Linear Algebra

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Outline

- Motivation
- Vector spaces
- Matrix operations
- Matrix decompositions
- Matrix transforms
- Layers built from linear transforms
- References

Disclaimer

- This set of slides is more accurately titled “A brief refresher of a subset of linear algebra for people already somewhat familiar with the topic followed by it’s specific application to xNN related items needed by the rest of the course”
- However, that’s not very catchy so we’ll just stick with “Linear algebra”
- In all seriousness, recognize that linear algebra is a very broad and deep topic that has and will continue to occupy many lifetimes of work; if interested in learning more, please consult the references to open a window into a much larger world

Motivation

Pre Processing

- Pre processing methods simplify feature extraction and prediction
- Understanding linear transformations is a key to understanding many popular pre processing methods
- Example pre processing methods
  - Discrete Fourier transform
  - Principal component analysis

Feature Extraction And Prediction

- CNNs are compositions of nonlinear functions (layers)
  - $y = f_{D-1}(\ldots(f_2(f_1(f_0(x, h_0), h_1), h_2), \ldots), h_{D-1})$
- Linear function with trainable parameters are a component of key layer types that control the network mapping from data space to feature space to information space
- Examples layers that include linear functions
  - Dense layers with single and multiple inputs
  - CNN style 2D convolution layers
  - RNN layers
  - Attention based layers
  - Average pooling layers

Vector Spaces

Preliminaries

- Notation
  - Scalars are not bold
  - Vectors are bold lower case
  - Matrices and tensors are bold upper case
  - Indices start at 0 and go from 0, ..., size – 1

Set

- A collection of distinct objects

Field

- A set with well defined addition and multiplication operations
  - Associativity: $a + (b + c) = (a + b) + c$ and $a\,(b\,c) = (a\,b)\,c$
  - Commutativity: $a + b = b + a$ and $a\,b = b\,a$
  - Additive identity: $a + 0 = a$
  - Additive inverse: $a + (-a) = 0$
  - Multiplicative identity: $1\,a = a$
  - Multiplicative inverse: $a\,a^{-1} = 1$
  - Distributivity: $a\,(b + c) = (a\,b) + (a\,c)$

- Elements of fields are generally referred to as scalars

- Examples: R (real scalars), C (complex scalars)

Vector

- K tuple of scalars
- Always a column
- Denoted by the field raised to the size
  - F^K
- Examples: R^K and C^K

Matrix

- M x K tuple of scalars

- Collection of K vectors of size M x 1 arranged in columns
  - Leads to column space and right null space
    - What can matrix vector multiplication reach and what can it not
  - Visualize using outer product of matrix vector multiplication

- Collection of M vectors of size K x 1 transposed and arranged as rows
  - Leads to row space and left null space
    - What can vector matrix multiplication reach and what can it not
  - Visualize using outer product of vector matrix multiplication

Tensor

- K_0 x ... x K_{D-1} array of scalars

- Ordering
  - Last dimension is contiguous in memory
  - Working from right to left goes from closest to farthest spacing in memory
  - Feature maps: batch x channel x row x column (sometimes referred to as NCHW ordering)
  - Filter coefficients: output channel x input channel x row x col

Function

- Mapping f: $X \rightarrow Y$ from domain to co domain
  - Injective: one to one; each y produced by at most one x
  - Surjective: onto; each y produced by at least one x
  - Bijective: one to one and onto (invertible)

- An infinite set is
  - Countably infinite if there's a bijection between the natural numbers and elements of the set
  - Un countably infinite if there's not

Vector Space

- Set of vectors and linear combinations of those vectors

- Satisfy
  - Associativity: $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}$
  - Commutativity: $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$
  - Additive identity: $\mathbf{x} + \mathbf{0} = \mathbf{x}$
  - Additive inverse: $\mathbf{x} + (-\mathbf{x}) = \mathbf{0}$
  - Multiplicative compatibility: $a\,(b\,\mathbf{x}) = b\,(a\,\mathbf{x})$
  - Multiplicative identity: $1\,\mathbf{x} = \mathbf{x}$
  - Distributivity: $(a + b)(\mathbf{x} + \mathbf{y}) = a\,\mathbf{x} + a\,\mathbf{y} + b\,\mathbf{x} + b\,\mathbf{y}$

- Examples: R^K, C^K, $R^{K\_0 \text{ x } \ldots \text{ x } K\_D-1}$

Vector Space

- Span
  - The span of a set of vectors $\{\mathbf{x}_0, \ldots, \mathbf{x}_{N-1}\}$ is the set of all finite linear combinations of the vectors
  - Vectors $\mathbf{x}$ in the span can be written as $\mathbf{x} = a_0 \mathbf{x}_0 + \ldots + a_{N-1} \mathbf{x}_{N-1}$
  - The span of a set of vectors is a vector space

- Rank
  - The rank of a matrix $\mathbf{X}$ is the dimension of the vector space generated by the span of the column vectors forming the matrix
  - It is the same as the dimension of the space spanned by the rows of $\mathbf{X}$

Vector Space

- Linear independence
  - A set of vectors is linearly dependent if at least 1 vector in the set is a linear combination of the others
  - A set of vectors is linearly independent if no vector in the set can be written as a linear combination of the others

- Basis
  - A basis for a vector space V is any linearly independent set of vectors that span V

- Dimension
  - The dimension of a vector space V is the number of vectors required to form a basis of V
  - Only finite dimensional vector spaces are considered here

