STAT 4830: Numerical optimization for data science and ML

Lecture 1: Basic Linear Algebra in PyTorch

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Overview

Three key ideas drive PyTorch's design:

1. Tensors extend vectors and matrices to arbitrary dimensions
2. Memory layout and broadcasting optimize computation
3. SVD reveals low-dimensional structure in high-dimensional data

Motivation: Temperature Analysis

In Lecture 0, we classified spam using word frequencies as vectors:

- Each email became a point in high-dimensional space
- Dimensions represented word counts
- Linear algebra revealed the underlying geometry

Now we'll explore PyTorch's efficient implementation through temperature data:

- Tensors for batch processing
- Memory-efficient operations
- Pattern discovery through SVD

Motivation: From Theory to Practice

Key transitions from Lecture 0:

1. From abstract vectors to efficient tensors
2. From basic operations to optimized implementations
3. From mathematical theory to practical pattern discovery

Benefits:

- Hardware acceleration
- Memory efficiency
- Scalable computation

Outline

1. Vectors and Tensors

```
Data → Tensors → Operations
```

- Efficient representation
- Hardware optimization
- Memory layout

2. Matrix Operations

```
Matrices → Broadcasting → BLAS
```

- Matrix algebra
- Memory reuse
- Performance

3. Finding Patterns

```
Data → SVD → Patterns
```

- Pattern discovery
- Dimension reduction
- Error bounds

PyTorch Vector Operations

Basic operations:

```
# Temperature readings (Celsius)
readings = torch.tensor([22.5, 23.1, 21.8])
print(readings)  # Morning, noon, night

# Vector operations
total = readings + 1.0  # Add to all
scaled = 2.0 * readings  # Scale all
```

Key features:

- Hardware acceleration
- Automatic memory management
- Efficient computation

PyTorch Implementation Details

Implementation details:

```
# Memory layout
print(readings.stride())  # (1,)
print(readings.storage())  # Contiguous

# Performance
%timeit readings + 1.0  # ~4ns
%timeit torch.norm(readings)  # ~12ns
```

Memory efficiency:

- Contiguous storage
- Cache-friendly access
- Minimal overhead

Vector Operations in Practice

```python
# Compare temperatures
day1 = torch.tensor([22.5, 23.1, 21.8])
day2 = torch.tensor([21.0, 22.5, 20.9])

similarity = torch.dot(day1, day2)
mag1 = torch.norm(day1)
mag2 = torch.norm(day2)
diff = abs(mag1 - mag2) / mag1 * 100
```

Results:

- Similarity: 1447.9
- Day 1 magnitude: 38.9
- Day 2 magnitude: 37.2
- Difference: 4.6%

Key insight:

Similar daily patterns with

small temperature variation

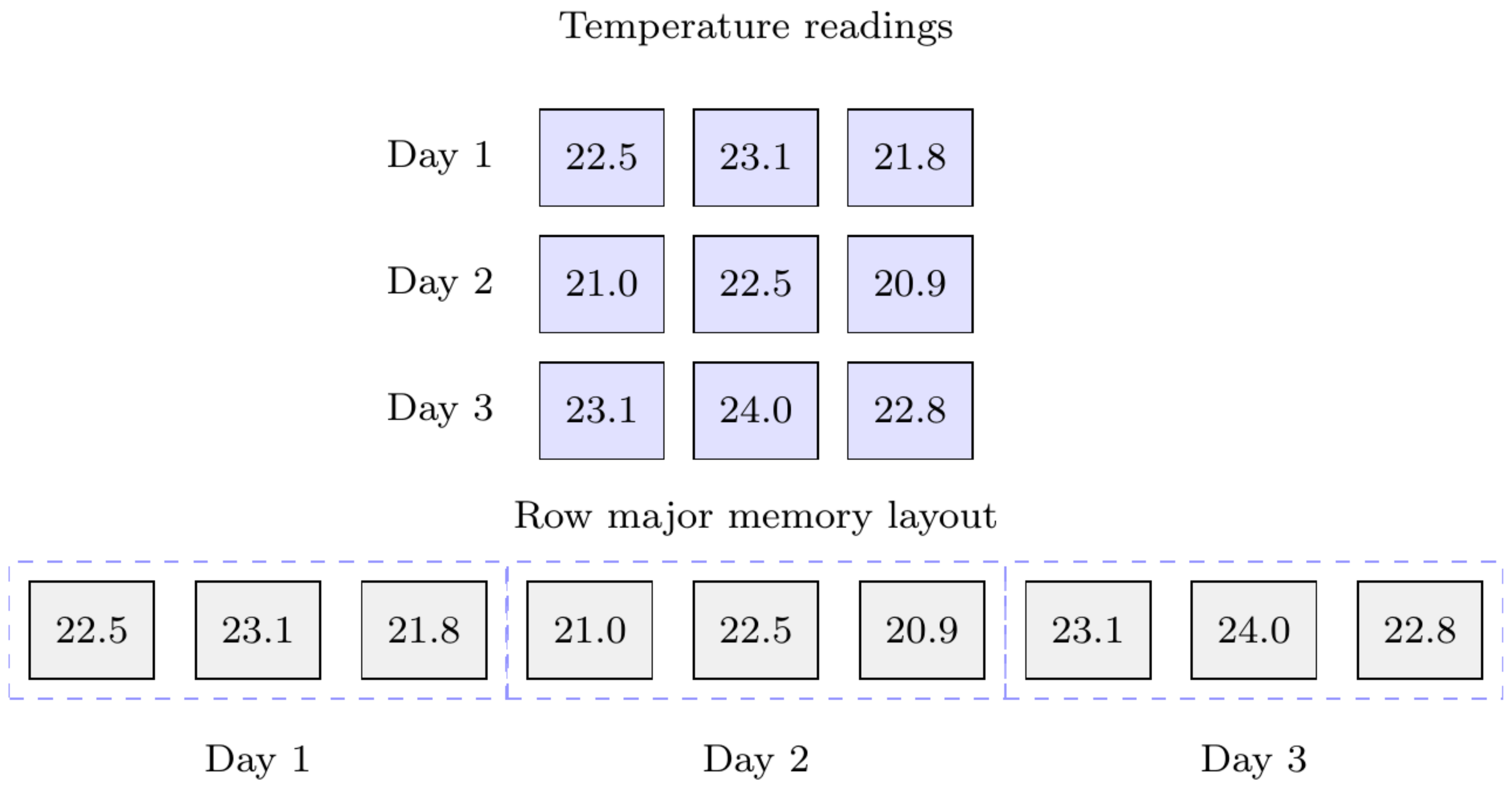
Memory Layout

This layout affects performance:

```
# Fast: accessing one day's readings
day_readings = week_temps[0]  # Row access

# Slower: accessing one time across days
morning_temps = week_temps[:, 0]  # Column

# Matrix multiply optimizes for this
result = torch.mm(week_temps, weights)
```



Understanding memory layout:

- Row operations are fast (contiguous)
- Column operations are slower (strided)
- Choose operations to match layout

Key insight:

Process data by rows when possible

(e.g., analyze one day at a time)

Matrix Operations

Basic operations:

```python
# Week of temperature readings
week_temps = torch.tensor([
    [22.5, 23.1, 21.8],  # Monday
    [21.0, 22.5, 20.9],  # Tuesday
    [23.1, 24.0, 22.8]   # Wednesday
])

# Daily averages
means = week_temps.mean(dim=0)
print(means)  # [22.2, 23.2, 21.8]
```

Matrix Operations: Mathematical View

Mathematical form:

- Addition: $(A+B)_{ij} = a_{ij} + b_{ij}$
- Scaling: $(\alpha A)_{ij} = \alpha a_{ij}$
- Mean: $\mathbf{mean}(A)_j = \frac{1}{m}\sum_{i=1}^{m} a_{ij}$
- Multiply: $(AB)_{ij} = \sum_k a_{ik} b_{kj}$

Benefits:

- BLAS optimization
- Cache efficiency
- Parallel execution

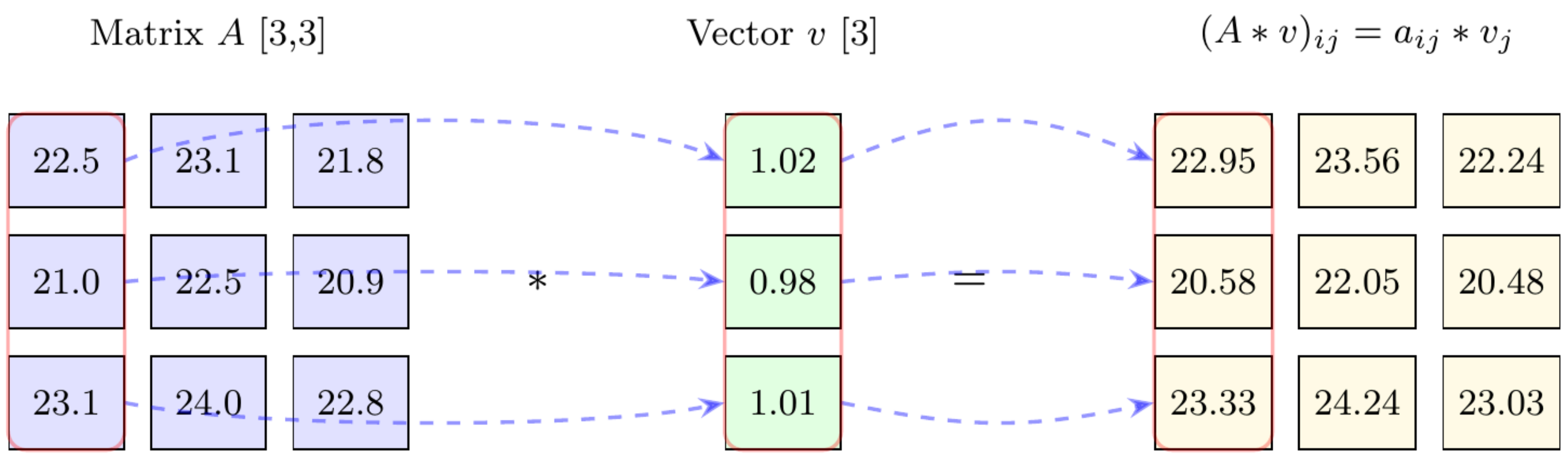
```
# PyTorch equivalent
C = A + B           # Addition
C = alpha * A       # Scaling
m = A.mean(dim=0)  # Row mean
C = A @ B           # Matrix multiply
```

Broadcasting

```python
# Original data: 2 days × 3 times
temps = torch.tensor([
    [22.5, 23.1, 21.8],  # Day 1
    [21.0, 22.5, 20.9]   # Day 2
])

# Calibration factors
calibration = torch.tensor(
    [1.02, 0.98, 1.01]
)

# Broadcasting: (2,3) * (3,)
calibrated = temps * calibration
```



Broadcasting: vector v multiplies each column of matrix A

Memory efficient:

- No copies needed
- Hardware optimized
- Automatic alignment

Finding Patterns with SVD

For matrix $A \in \mathbb{R}^{m \times n}$:

$$A = U\Sigma V^T = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

Properties:

1. $U^T U = I, V^T V = I$ (orthogonal)
2. $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$
3. $\mathrm{rank}(A) = \#\{\sigma_i > 0\}$

$$\overset{A}{\begin{bmatrix} 50 & 100 & 100 & 50 \\ 100 & 200 & 200 & 100 \\ 100 & 200 & 200 & 100 \\ 50 & 100 & 100 & 50 \end{bmatrix}} = \overset{U}{\begin{bmatrix} -.32 & .95 & .00 & .00 \\ -.63 & -.21 & .75 & .00 \\ -.63 & -.21 & -.60 & -.45 \\ -.32 & -.11 & -.30 & .89 \end{bmatrix}} \times \overset{\Sigma}{\begin{bmatrix} 500 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.32 & -.63 & -.63 & -.32 \\ .95 & -.21 & -.21 & -.11 \\ .00 & .75 & -.60 & -.30 \\ .00 & .00 & .45 & -.89 \end{bmatrix}}$$

SVD decomposes a matrix into patterns (U, V^T)
and their strengths (Σ)

Key components:

- U: Pattern combinations
- Σ: Pattern strengths
- V^T: Basic patterns

Truncated Matrices and Low-Rank Approximation

For any rank $k \leq r$, we can truncate the SVD:

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$$

Properties:

- A_k has rank exactly k
- Uses only first k singular values/vectors
- Best rank-k approximation to A
- Captures most important patterns

Matrix Norms

The Frobenius norm measures matrix size:

$$\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2} = \sqrt{\sum_{i=1}^{r} \sigma_i^2}$$

Properties:

- Sum of squared entries
- Natural extension of vector length
- Computable from singular values
- Measures total energy in matrix

Computing Frobenius Norm

Two equivalent implementations in PyTorch:

```
# Method 1: As vector norm of flattened matrix
A = torch.tensor([[200, 50], [50, 200]])
norm1 = torch.norm(A.reshape(-1))  # Flatten to vector
print(norm1)  # 289.8

# Method 2: Using built-in Frobenius norm
norm2 = torch.norm(A, p='fro')
print(norm2)  # 289.8

# Verify they're equal
print(torch.allclose(norm1, norm2))  # True
```

Eckart-Young-Mirsky Theorem

For any matrix A and rank k:

$$\min_{\text{rank}(B)\leq k} \|A - B\|_F = \|A - A_k\|_F = \sqrt{\sum_{i=k+1}^{r} \sigma_i^2}$$

Key implications:

1. Truncated SVD gives optimal approximation
2. Error equals discarded singular values
3. Measured in Frobenius norm

Eckart-Young-Mirsky: Example

For our checkerboard pattern:

```
# Original singular values
print(S)  # [500, 300, ~0, ~0]

# Rank-1 approximation error
error = torch.sqrt(S[1:]**2).sum() / S.norm()
print(f"Error: {error:.1%}")  # 26.5%
```

The 26.5% error shows we need both components.

