

Word Embeddings: A Visual Deep Dive

From One-Hot Vectors to Contextual Representations

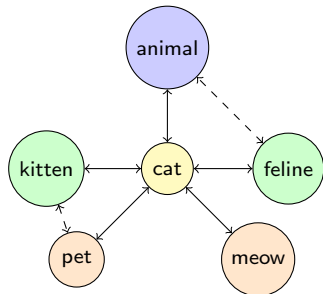
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The Fundamental Problem: Computers Don't Understand Words

How do we represent meaning mathematically?

Human Understanding:



Rich semantic connections!

Goal: Capture meaning in numbers so computers can process language

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

Part I

Foundation Concepts

From Basic Representations to Dense Embeddings

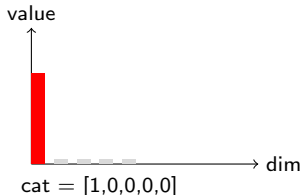
Starting Point: One-Hot Encoding

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:

❶ No Similarity:

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

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

Both are equally dissimilar!

❷ Huge Dimensions:

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

❸ No Relationships:

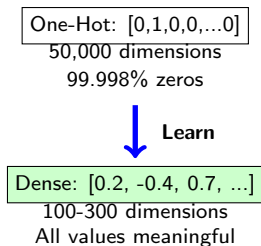
$$\text{cat} + \text{kitten} = [1, 0, 0, \dots] + [0, 1, 0, \dots] = [1, 1, 0, \dots]$$

Meaningless!

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

Dense Embeddings: The Solution

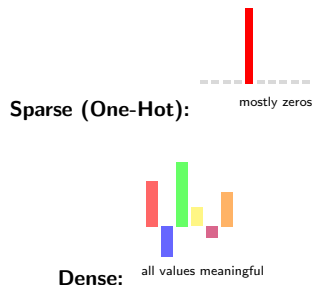
From Sparse to Dense - Capturing Meaning in Vectors The Transformation:



Benefits:

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

Visual Comparison:



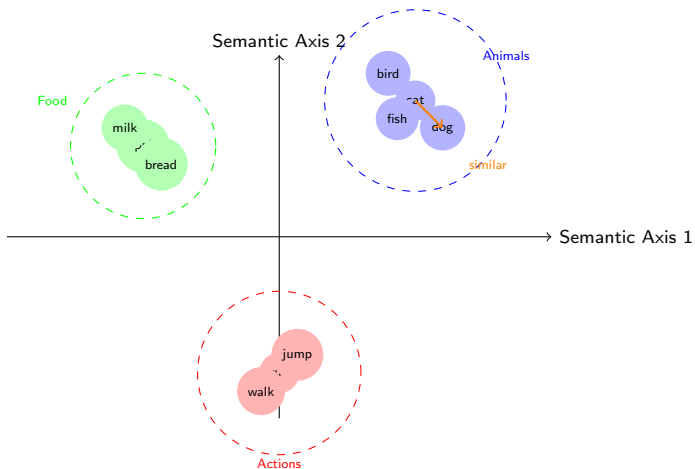
Example Vector:

cat = [0.21, -0.43, 0.67, 0.15, -0.22, ...]

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:**

man	\longrightarrow	woman
\uparrow		\uparrow
king	\longrightarrow	queen
\downarrow		\downarrow

Gender direction is consistent!

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

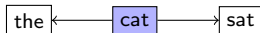
How Do We Learn These Vectors?

The Distributional Hypothesis:

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

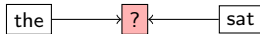
Two Approaches:

1. Skip-gram: Predict context from word



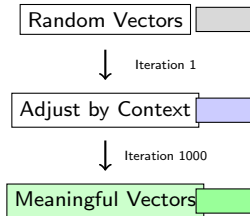
Given "cat", predict context

2. CBOW: Predict word from context



Given context, predict "cat"

Training Process Visualization:



Objective Function:

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

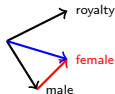
Maximize probability of context words

Vector Arithmetic: The Surprising Discovery

Embeddings Capture Analogies!

Famous Examples:

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

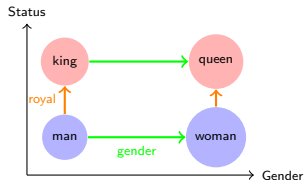


More Analogies:

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

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

Why Does This Work?