Normed Vector Space

- A vector space with a notion of distance
- A norm maps an element of the vector space to a scalar
- Satisfies
  - Non negativity: $||\mathbf{x}|| \geq 0$ and $||\mathbf{x}|| = 0$ iff $\mathbf{x} = \mathbf{0}$
  - Absolute scalability: $||a\,\mathbf{x}|| = |a|\ ||\mathbf{x}||$
  - Triangle inequality: $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$
- Example: l_p norm (common p = 1, 2 and ∞)
  - $||\mathbf{x}||_p = (\Sigma_n(|x(n)|^p))^{1/p}$, $p \geq 1$

Normed Vector Space

- The matrix norm induced by the l_p vector norm for a M x K matrix **H** is
  - $|| \mathbf{H} ||_p = \sup_{\mathbf{x} \neq \mathbf{0}} || \mathbf{H}\,\mathbf{x} ||_p / || \mathbf{x} ||_p$
  - The l_1 induced matrix norm is the maximum absolute column sum of **H**
  - The l_2 induced matrix norm is the largest singular value of **H**
  - The l_∞ induced matrix norm is the maximum absolute row sum of **H**

- The matrix norm expressed as a vector norm applied first across columns then to the resulting vector is
  - $|| \mathbf{H} ||_{p,q} = (\Sigma_k (\Sigma_m |H(m, k)|^p)^{q/p})^{1/q}$, $1 \leq p, q \leq \infty$
  - If p = q = 1 then the matrix norm is the absolute value of all matrix entries
  - If p = q = 2 then the matrix norm is the square root of the sum of the squares of all matrix entries and referred to as the Frobenius norm
  - If p = q = ∞ then the matrix norm is the maximum of the absolute value of all matrix entries

Inner Product Space

- A vector space with a notion of distance and angle
- An inner product maps 2 elements of a vector space to a scalar
- Satisfies
  - Positive definiteness: $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$ and $\langle \mathbf{x}, \mathbf{x} \rangle = 0$ iff $\mathbf{x} = 0$
  - Conjugate symmetry: $\langle \mathbf{x}, \mathbf{y} \rangle = \text{conj}(\langle \mathbf{y}, \mathbf{x} \rangle)$
  - Linearity: $\langle a\, \mathbf{x}, \mathbf{y} \rangle = a \langle \mathbf{x}, \mathbf{y} \rangle$ and $\langle \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle$
- Inner products induce norms on a vector space
  - But not all norms have associated inner products (e.g., l_∞)
- Example: dot product
  - $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x} \bullet \mathbf{y} = \mathbf{x}^H \mathbf{y} = \Sigma_n (\text{conj}(x(n))\, y(n)) = ||\mathbf{x}||_2\, ||\mathbf{y}||_2 \cos(\theta)$

Inner Product Space

- Matrix inner product is the Frobenius inner product
  - $\langle \mathbf{H}, \mathbf{G} \rangle_F = \Sigma_m \Sigma_k \mathrm{conj}(H(m, k))\, G(m, k)$
  - If the matrices were flattened by stacking the rows or columns end to end then the Frobenius inner product would be equivalent to the vector dot product

Matrix Operations

Transpose

- Definition
  - The transpose of matrix **A** with entries A(m, k) is matrix $\mathbf{A}^T$ with entries conj(A(k, m))
  - Also referred to as the Hermitian adjoint

- Properties
  - $\mathbf{C}^T = (\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$
  - $\mathbf{C}^T = (\mathbf{A}\ \mathbf{B})^T = \mathbf{B}^T\ \mathbf{A}^T$

Addition

- Definition
  - **C** = **A** + **B** where $C(m, k) = A(m, k) + B(m, k)$

Multiplication – Matrix Scalar

- Definition
  - **C** = a **B** where C(m, k) = a B(m, k)

Multiplication – Matrix Vector

Matrix vector multiplication

- Definition
  - **c** = **A b** where $c(m) = \Sigma_k A(m, k)\, b(k)$
  - $$\begin{bmatrix} c(0) \\ \vdots \\ c(M-1) \end{bmatrix} = \begin{bmatrix} A(0,0) & \cdots & A(0,K-1) \\ \vdots & & \vdots \\ A(M-1,0) & \cdots & A(M-1,K-1) \end{bmatrix} \begin{bmatrix} b(0) \\ \vdots \\ b(K-1) \end{bmatrix}$$
- Comments
  - M (output dimension), K (input dimension) is setting up for BLAS notation
  - Inner product of matrix row and vector input to produce each output

Multiplication – Matrix Vector

Matrix vector multiplication

- Arithmetic intensity
  - Compute = MK (MACs = multiply accumulates)
  - Data movement = K + MK + M (elements)
  - Ratio = (MK)/(K + MK + M) (consider M and K large)
    ≈ 1 (memory wall)

- Implementation preview
  - If you want to make matrix vector multiplication run fast, you need to build a fast memory subsystem
  - Typically not an efficient thing to do from an operation per power perspective

Multiplication – Matrix Matrix

Matrix matrix multiplication

- Definition
  - **C** = **A B** where C(m, n) = Σ_k A(m, k) B(k, n)
  - $$\begin{bmatrix} C(0,0) & \cdots & C(0,N-1) \\ \vdots & & \vdots \\ C(M-1,0) & \cdots & C(M-1,N-1) \end{bmatrix} = \begin{bmatrix} A(0,0) & \cdots & A(0,K-1) \\ \vdots & & \vdots \\ A(M-1,0) & \cdots & A(M-1,K-1) \end{bmatrix} \begin{bmatrix} B(0,0) & \cdots & B(0,N-1) \\ \vdots & & \vdots \\ B(K-1,0) & \cdots & B(K-1,N-1) \end{bmatrix}$$
- Comments
  - M (output dimension), K (input dimension), N (number of inputs and outputs) is setting up for BLAS notation
  - Can view as matrix vector multiplication applied to multiple inputs stacked next to each other (in the N dimension) with matrix vector multiplication as a special case with N = 1
  - A discussion of different computational options for matrix matrix multiplication (inner product based, outer product based, block based, Strassen style) will be deferred to the implementation section

