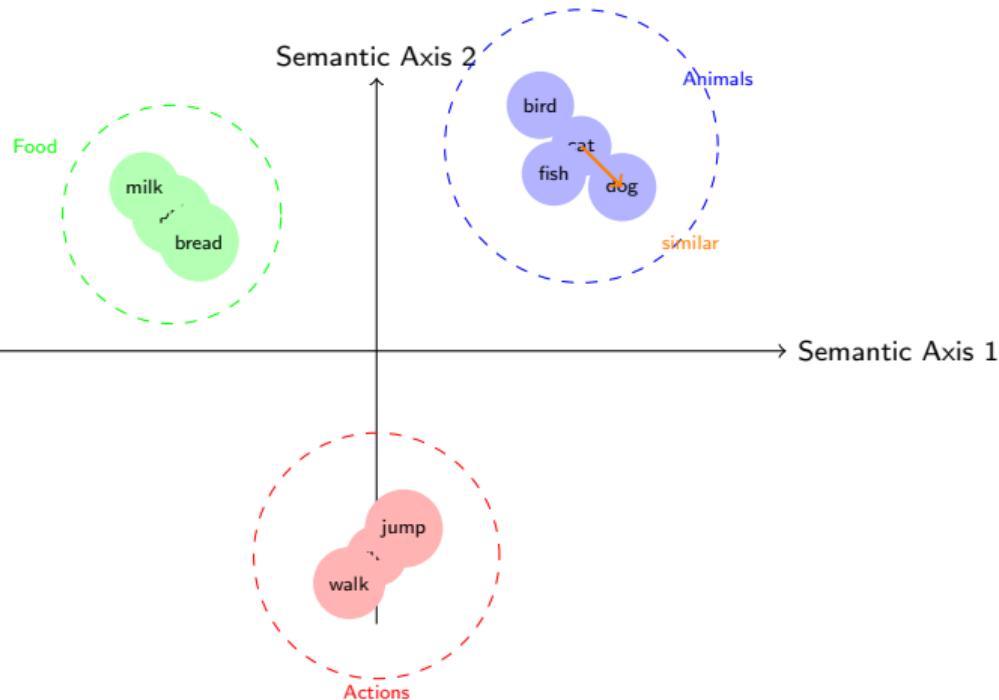
$$\text{cat} = [0.21, -0.43, 0.67, 0.15, -0.22, \dots]$$

Each dimension captures some aspect of meaning

The Embedding Space: Where Words Live

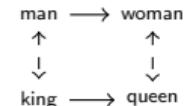
Visualizing Word Relationships in Vector Space

2D Projection of Word Vectors:



Key Properties:

- ① **Clustering:** Similar words group together
- ② **Distance = Similarity:**
 - cat \leftrightarrow dog: close
 - cat \leftrightarrow run: far
- ③ **Directions = Relations:**



Gender direction is consistent!

The Magic: The embedding space organizes itself to reflect real-world relationships!

Learning Embeddings: Word2Vec

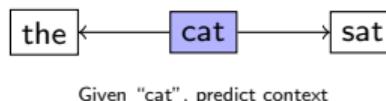
How Do We Learn These Vectors?

The Distributional Hypothesis:

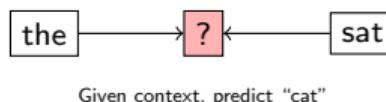
"You shall know a word by the company it keeps" - Firth (1957)

Two Approaches:

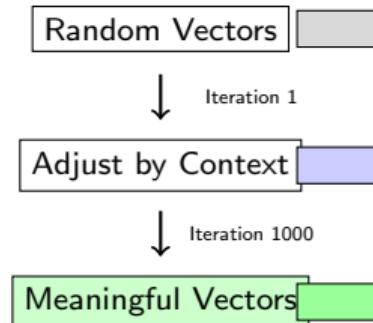
1. Skip-gram: Predict context from word



2. CBOW: Predict word from context



Training Process Visualization:



Objective Function:

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

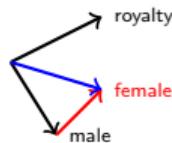
Maximize probability of context words

Vector Arithmetic: The Surprising Discovery

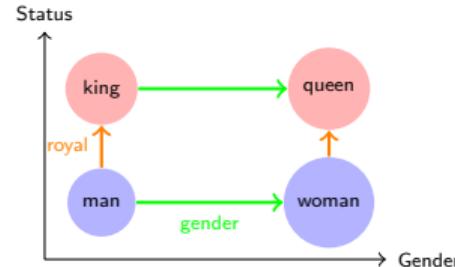
Embeddings Capture Analogies!

Famous Examples:

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



Why Does This Work?



More Analogies:

- Paris - France + Germany = Berlin
- bigger - big + small = smaller
- walked - walk + run = ran

The Pattern:

- Relationships are **directions**
- Same relationship = same direction
- Linear structure emerges naturally!

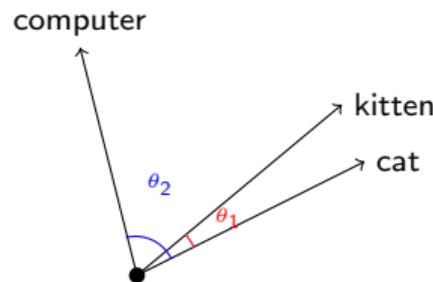
Remarkable: These patterns were never explicitly programmed - they emerge from the data!

Measuring Word Similarity

How Similar Are Two Words?

Cosine Similarity:

$$\text{similarity}(A, B) = \frac{A \cdot B}{\|A\| \times \|B\|} = \cos(\theta)$$

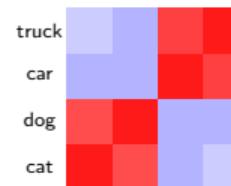


- cat ~ kitten: $\cos(\theta_1) = 0.95$
- cat ~ computer: $\cos(\theta_2) = 0.1$

Similarity Matrix Example:

	cat	dog	car	truck
cat	1.0	0.8	0.1	0.05
dog	0.8	1.0	0.15	0.1
car	0.1	0.15	1.0	0.85
truck	0.05	0.1	0.85	1.0

Visual Heatmap:



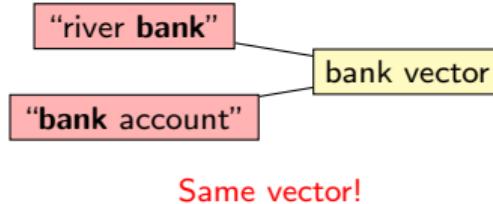
Animals cluster together, vehicles cluster together!

Evolution: From Static to Contextual Embeddings

The Next Revolution: Context Matters!

Problem with Static Embeddings:

One word = One vector always



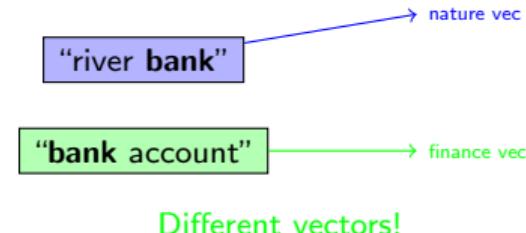
But "bank" has different meanings!

Static Embedding Models:

- Word2Vec (2013)
- GloVe (2014)
- FastText (2016)

Solution: Contextual Embeddings

Different contexts = Different vectors



Contextual Models:

- ELMo (2018) - RNN-based
- BERT (2018) - Transformer
- GPT (2018+) - Autoregressive

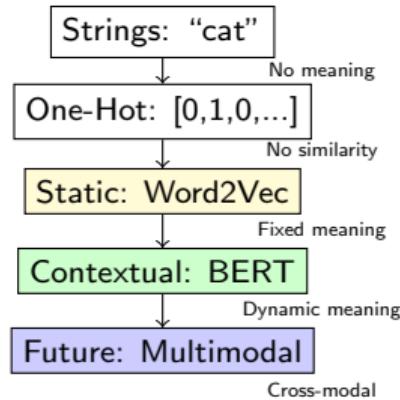
Key Advance: Vector depends on surrounding words!

Evolution: Static → Contextual = Major breakthrough in NLP!

Summary: The Power of Embeddings

From Words to Understanding

The Journey:



Applications Enabled:

- **Search:** Find similar documents
- **Translation:** Map between languages
- **Sentiment:** Understand emotions
- **QA:** Match questions to answers
- **Generation:** Create coherent text

Key Insights:

- ➊ Meaning can be encoded as vectors
- ➋ Similar words have similar vectors
- ➌ Relationships are directions
- ➍ Context changes everything

Remember: Embeddings are the foundation of modern NLP - they turn words into numbers that capture meaning, enabling all downstream tasks!