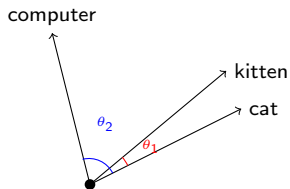
The Pattern:

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

Measuring Word Similarity

How Similar Are Two Words? Cosine Similarity:

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

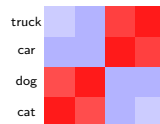


- cat \sim kitten: $\cos(\theta_1) = 0.95$
- cat \sim computer: $\cos(\theta_2) = 0.1$

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:



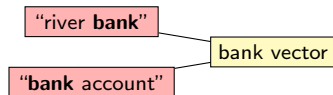
Animals cluster together, vehicles cluster together!

Evolution: From Static to Contextual Embeddings

The Next Revolution: Context Matters!

Problem with Static Embeddings:

One word = One vector always



Same vector!

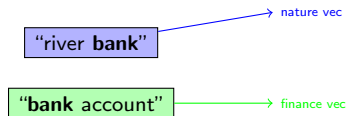
But "bank" has different meanings!

Static Embedding Models:

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

Solution: Contextual Embeddings

Different contexts = Different vectors



Different vectors!

Contextual Models:

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

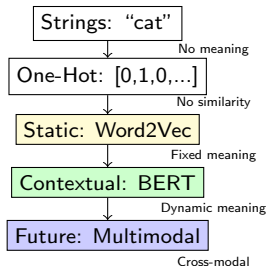
Key Advance: Vector depends on surrounding words!

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:

- 1 Meaning can be encoded as vectors
- 2 Similar words have similar vectors
- 3 Relationships are directions
- 4 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!

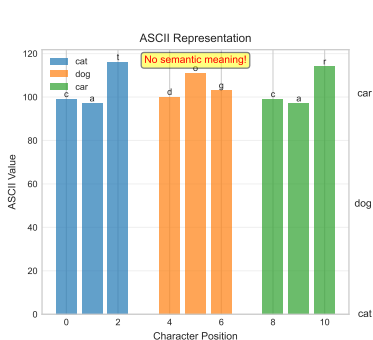
Part II

Advanced Theory & Visualizations

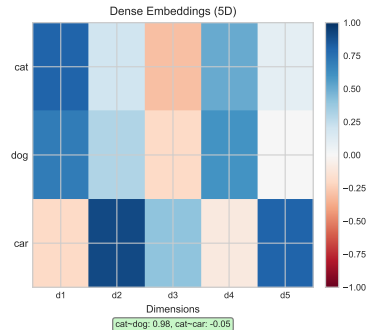
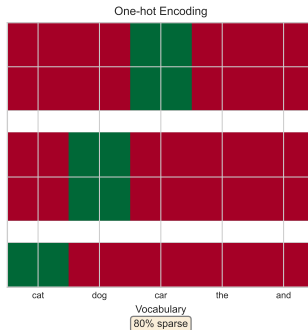
Deeper Insights into Embedding Mathematics

Beyond ASCII: From Characters to Meaning

How Computers See Text: Three Approaches



From Characters to Meaning: Representation Methods



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

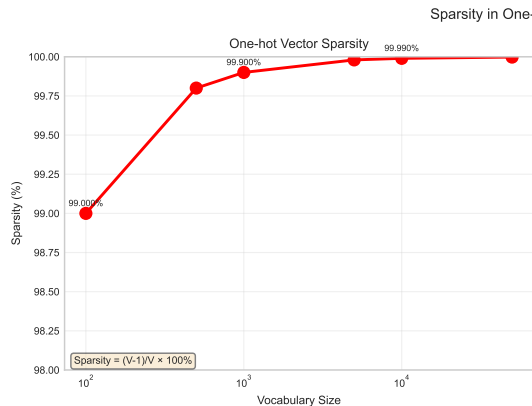
Dense Embedding:

- 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



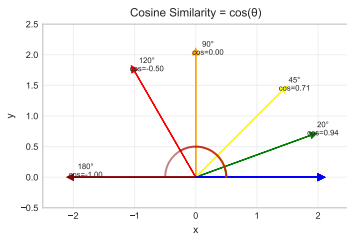
Mathematical Analysis:

- 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

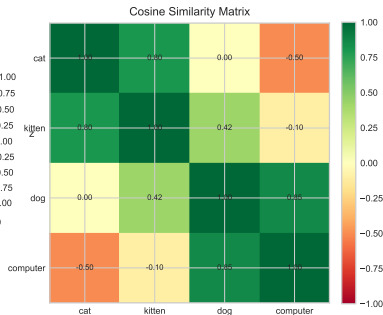
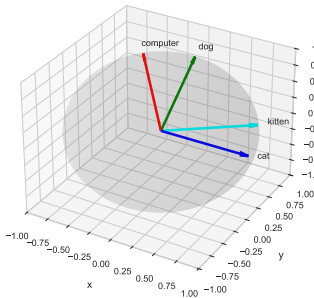
Key Insight:

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

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

Context Window Sizes in Skip-gram Training

Window Size = 1 (Total pairs: 16)

Window Size = 2 (Total pairs: 30)

The quick brown fox jumps over the lazy dog

fox jumps over



Context words: ± 1 positions

Window Size = 3 (Total pairs: 42)

The quick brown fox jumps over the lazy dog

brown fox jumps over the



Context words: ± 2 positions

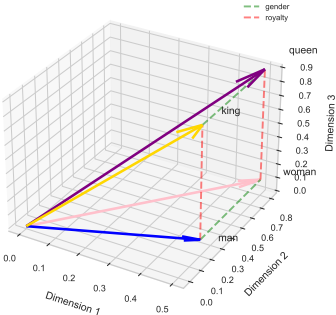
Window Size = 5 (Total pairs: 60)

Vector Arithmetic: The Surprising Discovery

Embeddings Can Do Analogies!

Vector Arithmetic: Mathematical Demonstration

Vector Relationships in 3D Space



Vector Arithmetic:

king - man + woman = ?

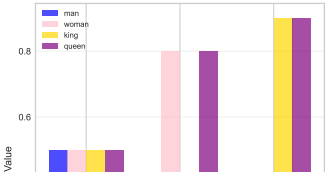
Step 1: king - man
[0.5, 0.2, 0.9] - [0.5, 0.2, 0.1]
= [0.0, 0.0, 0.8] (royal vector)

Step 2: + woman
[0.0, 0.0, 0.8] + [0.5, 0.8, 0.1]
= [0.5, 0.8, 0.9]

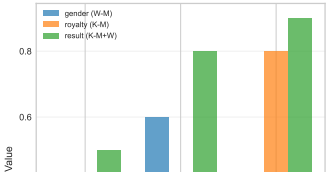
Result = queen vector!
[0.5, 0.8, 0.9]

Similarity = 1.0 (perfect match)

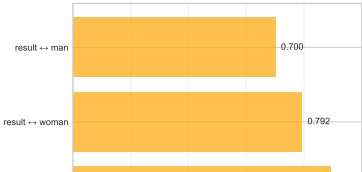
Vector Components



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: $\vec{g} = \text{woman} - \text{man}$
- Royalty vector: $\vec{r} = \text{king} - \text{man}$

Step-by-Step Derivation:

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

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

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

$$= \vec{\text{king}} - \vec{\text{man}} + \vec{\text{woman}} \quad (4)$$

Why Linear Structure Emerges:

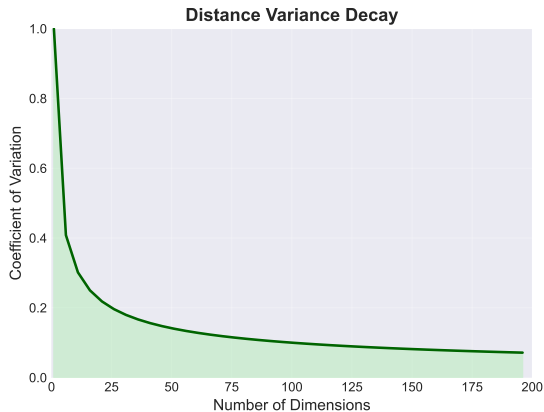
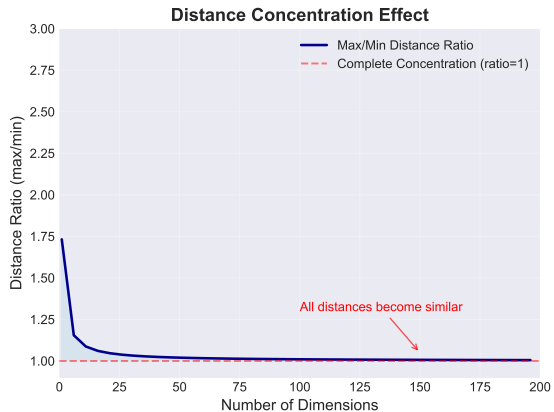
- Co-occurrence patterns are approximately linear
- Skip-gram objective encourages linear relationships
- High-dimensional spaces tend toward linearity (concentration of measure)

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:

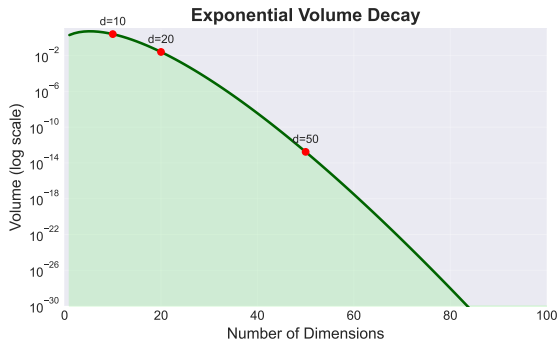
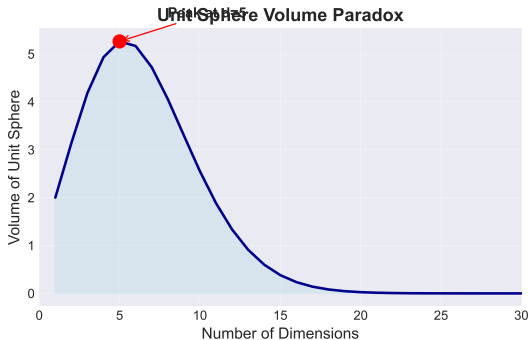
- Nearest neighbor search becomes meaningless
- Traditional distance metrics fail
- Need specialized techniques:
 - Locality-Sensitive Hashing (LSH)
 - Approximate nearest neighbors
 - Learned distance metrics
- Explains why high-D embeddings need normalization

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



d=100

The Volume Formula:

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

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!

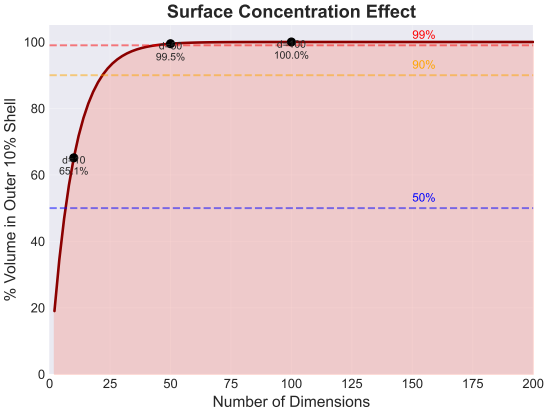
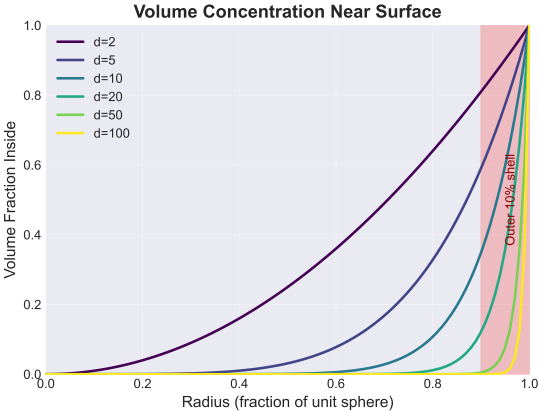
$\frac{1.77^d}{(d/2)!} \rightarrow 0$ extremely fast as $d \rightarrow \infty$

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

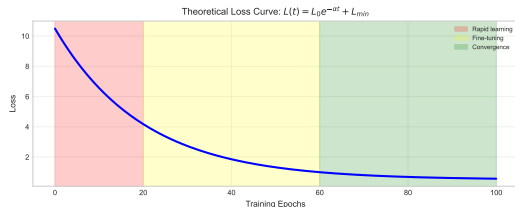
Higher Dimensions (768-1024+):

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

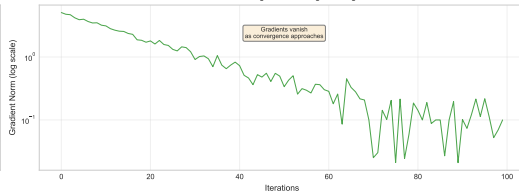
Rapid Learning: Gradient Dynamics (Epochs 0-20)

Why Training Starts Fast

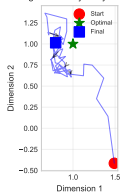
Training Process: Theoretical Dynamics



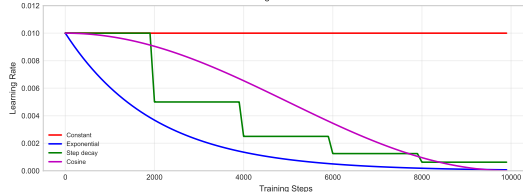
Gradient Magnitude During Training



Embedding Vector Trajectory During Training



Learning Rate Schedules



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%

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

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%

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%

Optimization Dynamics:

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

Mathematical Characterization:

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

Logarithmic improvement phase

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

Stopping Criteria:

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

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

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:

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

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:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) W^O$$

$$\text{head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

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

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:

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

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

This is a linear transformation of PE_{pos} !