Multiplication – Matrix Matrix

Matrix vector multiplication

- Arithmetic intensity
  - Compute = MNK (MACs)
  - Data movement = KN + MK + MN (elements)
  - Ratio = (MNK)/(KN + MK + MN) (cube in num, squares in den)
    = $N^3/(3*N^2)$ (special case M = N = K)
    = N/3 (ratio maxed with sq matrix)

- Implementation preview
  - If you want to make matrix matrix mult run fast, if it's possible choose a large matrix size such that you get multiple ops per element of data moved

- Why are bubbles spherical? Min surface area per volume enclosed
  - Think of surface area as data movement and volume as MACs

Inversion

- Square
  - A K x K square matrix **A** has an inverse matrix **B** = $\mathbf{A}^{-1}$ when the column vectors comprising **B** are linearly independent
  - $\mathbf{A}\,\mathbf{B} = \mathbf{B}\,\mathbf{A} = \mathbf{I}_K$
  - Properties
    - $(\mathbf{A}^T)^{-1} = (\mathbf{A}^{-1})^T$
    - $(\mathbf{A}^{-1})^{-1} = \mathbf{A}$
    - $(\mathbf{A}\,\mathbf{B})^{-1} = \mathbf{B}^{-1}\,\mathbf{A}^{-1}$
  - Diagonal
    - Invertible if diagonal entries are non zero
    - B(k, k) = 1/A(k, k)

Inversion

- Non square
  - A M x K matrix **A**
  - When the rank of **A** is M then **A** has a right inverse **B** such that $\mathbf{A}\,\mathbf{B} = \mathbf{I}_M$
  - When the rank of **A** is K then **A** has a left inverse **B** such that $\mathbf{B}\,\mathbf{A} = \mathbf{I}_K$
- Unitary
  - A K x K unitary matrix **U** has orthogonal unit norm columns
  - $\mathbf{U}^H\,\mathbf{U} = \mathbf{U}\,\mathbf{U}^H = \mathbf{I}_K$
  - Unitary matrices preserve inner products $\langle \mathbf{U}\,\mathbf{x}, \mathbf{U}\,\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$
- Orthogonal
  - A K x K orthogonal matrix **Q** has orthogonal unit norm columns with only real valued elements
  - $\mathbf{Q}^T\,\mathbf{Q} = \mathbf{Q}\,\mathbf{Q}^T = \mathbf{I}_K$
  - Orthogonal matrices preserve inner products $\langle \mathbf{Q}\,\mathbf{x}, \mathbf{Q}\,\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$

Hadamard or Schur Product

- Definition
  - **C** = **A** $\odot$ **B** where C(m, k) = A(m, k) B(m, k)

- Comments
  - Can be thought of as a point wise or element wise product
  - Used in many FFT algorithms for twiddle factor multiplication
  - Used to combine a gate ([0, 1] limited vector) with an input or output

Kronecker Product

- Definition
  - **C** = **A** $\otimes$ **B** where **C**(m, k) = A(m, k) **B**

- Comments
  - Generalizes vector outer products to matrix outer products
  - Not commutative in general

Vectorization

- Definition
    - $\mathbf{y} = \text{vec}(\mathbf{A})$ where $\mathbf{y}$ is formed from stacking columns of $\mathbf{A}$

- Identities
    - $$\begin{aligned}\text{vec}(\mathbf{A}\,\mathbf{B}\,\mathbf{C}) &= (\mathbf{C}^T \otimes \mathbf{A})\,\text{vec}(\mathbf{B}) \\ &= (\mathbf{I}_N \otimes \mathbf{A}\,\mathbf{B})\,\text{vec}(\mathbf{C}) \\ &= (\mathbf{B}^T\,\mathbf{C}^T \otimes \mathbf{I}_K)\,\text{vec}(\mathbf{A})\end{aligned}$$

Trace

- Definition
    - The trace of a K x K matrix **A** is the sum of the elements on the principal diagonal
- Comments
    - The trace is also equal to the sum of the eigenvalues of **A**

Determinant

- Definition
  - The determinant of a K x K matrix **A** is the product of the matrix eigenvalues

- Comments
  - Can be thought of as the volume of a polytope defined by the column vectors of **A**

Matrix Decompositions

Eigen Decomposition

- An eigenvector **v** of a K x K matrix **A** is a nonzero vector that satisfies $\mathbf{A}\,\mathbf{v} = \lambda\,\mathbf{v}$
  - λ is a scalar referred to as the associated eigenvalue
  - Matrix **A** simply scales the eigen vector **v** but does not change it's direction

- If **A** has K linearly independent eigenvectors then **A** can be factored as $\mathbf{A} = \mathbf{Q}\,\mathbf{D}\,\mathbf{Q}^{-1}$
  - **Q** is an orthogonal matrix with eigenvectors as columns
  - **D** is a diagonal matrix with associated eigenvalues as diagonal elements
  - The eigen decomposition is frequently calculated via a power method and deflation

- Given an eigen decomposition of **A** it's straightforward to find the inverse of **A**
  - $\mathbf{A}^{-1} = (\mathbf{Q}\,\mathbf{D}\,\mathbf{Q}^{-1})^{-1}$
    $= \mathbf{Q}\,\mathbf{D}^{-1}\,\mathbf{Q}^{-1}$
  - This exploits the inversion formula for orthogonal and diagonal matrices and products of matrices