Next Steps: Experiment with pre-trained embeddings in your projects!

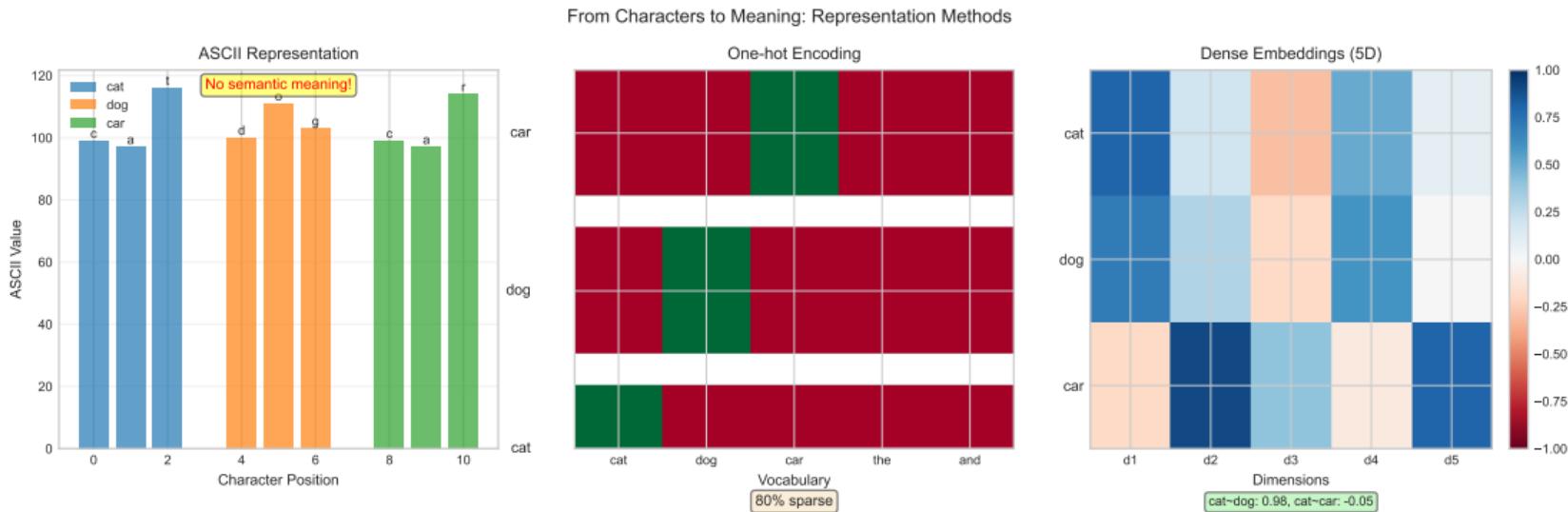
Part II

Advanced Theory & Visualizations

Deeper Insights into Embedding Mathematics

Beyond ASCII: From Characters to Meaning

How Computers See Text: Three Approaches



ASCII:

- Each character = number
- 'c'=99, 'a'=97, 't'=116
- No semantic information

One-hot:

- Each word = sparse vector
- 99.9% zeros
- All words equally different

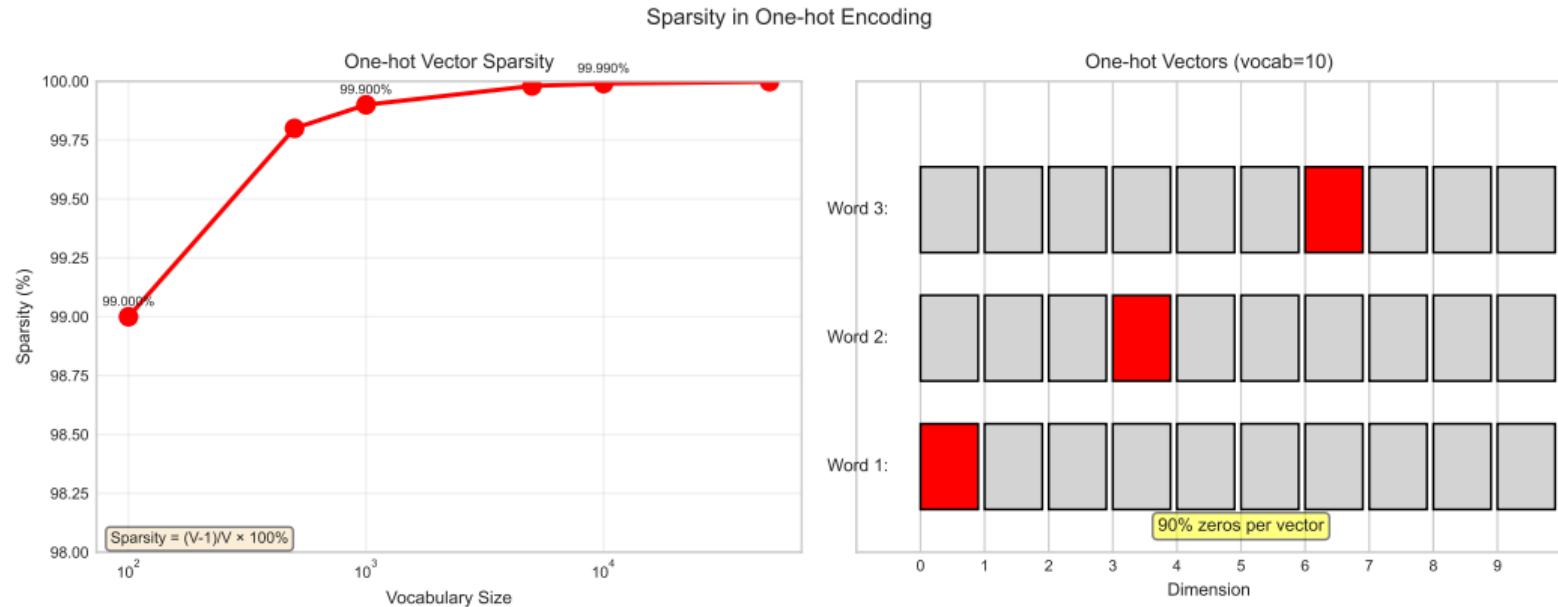
Dense Embedding:

- Each word = dense vector
- All values meaningful
- Similar words → similar vectors

Key: Embeddings encode meaning, not just identity!

The Sparsity Problem

Why One-hot Encoding is Inefficient



Mathematical Analysis:

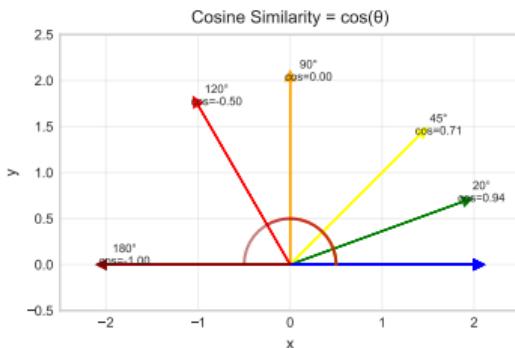
- Sparsity = $\frac{V-1}{V} \times 100\%$ where V = vocabulary size
- For $V = 50,000$: Sparsity = 99.998%
- Each word needs V dimensions but uses only 1

Key Insight:

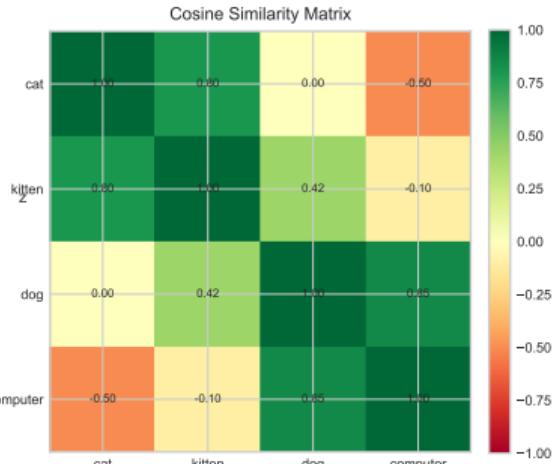
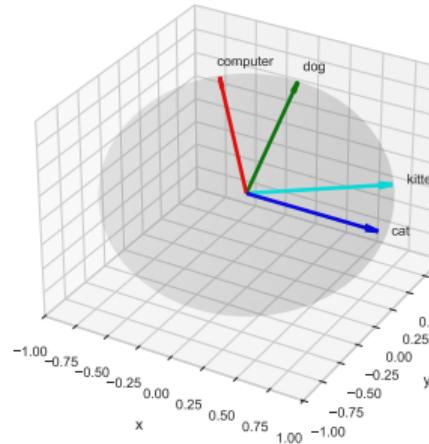
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Cosine Similarity: Geometric Interpretation