BERT: Bidirectional Training Mathematics

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:

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

Truncated SVD for Embeddings:

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

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:

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

Spectral Norm Regularization:

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

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:

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

where:

- $\mathbf{h}_{k,j}^{\text{LM}}$ 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: $\tilde{\mathbf{W}} = (\mathbf{W} - \mu) \Sigma^{-1/2}$

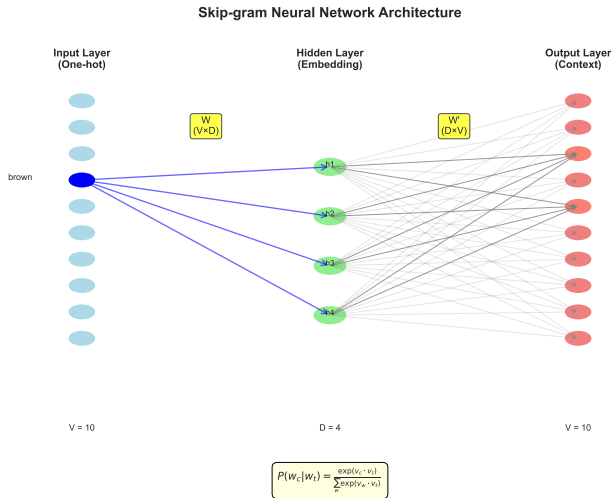
Intrinsic Dimension:

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

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

Skip-gram Neural Network Architecture

How the Network Processes Words



Key Components:

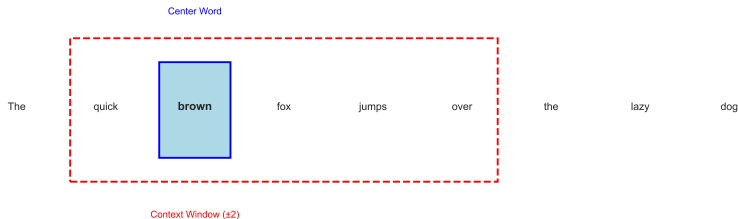
• **Input:** One-hot word (V dimensions)

Joerg R. Osterrieder (www.joergosterrieder.com)

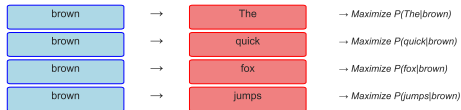
From Text to Training Data

Extracting (Center, Context) Pairs

Creating Training Pairs from Text Sliding Window for Training Pair Extraction



Training Pairs Generated:

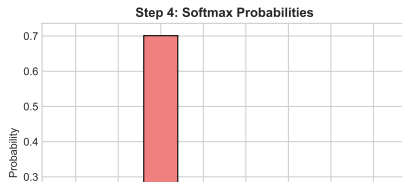
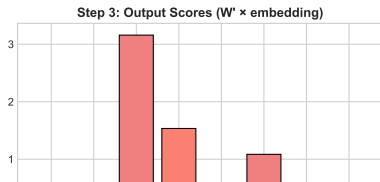
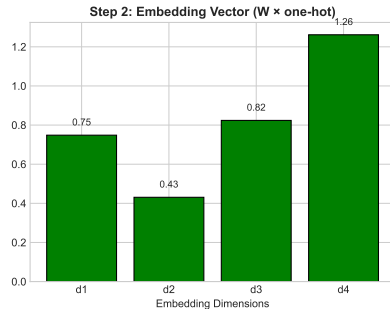
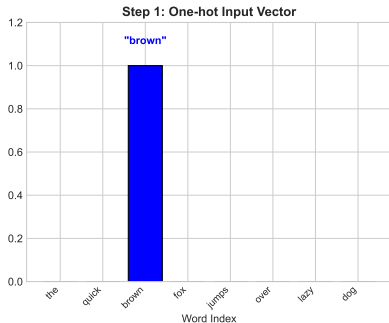


Input

Target

Forward Pass: Computing Context Probabilities

Forward Pass: Computing Context Probabilities



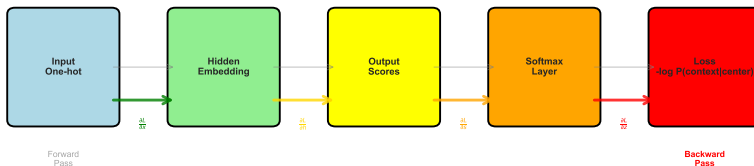
Backpropagation: Learning the Embeddings

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: $(y_i - 1) \cdot v_j$

Negative sample: $y_i \cdot v_j$

Updates:

How Embeddings Evolve

Evolution of Word Embeddings During Training