Singular Value Decomposition

- The SVD of a M x K matrix **A** is the weighted outer product $\mathbf{A} = \mathbf{U}\ \mathbf{S}\ \mathbf{V}^H$
  - **U** is a M x M orthogonal matrix
  - **S** is a M x K diagonal matrix is singular values
  - $\mathbf{V}^H$ is a K x K orthogonal matrix
- The columns of **U** are the eigenvectors of $\mathbf{A}\ \mathbf{A}^H = \mathbf{U}\ \mathbf{S}\ \mathbf{V}^H\ \mathbf{V}\ \mathbf{S}^H\ \mathbf{U}^H = \mathbf{U}\ \mathbf{S}\ \mathbf{S}^H\ \mathbf{U}^H$
  - Let $\mathbf{Q} = \mathbf{U}$, $\mathbf{D} = \mathbf{S}\ \mathbf{S}^H$ and $\mathbf{Q}^{-1} = \mathbf{U}^H$ in the eigen decomposition
  - Initial columns corresponding to nonzero singular values span the column space of **A**
  - Last columns corresponding to zero singular values span the left null space of **A**
- The number of nonzero singular values is the rank of **A** and the ratio of the largest to smallest singular value is the condition number of **A**
- The columns of $\mathbf{V}^H$ are the eigenvectors of $\mathbf{A}^H\ \mathbf{A} = \mathbf{V}\ \mathbf{S}^H\ \mathbf{U}^H\ \mathbf{U}\ \mathbf{S}\ \mathbf{V}^H = \mathbf{V}\ \mathbf{S}^H\ \mathbf{S}\ \mathbf{V}^H$
  - Let $\mathbf{Q} = \mathbf{V}$, $\mathbf{D} = \mathbf{S}^H\ \mathbf{S}$ and $\mathbf{Q}^{-1} = \mathbf{V}^H$ in the eigen decomposition
  - Initial columns corresponding to nonzero singular values span the row space of **A**
  - Last columns corresponding to zero singular values span the null space of **A**

Matrix Transforms

Linear

- Important to understand matrices in the context of linear maps (transforms)
  - Every linear map can be represented as a matrix
  - Every matrix represents a linear map

- T: $V_1 \rightarrow V_2$ is a linear map between vector spaces V_1 and V_2
  - Let $\mathbf{x}$ and $\mathbf{y}$ be vectors in V_1 and a be a scalar
  - Then T satisfies the following properties
    - Additivity: $T(\mathbf{x} + \mathbf{y}) = T(\mathbf{x}) + T(\mathbf{y})$
    - Homogeneity: $T(a\,\mathbf{x}) = a\,T(\mathbf{x})$

Linear

- 4 fundamental subspaces
  - The column space, image or range of T is the vector subspace of V_2 comprising all vectors T can produce and is denoted by range(T) = $\{T(\mathbf{x}) \in V_2 : \mathbf{x} \in V_1\}$
  - The null space or right null space of T is the vector subspace of V_1 comprising all vectors T maps to **0** and is denoted by null(T) = $\{\mathbf{x} \in V_1 : T(\mathbf{x}) = \mathbf{0}\}$
  - The row space or co image of T is the vector subspace of V_1 comprising all vectors T^T can produce and is denoted by range(T^T) = $\{T^T(\mathbf{y}) \in V_1 : \mathbf{y} \in V_2\}$
  - The left null space or co kernel of T is the vector subspace of V_2 comprising all vectors T^T maps to **0** and is denoted by null(T^T) = $\{\mathbf{y} \in V_2 : T^T(\mathbf{y}) = \mathbf{0}\}$

- Consider the linear transformation between finite dimensional vector spaces $\mathbf{y} = \mathbf{A}\,\mathbf{x}$
  - **A** is a M x K matrix representing linear map T, **x** is a length K input and **y** is a length M output
  - The range of **A** is the vector space formed by the span of the column vectors of **A**
  - The number of linearly independent columns of **A** is the rank of **A** and satisfies rank(**A**) ≤ min(M, K)

Affine

- An affine transformation is a linear transformation + an offset or bias
  - $\mathbf{y} = \mathbf{A}\,\mathbf{x} + \mathbf{b}$
- Can be implemented as a linear transformation augmented with a nonzero constant input
  - $\mathbf{y} = \mathbf{A}\,\mathbf{x} + \mathbf{b}$
    $= [\mathbf{A}\ \mathbf{b}]\ [\mathbf{x};\ \mathbf{1}]$
    $= \mathbf{A}_{aug}\ \mathbf{x}_{aug}$
  - Note the input dimension has increased from K to K + 1
- Many xNN layers take the form of an affine transformation followed by a nonlinearity

Compositions

- Multiple linear transformations can be composed into a single linear transformation
  - $\mathbf{y} = \mathbf{A}_{D-1} \ldots \mathbf{A}_1 \mathbf{A}_0 \mathbf{x}$
    $= \mathbf{A}\,\mathbf{x}$, where $\mathbf{A} = \mathbf{A}_{D-1} \ldots \mathbf{A}_1 \mathbf{A}_0$
- Comments
  - A reason why nonlinearities are included in xNNs
  - Otherwise there would be no depth