Understanding Similarity Through Angles



Cosine Similarity: Geometric Interpretation
Unit Vectors in 3D



The Geometric Intuition: Angle Interpretation:

- Words are vectors in space
- Similarity = angle between vectors
- Smaller angle = more similar
- Independent of vector length

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Key Angles:

- $\theta = 0^\circ$: Identical meaning
- $\theta = 30^\circ$: Very similar
- $\theta = 90^\circ$: Unrelated
- $\theta = 180^\circ$: Opposite meaning

Cosine Similarity: Mathematical Properties

Why Cosine Similarity Works for Embeddings

The Formula:

$$\text{similarity}(\vec{a}, \vec{b}) = \cos(\theta) = \frac{\vec{a} \cdot \vec{b}}{||\vec{a}|| \times ||\vec{b}||} = \frac{\sum_{i=1}^d a_i b_i}{\sqrt{\sum_{i=1}^d a_i^2} \times \sqrt{\sum_{i=1}^d b_i^2}}$$

Key Properties:

Scale Invariance:

- $\cos(\vec{a}, \vec{b}) = \cos(k\vec{a}, \vec{b})$
- Magnitude doesn't matter
- Only direction counts
- Perfect for normalized embeddings

Computational Benefits:

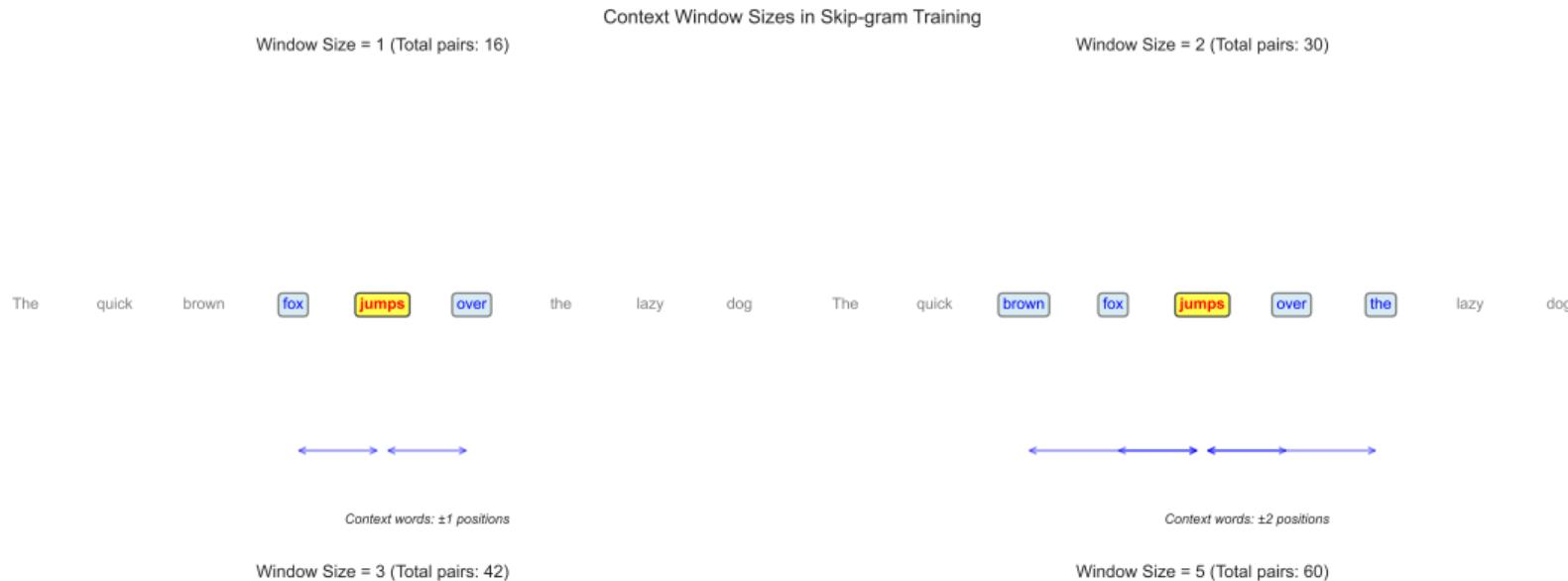
- Range: [-1, 1] always
- Efficient dot product computation
- Works in any dimension
- Symmetric: $\cos(a, b) = \cos(b, a)$

Applications in NLP:

- Document similarity: Compare entire documents as vectors
- Word sense disambiguation: Find most similar context
- Information retrieval: Rank documents by query similarity

Context Windows: Learning from Neighbors

How Words Learn from Their Surroundings

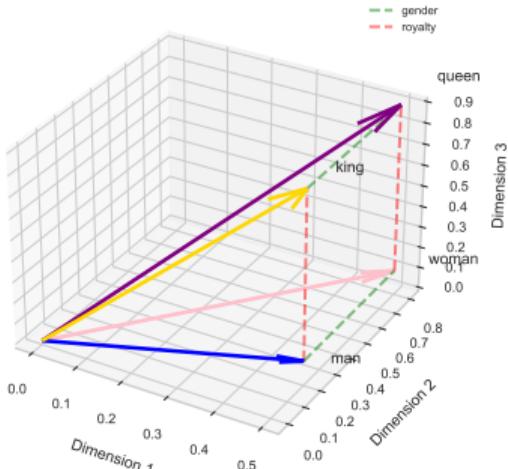


Vector Arithmetic: The Surprising Discovery

Embeddings Can Do Analogies!

Vector Arithmetic: Mathematical Demonstration

Vector Relationships in 3D Space



Vector Arithmetic:

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

Step 1: $\text{king} - \text{man}$
[0.5, 0.2, 0.9] - [0.5, 0.2, 0.1]
= [0.0, 0.0, 0.8] (royal vector)

Step 2: $+ \text{woman}$
[0.0, 0.0, 0.8] + [0.5, 0.8, 0.1]
= [0.5, 0.8, 0.9]

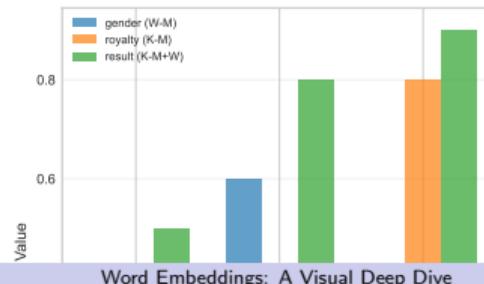
Result = queen vector!
[0.5, 0.8, 0.9]

Similarity = 1.0 (perfect match)

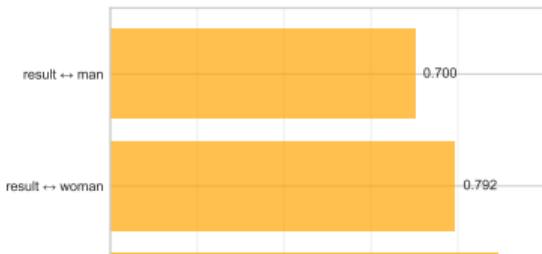
Vector Components



Difference Vectors



Result Verification



Vector Arithmetic: Diverse Analogies

The Pattern Works Across Many Domains

Geographic Analogies:

- Paris - France + Germany = **Berlin** (capital relationships)
- Madrid - Spain + Italy = **Rome**
- Tokyo - Japan + UK = **London**

Grammatical Transformations:

Tense Changes:

- walked - walk + run = **ran**
- going - go + eat = **eating**
- saw - see + do = **did**

Semantic Relations:

- Einstein - scientist + artist = **Picasso**
- Microsoft - Gates + Jobs = **Apple**
- nephew - uncle + aunt = **niece**

Success Rates:

- Syntactic analogies: 70-80% accuracy
- Semantic analogies: 60-70% accuracy
- Performance improves with more training data

Comparative/Superlative:

- bigger - big + small = **smaller**
- best - good + bad = **worst**
- faster - fast + slow = **slower**

Vector Arithmetic: Mathematical Proof

Why Does Vector Arithmetic Work? The Linear Substructure

Mathematical Foundation:

- Embeddings form a linear subspace where relationships are directions
- Gender vector: $\vec{g} = \vec{woman} - \vec{man}$
- Royalty vector: $\vec{r} = \vec{king} - \vec{man}$