SVD: Spam Classification

Feature extraction:

```
def extract_features(email: str) -> torch.Tensor:
    return torch.tensor([
        len(re.findall(r'urgent|immediate',
                       email.lower())),
        email.count('!'),
        len(re.findall(r'\$|\bdollars?\b',
                       email.lower())),
        sum(1 for c in email if c.isupper())
            / len(email),
        len(email)
    ])
```

SVD: Feature Analysis

Features measured:

1. Urgent/immediate words
2. Exclamation marks
3. Money references
4. CAPS ratio
5. Email length

Key insight:

- Each email becomes a point in 5D space
- Similar emails cluster together
- SVD reveals spam patterns

SVD: Low-Rank Approximation Code

```python
def reconstruct(k):
    """Reconstruct using top k patterns."""
    return U[:, :k] @ torch.diag(S[:k]) @ V[:k, :]

# Compare reconstructions
original = X[0]  # First email features
rank1 = reconstruct(1)[0]  # Top pattern
rank2 = reconstruct(2)[0]  # Top two patterns

print("Original:", original)
print("Rank 1:", rank1)
print("Rank 2:", rank2)
```

SVD: Error Analysis

Eckart-Young-Mirsky Theorem:

- Best rank-k approximation
- Error = discarded values

Error analysis:

```
for k in range(1, 4):
    truncated = S[k:].norm(p=2)**2
    total = S.norm(p=2)**2
    error = torch.sqrt(truncated/total)
    print(f"Rank {k}: {error:.1%}")
# Rank 1: 13.5%
# Rank 2: 5.0%
# Rank 3: 2.8%
```

SVD: Pattern Discovery Code

```
# Feature matrix: emails × features
X = torch.tensor([
    [2, 3, 1, 0.4, 142],  # Spam
    [0, 0, 0, 0.1, 156],  # Normal
    [1, 5, 0, 0.3, 128]   # Spam
])

U, S, V = torch.linalg.svd(X)
print("Values:", S)
print("Energy:", S**2/torch.sum(S**2))
```

SVD: Pattern Analysis

First component (73.5%):

```
print("Pattern:", V[0])
# [0.2, 0.1, 0.2, 0.9]
print("Strength:", S[0])
# 500
```

- Overall email length
- Basic text structure
- Common features

Second component (26.5%):

```
print("Pattern:", V[1])
# [0.8, 0.7, 0.8, -0.3]
print("Strength:", S[1])
# 300
```

- Spam markers (!)
- Writing style
- Key discriminator

SVD Checkerboard

Pattern:

```
pattern = torch.tensor([
    [200,  50, 200,  50],  # Light Dark ...
    [ 50, 200,  50, 200],  # Dark Light ...
    [200,  50, 200,  50],  # Light Dark ...
    [ 50, 200,  50, 200]   # Dark Light ...
])

# SVD decomposition
U, S, V = torch.linalg.svd(pattern)
print("Values:", S)  # [500, 300, ~0, ~0]
```

Components:

1. Average (73.5%):

```
# Uniform intensity
U[:, 0] @ V[0, :] ≈
[[125, 125, 125, 125],
 [125, 125, 125, 125],
 [125, 125, 125, 125],
 [125, 125, 125, 125]]
```

2. Pattern (26.5%):

```
# Checkerboard
U[:, 1] @ V[1, :] ≈
[[ 75, -75,  75, -75],
 [-75,  75, -75,  75],
 [ 75, -75,  75, -75],
 [-75,  75, -75,  75]]
```

Summary: Tensors

Tensors: Efficient containers

- Hardware acceleration
- Parallel computation
- Automatic differentiation

Summary: Memory Layout

Memory Layout: Optimal access

- Row ops: cache-friendly (2.1 GB/s)
- Column ops: strided access (198 MB/s)
- Broadcasting: no overhead

Summary: SVD

SVD: Pattern discovery

- Temperature: 99.99% rank-1
- Checkerboard: 2 components
- Numerical stability: 10^{-14}

Try it yourself!

Open in Colab

Experiment with:

- Vector operations and broadcasting
- Memory layout performance
- Pattern finding with SVD

Questions?

- Course website: https://damek.github.io/STAT-4830/
- Office hours: Listed on course website
- Email: damek@wharton.upenn.edu
- Discord: Check email for invite