Principal Component Analysis

- Note
  - Some of this is dependent on probability for parts of the understanding
- Setup
  - M x K data matrix **X**
  - Each row is a different trial (ex: point in time)
  - Each column is a different measurement from that trial (ex: different stock)
  - Columns are normalized to 0 mean
  - Columns are potentially linearly correlated
- Goal
  - Linearly transform to a new M x K matrix **Y** via a K x K matrix **Q** by **Y** = **X Q**
  - **Q** is chosen such that columns of **Y** are orthogonal and ordered from largest to smallest variance
  - For dimensionality reduction keep first L < K columns

Principal Component Analysis

- Mechanics for finding **Q**
  - Decompose **X** via the SVD as $\mathbf{X} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^T$
  - Select $\mathbf{Q} = \mathbf{V}$ such that $\mathbf{Y} = \mathbf{X}\,\mathbf{Q} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^T\,\mathbf{V} = \mathbf{U}\,\mathbf{S}$

- Example
  - Statistical arbitrage (e.g., SPY, MDY and IJR)
  - Stock 0 time series in col 0, stock 1 time series in col 1, …, stock K – 1 time series in col K – 1
  - 0 th principal component for trend trading (you would keep this for feature extract)
  - K – 1 th principal component for stat arb (throw away for feature extract)

Discrete Fourier Transform

- The DFT is a linear transformation from domain to 1/domain via a projection onto a complex exponential basis: $y(k) = (1/\mathrm{sqrt}(K)) \Sigma_n x(n) e^{-i(2\pi/K)nk}$
  - k = 0, ..., K – 1 and n = 0, ..., K – 1
  - Example domains: time to 1/time = frequency

- Equivalent to a K x K DFT matrix $\mathbf{F}_K$ that transforms input vectors **x** to output vectors **y**
  - $\mathbf{y} = \mathbf{F}_K \mathbf{x}$ where $F_K(a, b) = (1/\mathrm{sqrt}(K)) e^{-i(2\pi/K)ab}$
  - $\mathbf{F}_K$ is a unitary matrix so it's invertible (conj transpose = inverse, called the IDFT)
  - Output is typically circular complex Gaussian (will discuss implications later)
  - Efficient implementations are possible
    - O(K log K) for fast Fourier transform (FFT)
    - Vs $O(K^2)$ for DFT

Discrete Fourier Transform

- Use: data transformation
  - Sometimes it's easier to do feature extraction in the frequency domain vs time domain
    - Common example of this is speech to text
    - DFTs are used for creating MFCCs
  - Unitary so invertible (no information lost (until you read the next bullet point))
    - Effectively lets the network decide what data to keep and what data to throw away

- Use: dimensionality reduction
  - The DFT frequently concentrates the majority of information in naturally occurring signals to $L < K$ basis components
  - A common dimensionality reduction strategy is to keep the L main components and get rid of the rest

CNN Style 2D Convolution

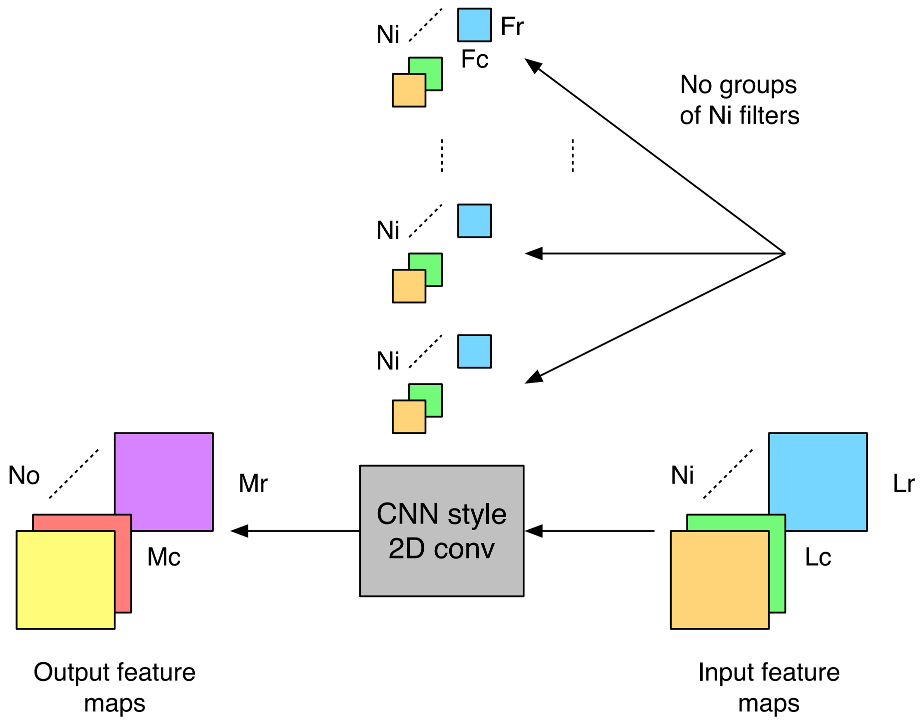
- Common types of filtering / convolution
  - 1D
  - 2D
  - CNN style 2D

- Common methods for speeding up filtering / convolution for various cases
  - Frequency domain
  - Winograd

- This set of slides will only consider CNN style 2D convolution in the time domain
  - 1D and 2D convolution can be viewed as special cases
  - Tensor to matrix lowering for computation is also included