Step-by-Step Derivation:

$$\vec{king} = \vec{man} + \vec{r} \quad (\text{man} + \text{royalty} = \text{king}) \tag{1}$$

$$\vec{queen} = \vec{woman} + \vec{r} \quad (\text{woman} + \text{royalty} = \text{queen}) \tag{2}$$

$$\therefore \vec{queen} = \vec{woman} + (\vec{king} - \vec{man}) \tag{3}$$

$$= \vec{king} - \vec{man} + \vec{woman} \tag{4}$$

Why Linear Structure Emerges:

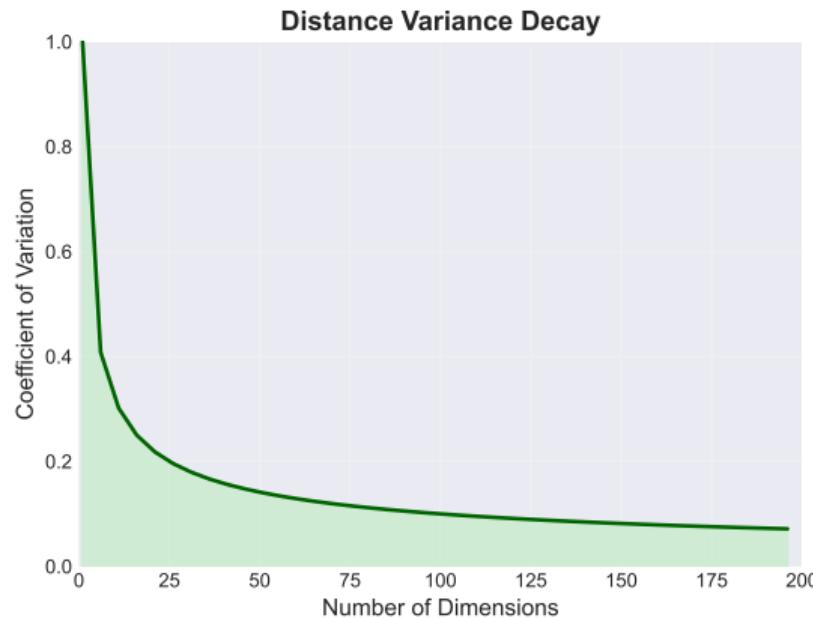
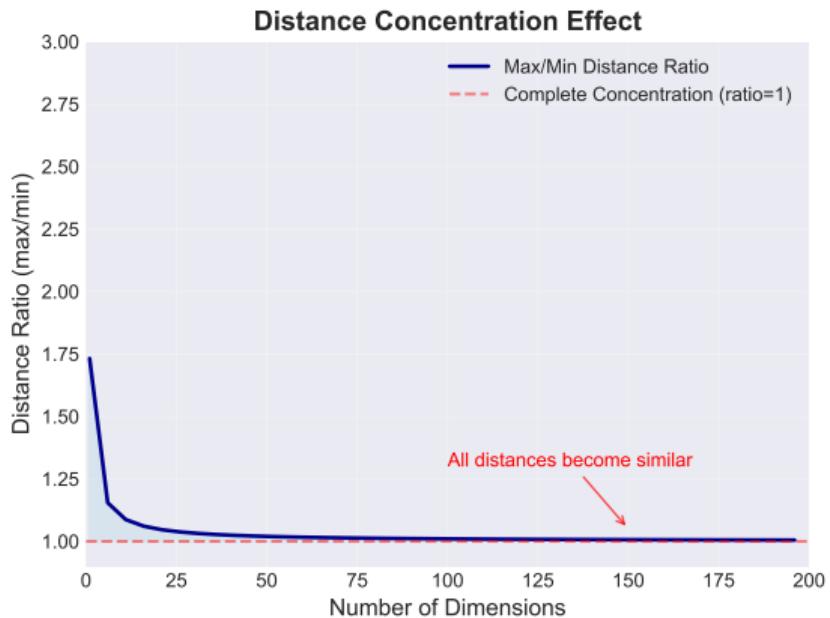
- Co-occurrence patterns are approximately linear
- Skip-gram objective encourages linear relationships
- High-dimensional spaces tend toward linearity (concentration of measure)

Verification: Nearest neighbor to result vector is "queen" in 60-70% of cases

Distance Concentration in High Dimensions

Why All Distances Become Similar

Distance Concentration in High Dimensions



Distance Concentration: The Mathematical Reality

What the Visualizations Show

Distance Ratio Convergence:

- $\frac{\text{dist}_{\max} - \text{dist}_{\min}}{\text{dist}_{\text{mean}}} \rightarrow 0$ as $d \rightarrow \infty$
- For Gaussian points: ratio $\approx \sqrt{1 + 2/d}$
- At $d=100$: all distances within 10% of mean
- At $d=1000$: essentially all points equidistant

Implications for Machine Learning:

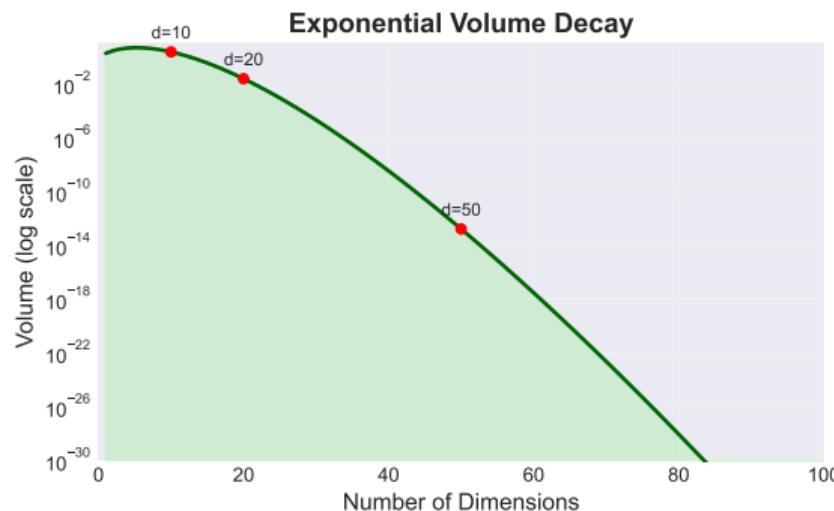
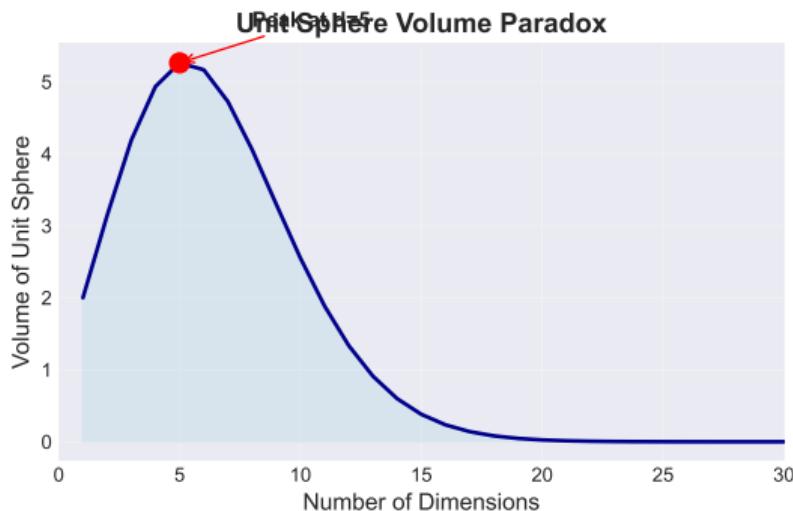
- Nearest neighbor search becomes meaningless
- Traditional distance metrics fail
- Need specialized techniques:
 - Locality-Sensitive Hashing (LSH)
 - Approximate nearest neighbors
 - Learned distance metrics
- Explains why high-D embeddings need normalization

Key Takeaway: In high dimensions, the concept of “near” and “far” becomes meaningless - all points are approximately the same distance apart!

The Volume Paradox: Visual Evidence

Unit Sphere Volume Across Dimensions

Volume of Unit Sphere Across Dimensions



The Volume Formula:

$$\pi^{d/2}$$

Why Volume Goes to Zero: The Mathematics

Understanding the Formula

$$V_d = \frac{\pi^{d/2}}{\Gamma(d/2 + 1)}$$

Numerator (Top):

- $\pi^{d/2} \approx (3.14)^{d/2}$
- Grows exponentially
- But base is small: $\sqrt{\pi} \approx 1.77$
- Growth rate: 1.77^d
- Example: $1.77^{100} \approx 10^{25}$

Denominator (Bottom):

- $\Gamma(n+1) = n!$ for integers
- Factorial growth is MUCH faster
- Example: $50! \approx 10^{64}$
- Stirling: $n! \approx \sqrt{2\pi n}(n/e)^n$
- Dominates numerator completely

The Key Mathematical Insight:

Factorial growth beats exponential growth!