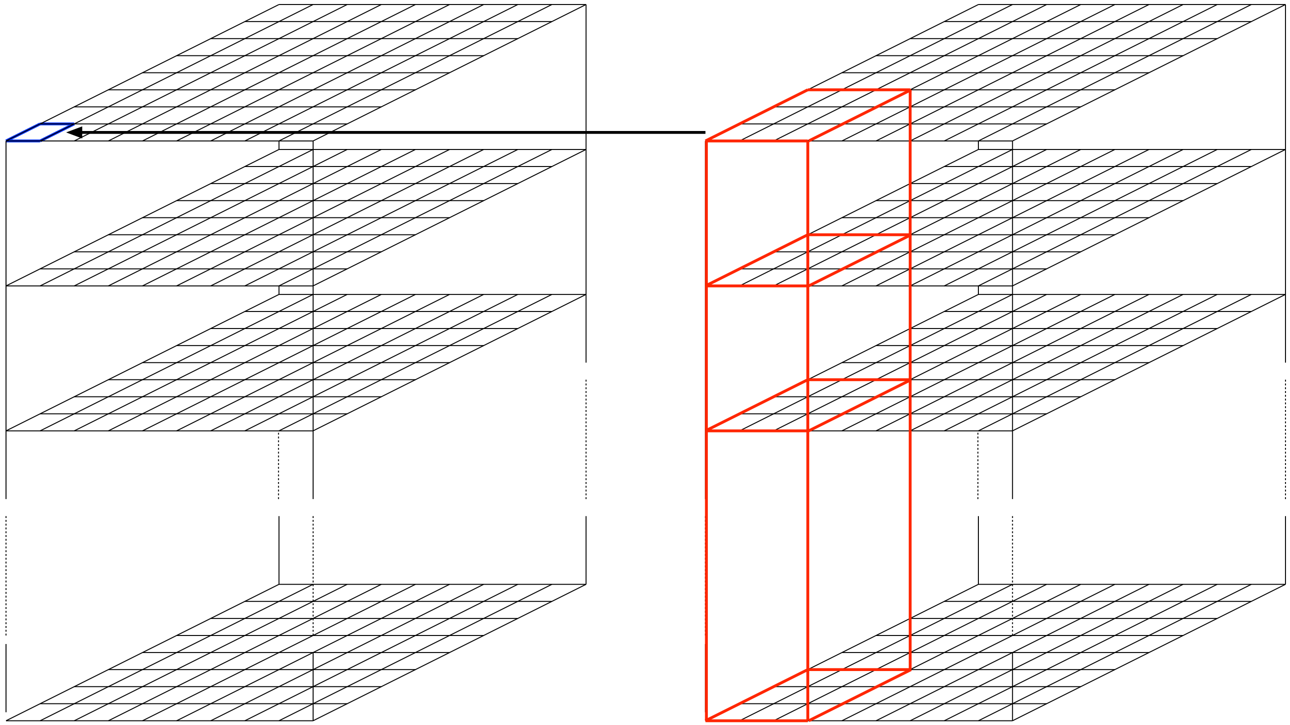
CNN Style 2D Convolution

- Input feature maps
  - 3D tensor
  - N_i inputs x L_r rows x L_c cols
- Filter coefficients
  - 4D tensor
  - N_o outputs x N_i inputs x F_r rows x F_c cols
- Output feature maps
  - 3D tensor
  - N_o outputs x M_r rows x M_c cols



CNN Style 2D Convolution

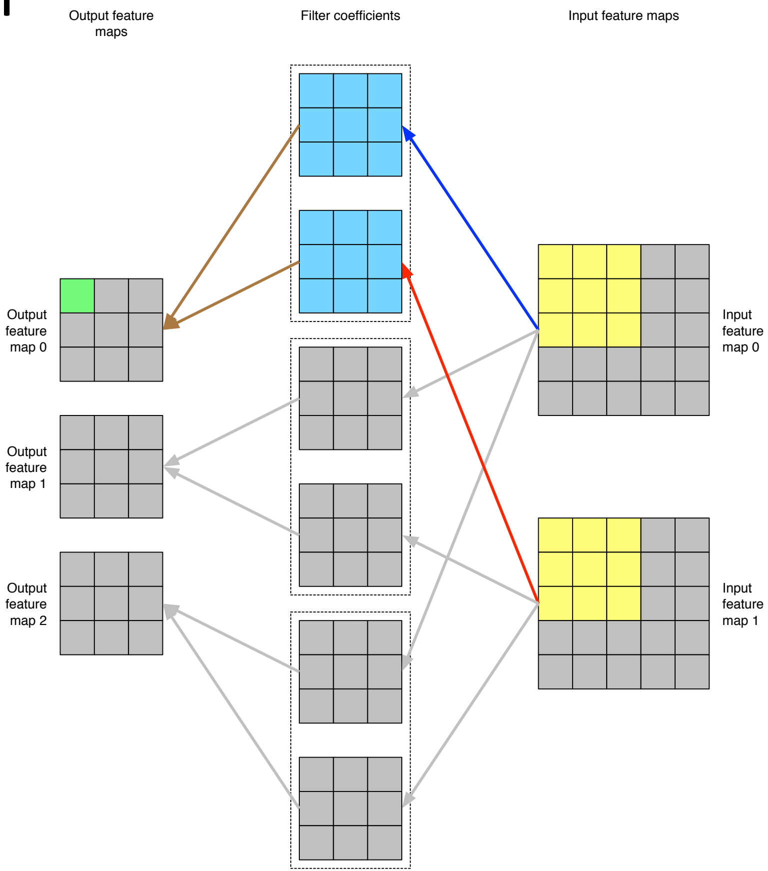
An illustration of the input features used by CNN style 2D convolution with 3x3 filters to produce each output feature



CNN Style 2D Convolution

- An example showing CNN style 2D convolution is matrix matrix multiplication using 2 x 5 x 5 input feature maps, 3 x 2 x 3 x 3 filters and 3 x 3 x 3 output feature maps

- This sequence of figures illustrates the specific set of inputs and filter coefficients used to generate each output



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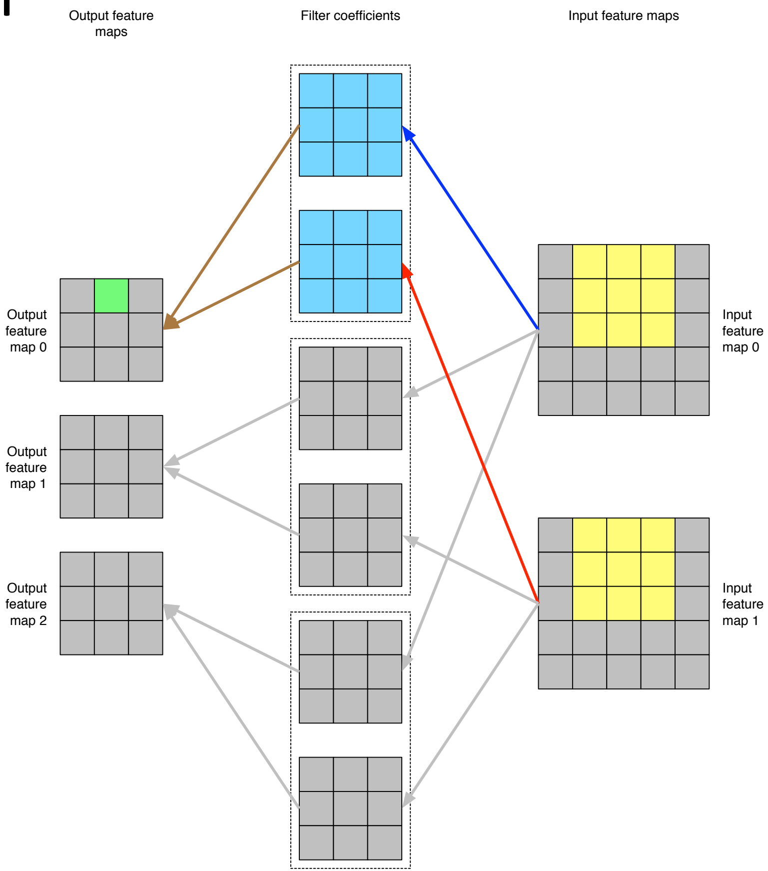

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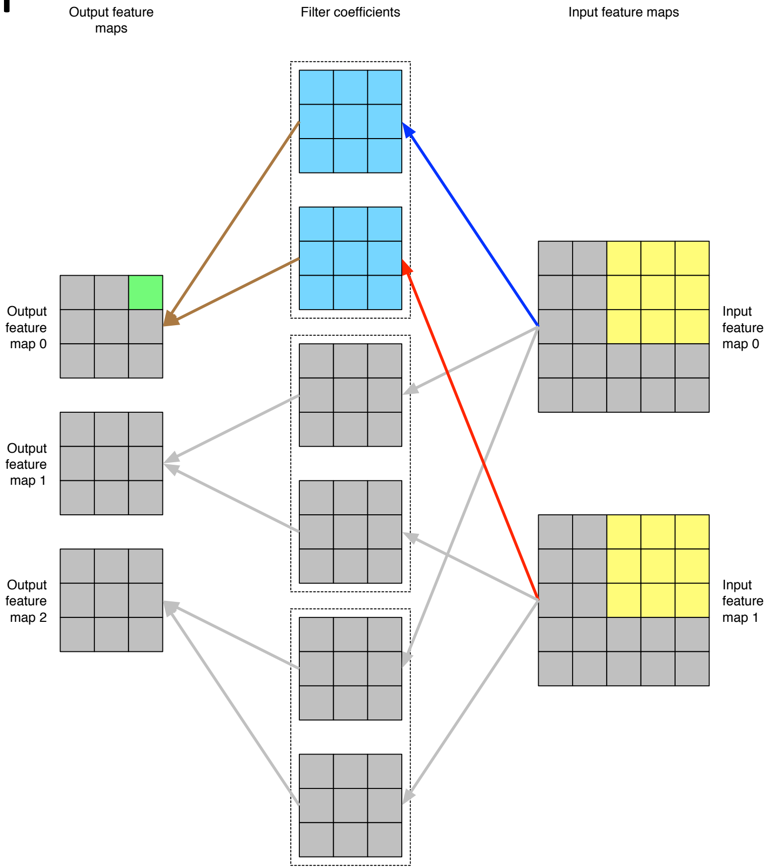

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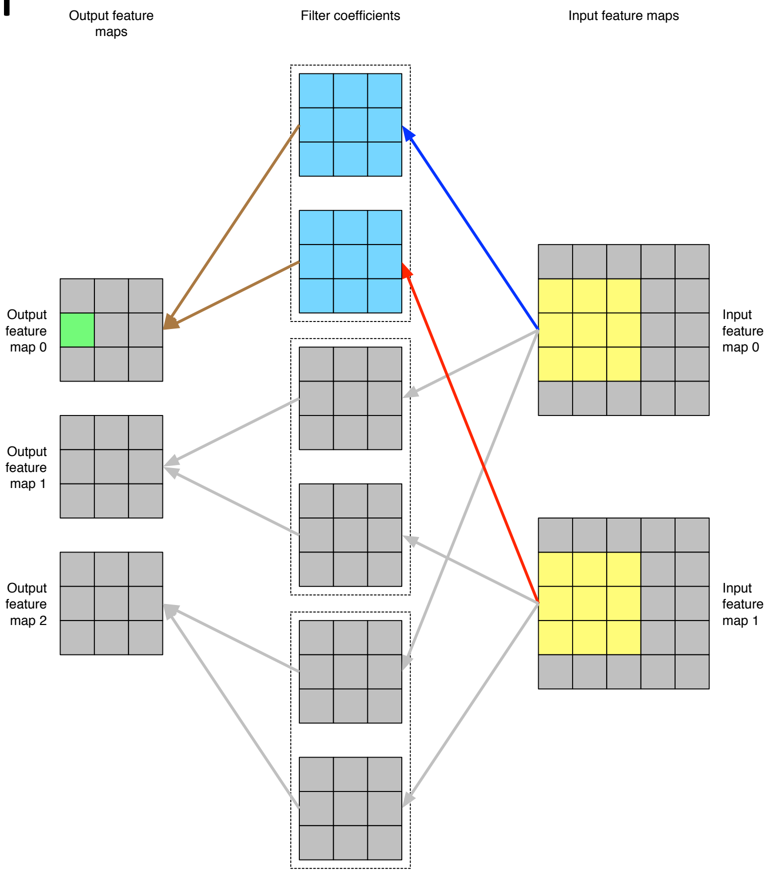