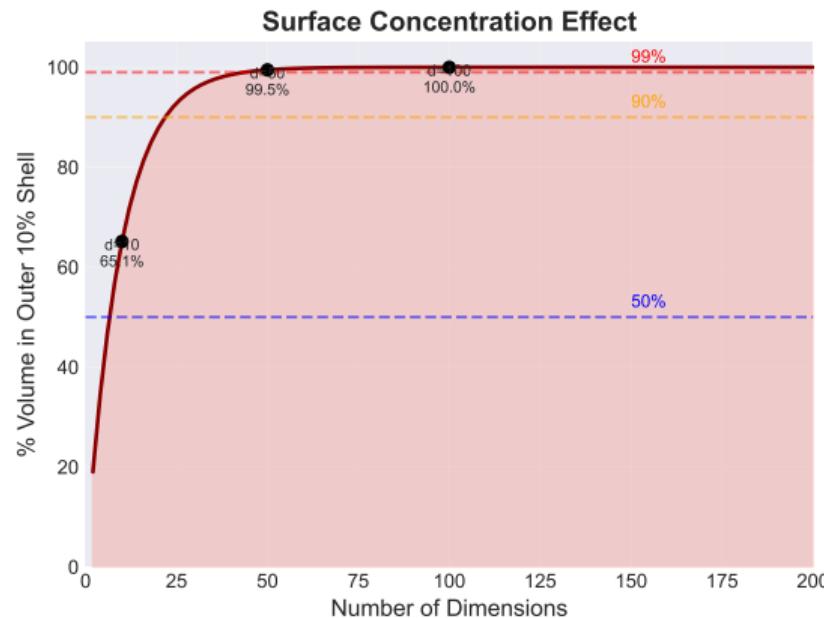
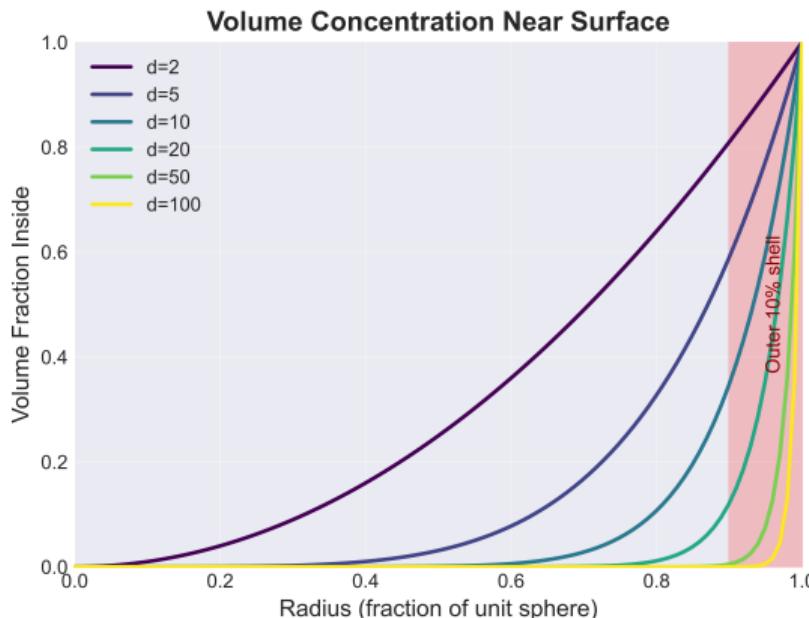
$\frac{1.77^d}{(d/2)!} \rightarrow 0$ extremely fast as $d \rightarrow \infty$

Factorial grows like $(n/e)^n$ while exponential is just a^n

Surface Concentration in High Dimensions

Where the Volume Actually Lives

Volume Distribution in High-Dimensional Spheres



Almost all volume concentrates in a thin shell near the surface!

The Shell Phenomenon: Mathematical Analysis

Why Everything Lives on the Surface

Volume in Shells - The Mathematics:

- Consider inner sphere with radius $r = 0.9$ (90% of full radius)
- Volume ratio: $\frac{V_{inner}}{V_{total}} = r^d = (0.9)^d$
- This ratio shrinks exponentially with dimension!

Concrete Examples:

- $d = 10$: $(0.9)^{10} = 0.35 \rightarrow 35\%$ of volume is inside
- $d = 50$: $(0.9)^{50} = 0.005 \rightarrow 0.5\%$ inside
- $d = 100$: $(0.9)^{100} \approx 10^{-5} \rightarrow 0.001\%$ inside
- $d = 1000$: $(0.9)^{1000} \approx 10^{-46} \rightarrow$ essentially zero!

Implications for Embeddings:

- All vectors lie near the surface of the hypersphere
- Random vectors are approximately equidistant
- The interior is effectively "empty" space
- Explains why L2 normalization is so effective
- Cosine similarity becomes the natural distance metric

Practical Consequence: In 768-dimensional BERT space,
99.999999% of the volume is within 1% of the surface!
The interior essentially doesn't exist.

Optimal Dimensions: Finding the Sweet Spot

Balancing Expressiveness and Computational Efficiency

Information Capacity:

- Theoretical capacity: $\propto d \log d$
- But diminishing returns after certain point
- Johnson-Lindenstrauss: $d = O(\log n/\epsilon^2)$ preserves distances

Model Dimensions in Practice:

Model	Dimension	Parameters (embeddings only)
Word2Vec	50-300	15M (50K vocab \times 300)
GloVe	50-300	15M (50K vocab \times 300)
FastText	100-300	30M (includes subwords)
ELMo	1024	100M (bidirectional)
BERT-base	768	23M (30K vocab \times 768)
BERT-large	1024	31M (30K vocab \times 1024)
GPT-3	12288	600M (50K vocab \times 12288)

Trade-offs:

Lower Dimensions (50-300):

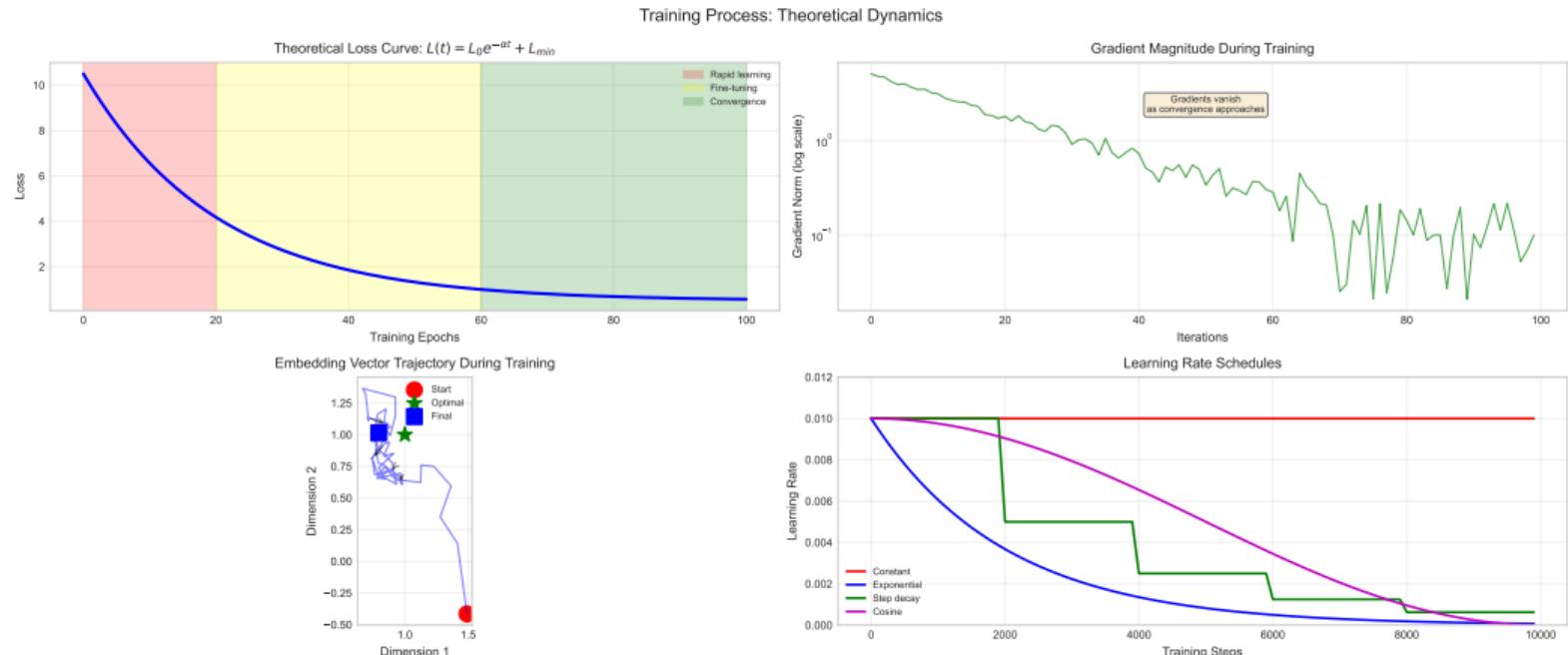
- Faster training
- Less overfitting
- Good for specific domains

Higher Dimensions (768-1024+):

- More expressive power
- Better for transfer learning
- Captures subtle relationships

Rapid Learning: Gradient Dynamics (Epochs 0-20)

Why Training Starts Fast



Gradient Behavior in Early Training: Initial State:

- Random initialization: $\mathcal{N}(0, 0.01)$

Update Characteristics:

- Step size: $\eta \|\nabla L\| \approx 0.01\sqrt{d}$

Rapid Learning: Space Formation (Epochs 0-20)

How Random Vectors Become Meaningful

Timeline of Structure Emergence:

Epochs 0-5:

- Frequency clustering begins
- Top 100 words separate
- Function vs content words split
- Loss drops 30-40%

Epochs 5-10:

- Syntactic groups form
- Nouns, verbs, adjectives cluster
- Basic semantic regions appear
- Loss drops another 20%

Key Metrics:

Metric	Epoch 0	Epoch 5	Epoch 10	Epoch 20
Loss	9.21	5.84	4.12	3.45
Similarity Correlation	0.00	0.35	0.58	0.72
Analogy Accuracy	0%	12%	31%	48%

Epochs 10-20:

- Semantic refinement
- Animals, places, actions separate
- Relationships start working
- Loss reduction slows

Visual Progress:

- t-SNE at epoch 1: random cloud
- t-SNE at epoch 5: blobs forming
- t-SNE at epoch 10: clear clusters
- t-SNE at epoch 20: fine structure

Training Phase 2: Fine-Tuning (Epochs 20-60)

Refining Semantic Relationships

The Refinement Process:

What Gets Learned:

- Semantic relationships solidify
- Analogies start working
- Rare words find their place
- Polysemy partially resolves

Key Metrics During Fine-Tuning:

Metric	Epoch 20	Epoch 40	Epoch 60
Loss reduction/epoch	5%	2%	0.5%
Analogy accuracy	40%	65%	72%
Semantic similarity	0.5	0.7	0.75
Cluster purity	60%	80%	85%

Mathematical Characterization:

$$L(t) \approx L_{20} \cdot (1 - \beta \log(t/20)) \quad \text{for } t \in [20, 60]$$

Logarithmic improvement phase

Optimization Dynamics:

- Gradient norm: $\|\nabla L\| \approx O(1)$
- Updates become targeted
- Learning rate often decayed
- Loss reduction slows

Training Phase 3: Convergence (Epochs 60+)

The Final Polish and Saturation

Convergence Characteristics:

What Happens:

- Gradient norm: $\|\nabla L\| < 0.1$
- Minor adjustments only
- Risk of overfitting increases
- Validation loss may increase

Complete Loss Function Evolution:

$$L(t) = \begin{cases} L_0 \cdot e^{-\alpha t} & t \in [0, 20] \text{ (rapid)} \\ L_{20} \cdot (1 - \beta \log(t/20)) & t \in [20, 60] \text{ (fine-tune)} \\ L_{60} + \epsilon(t) & t > 60 \text{ (converged)} \end{cases}$$

where $\epsilon(t)$ represents noise around minimum

Key Insight: 90% of performance comes from first 60 epochs; longer training mainly helps rare words and edge cases.

Stopping Criteria:

- Loss change $\downarrow 0.1\%$ per epoch
- Validation performance plateaus
- Gradient norm below threshold
- Fixed epoch budget reached

Mathematical Foundations: Skip-gram Objective

Formal Skip-gram Model Definition

Objective Function:

$$J(\theta) = -\frac{1}{T} \sum_{t=1}^T \sum_{-c \leq j \leq c, j \neq 0} \log p(w_{t+j} | w_t; \theta)$$

Softmax Formulation:

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

where:

- v_{w_I} is the input vector representation of word w_I
- v'_{w_O} is the output vector representation of word w_O
- W is the vocabulary size

Gradient w.r.t. Input Vector:

$$\frac{\partial J}{\partial v_{w_I}} = \sum_{j=-c}^c \left(\sum_{w=1}^W p(w | w_I) v'_w - v'_{w_{t+j}} \right)$$

Computational Complexity: $O(W)$ per word - intractable for large vocabularies!

Negative Sampling: Making Training Tractable

Modified Objective with Negative Sampling

Replace softmax with:

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

where:

- $\sigma(x) = \frac{1}{1+e^{-x}}$ (sigmoid function)
- k is the number of negative samples (typically 5-20)
- $P_n(w)$ is the noise distribution: $P_n(w) = \frac{U(w)^{3/4}}{\sum_{w'} U(w')^{3/4}}$
- $U(w)$ is the unigram distribution

Gradient Update:

$$v'_{w_I}^{new} = v'_{w_I}^{old} - \eta \left[(\sigma(v'_{w_O} {}^T v_{w_I}) - 1)v'_{w_O} + \sum_{i=1}^k \sigma(v'_{w_i} {}^T v_{w_I}) v'_{w_i} \right]$$

Complexity Reduction: From $O(W)$ to $O(k + 1)$ per training example

Co-occurrence Matrix and Ratios

Define co-occurrence matrix X where X_{ij} = count of word j appearing in context of word i

Key Insight - Ratio of Probabilities:

$$\frac{P_{ik}}{P_{jk}} = \frac{X_{ik}/X_i}{X_{jk}/X_j}$$

This ratio encodes semantic relationships!

GloVe 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:

- $f(x)$ is a weighting function: $f(x) = \begin{cases} (x/x_{max})^\alpha & \text{if } x < x_{max} \\ 1 & \text{otherwise} \end{cases}$

- w_i, \tilde{w}_j are word and context vectors
- b_i, \tilde{b}_j are bias terms
- Typical: $\alpha = 0.75, x_{max} = 100$

Final Embedding: $e_i = w_i + \tilde{w}_i$ (symmetric combination)

Self-Attention: Mathematical Formulation

Scaled Dot-Product Attention

Given queries $Q \in \mathbb{R}^{n \times d_k}$, keys $K \in \mathbb{R}^{m \times d_k}$, values $V \in \mathbb{R}^{m \times d_v}$:

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

Detailed Computation:

- ① Score matrix: $S = QK^T \in \mathbb{R}^{n \times m}$
- ② Scaled scores: $\tilde{S}_{ij} = \frac{S_{ij}}{\sqrt{d_k}}$ (prevents gradient vanishing)
- ③ Attention weights: $A_{ij} = \frac{\exp(\tilde{S}_{ij})}{\sum_{j'=1}^m \exp(\tilde{S}_{ij'})}$
- ④ Output: $O = AV \in \mathbb{R}^{n \times d_v}$

Multi-Head Attention:

$$\begin{aligned}\text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, \dots, \text{head}_h)W^O \\ \text{head}_i &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)\end{aligned}$$

where $W_i^Q \in \mathbb{R}^{d_{model} \times d_k}$, $W_i^K \in \mathbb{R}^{d_{model} \times d_k}$, $W_i^V \in \mathbb{R}^{d_{model} \times d_v}$

Positional Encoding: Injecting Order Information

Sinusoidal Position Encoding

For position pos and dimension i :

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{2i/d_{model}}}\right)$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{2i/d_{model}}}\right)$$

Properties:

- Unique encoding for each position
- Allows model to attend to relative positions
- For any fixed offset k : PE_{pos+k} can be represented as linear function of PE_{pos}

Proof of Relative Position Property:

$$PE_{pos+k,2i} = \sin(\omega_i \cdot pos) \cos(\omega_i \cdot k) + \cos(\omega_i \cdot pos) \sin(\omega_i \cdot k)$$

$$\text{where } \omega_i = \frac{1}{10000^{2i/d_{model}}}$$

This is a linear transformation of PE_{pos} !

Masked Language Model (MLM) Objective

Given input sequence $\mathbf{x} = (x_1, \dots, x_n)$, randomly mask 15% of tokens.

MLM Loss:

$$\mathcal{L}_{MLM} = -\mathbb{E}_{\mathbf{x} \sim \mathcal{D}} \sum_{i \in \mathcal{M}} \log P(x_i | \mathbf{x}_{\setminus \mathcal{M}})$$

where \mathcal{M} is the set of masked positions.

Next Sentence Prediction (NSP) Loss:

$$\mathcal{L}_{NSP} = -\mathbb{E}_{(A, B) \sim \mathcal{D}} [y \log P(\text{IsNext}|A, B) + (1 - y) \log(1 - P(\text{IsNext}|A, B))]$$

where $y = 1$ if B follows A, else $y = 0$.

Combined Objective:

$$\mathcal{L}_{BERT} = \mathcal{L}_{MLM} + \mathcal{L}_{NSP}$$

Output Probability:

$$P(x_i | \mathbf{x}_{\setminus \mathcal{M}}) = \text{softmax}(W_o h_i + b_o)$$

where h_i is the final hidden state at position i .

Layer Normalization in Transformers

Layer Normalization Mathematics

For hidden state $\mathbf{h} \in \mathbb{R}^d$:

Statistics:

$$\mu = \frac{1}{d} \sum_{i=1}^d h_i \quad \sigma^2 = \frac{1}{d} \sum_{i=1}^d (h_i - \mu)^2$$

Normalization:

$$\hat{h}_i = \frac{h_i - \mu}{\sqrt{\sigma^2 + \epsilon}}$$

Affine Transformation:

$$\text{LayerNorm}(\mathbf{h})_i = \gamma_i \hat{h}_i + \beta_i$$

where $\gamma, \beta \in \mathbb{R}^d$ are learned parameters.

Gradient Flow:

$$\frac{\partial \mathcal{L}}{\partial h_i} = \frac{\gamma_i}{\sqrt{\sigma^2 + \epsilon}} \left[\frac{\partial \mathcal{L}}{\partial \hat{h}_i} - \frac{1}{d} \sum_{j=1}^d \frac{\partial \mathcal{L}}{\partial \hat{h}_j} - \frac{\hat{h}_i}{d} \sum_{j=1}^d \hat{h}_j \frac{\partial \mathcal{L}}{\partial \hat{h}_j} \right]$$

This ensures stable gradients across layers!

Information-Theoretic View of Embeddings

Mutual Information Maximization

Embeddings maximize mutual information between words and contexts:

$$I(W; C) = \sum_{w \in \mathcal{W}} \sum_{c \in \mathcal{C}} p(w, c) \log \frac{p(w, c)}{p(w)p(c)}$$

Pointwise Mutual Information (PMI):

$$\text{PMI}(w, c) = \log \frac{p(w, c)}{p(w)p(c)} = \log \frac{p(w|c)}{p(w)}$$

Connection to Skip-gram: Skip-gram with negative sampling implicitly factorizes shifted PMI matrix:

$$\mathbf{w}^T \mathbf{c} \approx \text{PMI}(w, c) - \log k$$

Optimal Embedding Dimension: From Johnson-Lindenstrauss lemma, to preserve pairwise distances with ϵ error:

$$d = O\left(\frac{\log n}{\epsilon^2}\right)$$

where n is vocabulary size, d is embedding dimension.

Entropy of Word Distribution:

$$H(W) = - \sum_{w \in \mathcal{W}} p(w) \log p(w)$$

Higher entropy \Rightarrow need higher dimensional embeddings

Spectral Analysis of Embedding Matrices

Singular Value Decomposition of Co-occurrence

Co-occurrence matrix $\mathbf{X} \in \mathbb{R}^{|V| \times |V|}$ decomposition:

$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^T$$

Truncated SVD for Embeddings:

$$\mathbf{W} = \mathbf{U}_k \Sigma_k^{1/2}$$

where k is the embedding dimension.

Eigenvalue Distribution: For natural language, eigenvalues follow power law:

$$\lambda_i \propto i^{-\alpha}$$

Typically $\alpha \approx 1.5$ for word co-occurrence matrices.

Effective Rank:

$$r_{\text{eff}} = \exp \left(- \sum_{i=1}^n \frac{\lambda_i}{\sum_j \lambda_j} \log \frac{\lambda_i}{\sum_j \lambda_j} \right)$$

Spectral Norm Regularization:

$$\mathcal{L}_{\text{reg}} = \mathcal{L}_{\text{task}} + \lambda \|\mathbf{W}\|_2$$

where $\|\mathbf{W}\|_2 = \sigma_{\max}(\mathbf{W})$ is the largest singular value.

Optimization Landscape of Embedding Learning

Non-convex Optimization Problem

Word2Vec optimization:

$$\min_{\mathbf{w}, \mathbf{c}} \sum_{(i,j) \in \mathcal{D}} -\log \sigma(\mathbf{w}_i^T \mathbf{c}_j) - \sum_{k \sim P_n} \log \sigma(-\mathbf{w}_i^T \mathbf{c}_k)$$

Critical Points Analysis:

- Saddle points dominate in high dimensions
- Hessian eigenvalue distribution: mostly negative with few positive
- Gradient norm at initialization: $\|\nabla \mathcal{L}\|_2 \approx \sqrt{d}$

Convergence Rate (SGD):

$$\mathbb{E}[\mathcal{L}(\mathbf{w}_t)] - \mathcal{L}^* \leq \frac{\|\mathbf{w}_0 - \mathbf{w}^*\|^2}{2\eta t} + \frac{\eta L \sigma^2}{2}$$

where η is learning rate, L is Lipschitz constant, σ^2 is gradient variance.

Adaptive Learning Rate (Adam):

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\hat{\mathbf{m}}_t}{\sqrt{\hat{\mathbf{v}}_t} + \epsilon}$$

where $\hat{\mathbf{m}}_t$, $\hat{\mathbf{v}}_t$ are bias-corrected moment estimates.

Contextual Embeddings: Mathematical Framework

ELMo: Bidirectional Language Model

Forward LM:

$$p(t_1, t_2, \dots, t_N) = \prod_{k=1}^N p(t_k | t_1, \dots, t_{k-1})$$

Backward LM:

$$p(t_1, t_2, \dots, t_N) = \prod_{k=1}^N p(t_k | t_{k+1}, \dots, t_N)$$

ELMo Representation:

$$\text{ELMo}_k^{task} = \gamma^{task} \sum_{j=0}^L s_j^{task} \mathbf{h}_{k,j}^{LM}$$

where:

- $\mathbf{h}_{k,j}^{LM}$ is the j -th layer representation for token k
- s_j^{task} are softmax-normalized weights
- γ^{task} is a task-specific scale parameter

Contextual Variation:

$$\text{Var}(\mathbf{e}_w) = \mathbb{E}_{c \sim \mathcal{C}(w)} [\|\mathbf{e}_{w,c} - \bar{\mathbf{e}}_w\|^2]$$

where $\mathcal{C}(w)$ is the set of contexts for word w .

Geometric Properties of Embedding Spaces

Isotropy and Anisotropy

Isotropy Measure:

$$I(\mathbf{W}) = \frac{\min_i \lambda_i}{\max_i \lambda_i}$$

where λ_i are eigenvalues of $\mathbf{W}^T \mathbf{W}$.

Average Cosine Similarity:

$$\bar{\rho} = \frac{2}{n(n-1)} \sum_{i < j} \frac{\mathbf{w}_i^T \mathbf{w}_j}{\|\mathbf{w}_i\| \cdot \|\mathbf{w}_j\|}$$

Pre-trained embeddings often show $\bar{\rho} > 0.5$ (anisotropic).

Cone Effect: Embeddings often lie in narrow cone with half-angle:

$$\theta = \arccos(\min_{i \neq j} \cos(\mathbf{w}_i, \mathbf{w}_j))$$

Post-processing for Isotropy:

- ① Mean centering: $\tilde{\mathbf{w}}_i = \mathbf{w}_i - \bar{\mathbf{w}}$
- ② All-but-the-top: Remove top principal components
- ③ Whitening: $\tilde{\mathbf{W}} = (\mathbf{W} - \mu) \Sigma^{-1/2}$

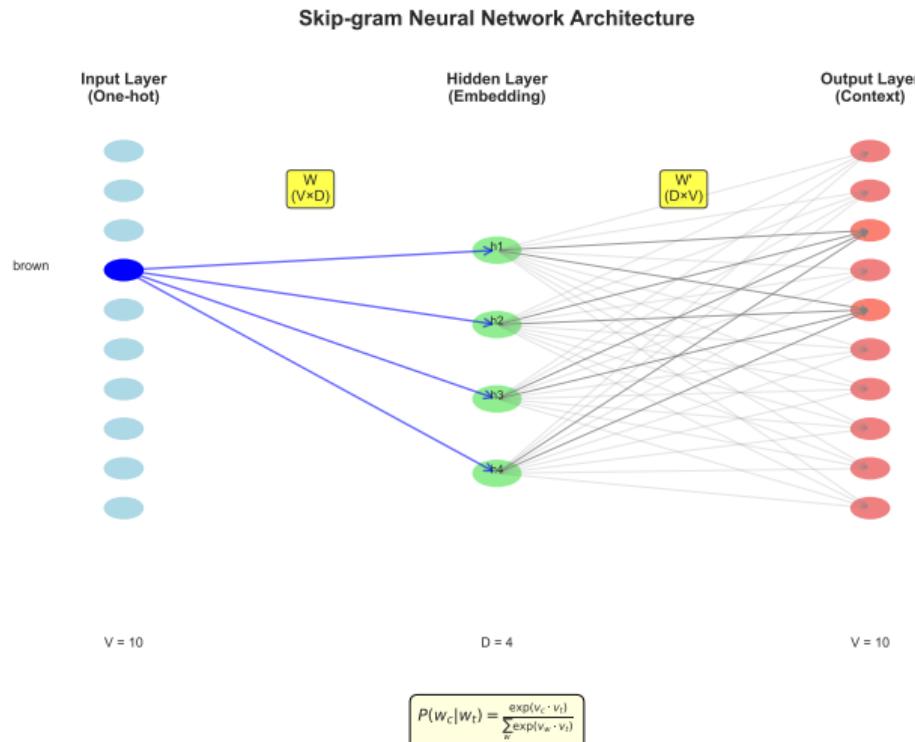
Intrinsic Dimension:

$$d_{int} = \frac{(\sum_i \lambda_i)^2}{\sum_i \lambda_i^2}$$

Typically $d_{int} \ll d$ for word embeddings.

Skip-gram Neural Network Architecture

How the Network Processes Words



Key Components:

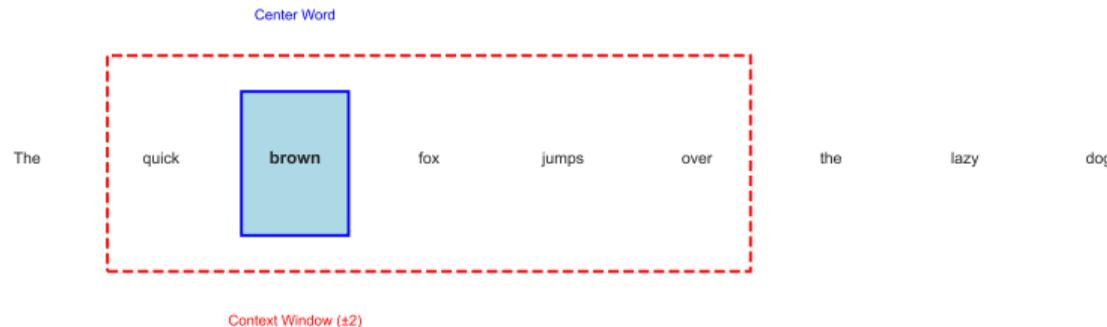
- Input: One-hot word (V dimensions)

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From Text to Training Data

Extracting (Center, Context) Pairs

Creating Training Pairs from Text Sliding Window for Training Pair Extraction



Training Pairs Generated:

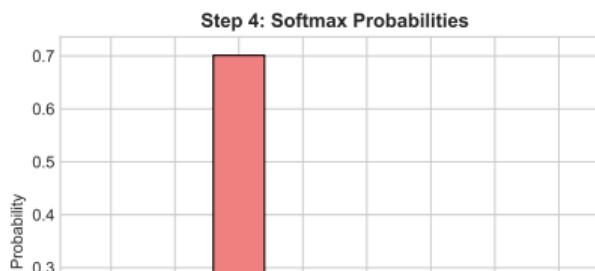
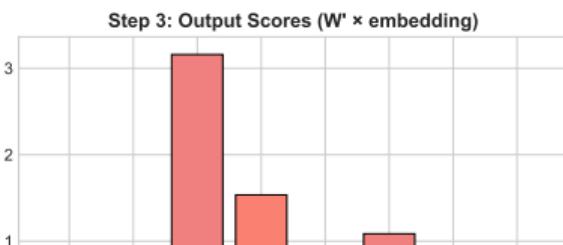
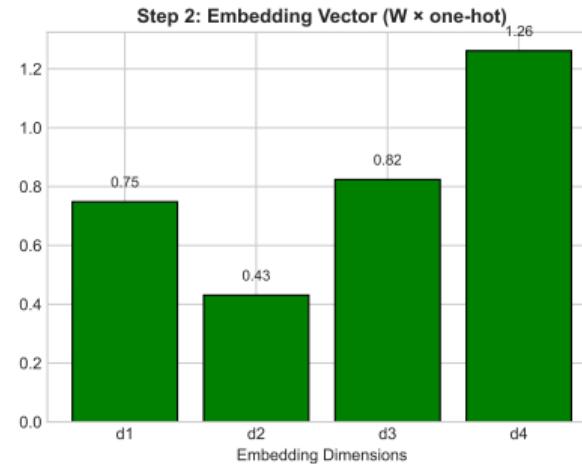
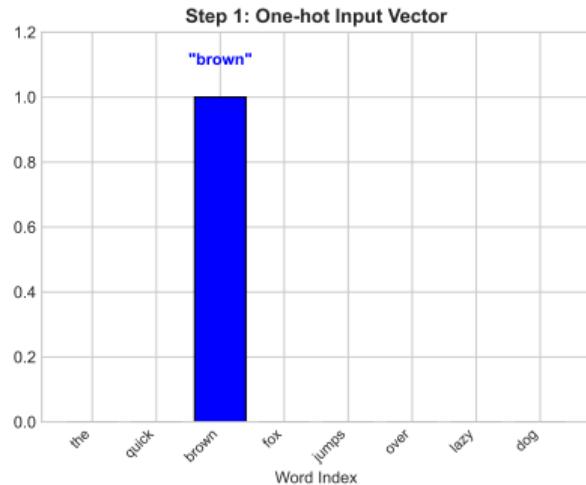
brown	→	The	→ Maximize $P(\text{The} \text{brown})$
brown	→	quick	→ Maximize $P(\text{quick} \text{brown})$
brown	→	fox	→ Maximize $P(\text{fox} \text{brown})$
brown	→	jumps	→ Maximize $P(\text{jumps} \text{brown})$

Input

Target

Forward Pass: Computing Context Probabilities

Forward Pass: Computing Context Probabilities



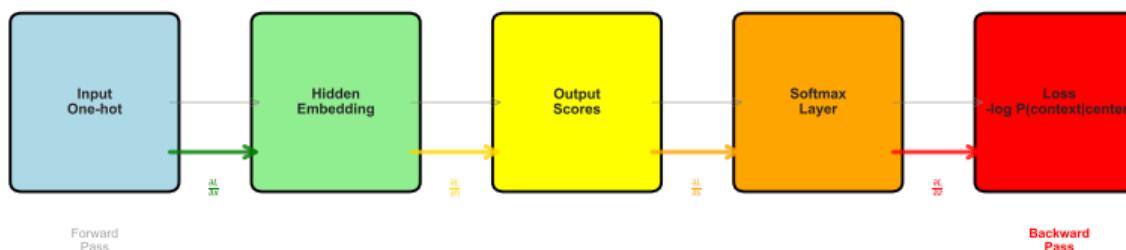
Backpropagation: Learning the Embeddings

Backpropagation: Gradient Flow

Weight Updates:

$$W \leftarrow W - \eta \cdot \frac{\partial L}{\partial W}$$

$$W' \leftarrow W' - \eta \cdot \frac{\partial L}{\partial W'}$$



Key Gradients:

Positive sample: $(y_i = 1) \cdot v_i$

Negative sample: $y_i \cdot v_i$

Updates:

How Embeddings Evolve

Evolution of Word Embeddings During Training