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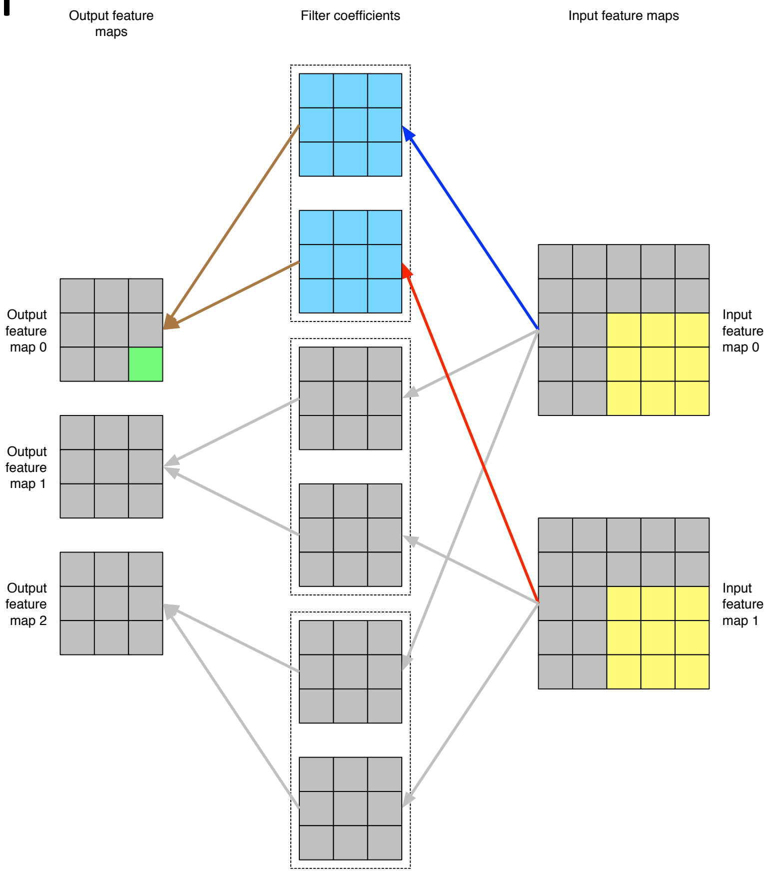

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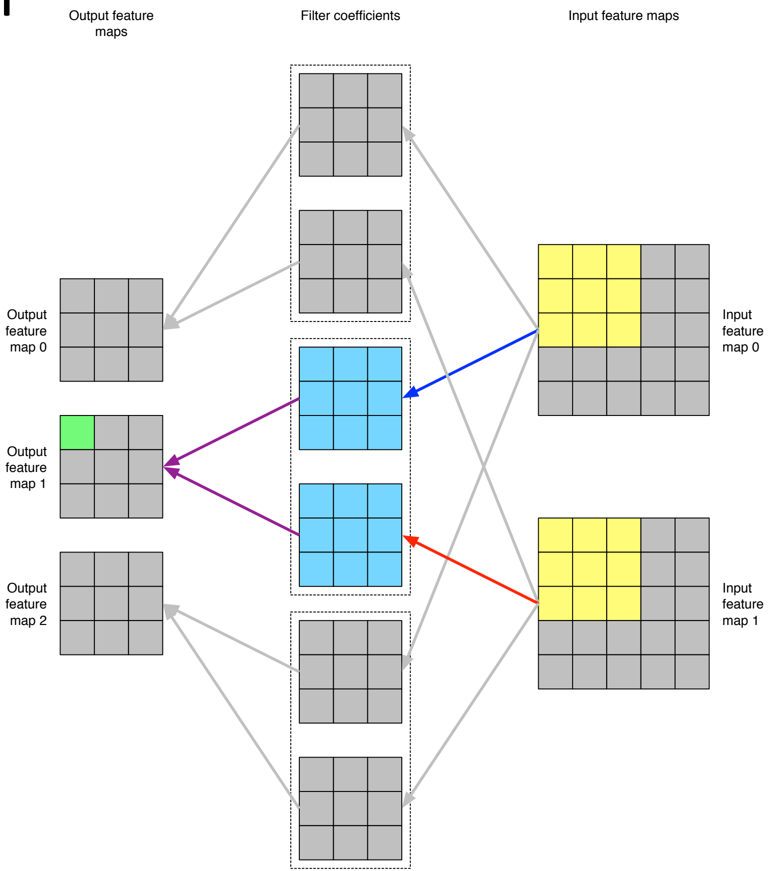

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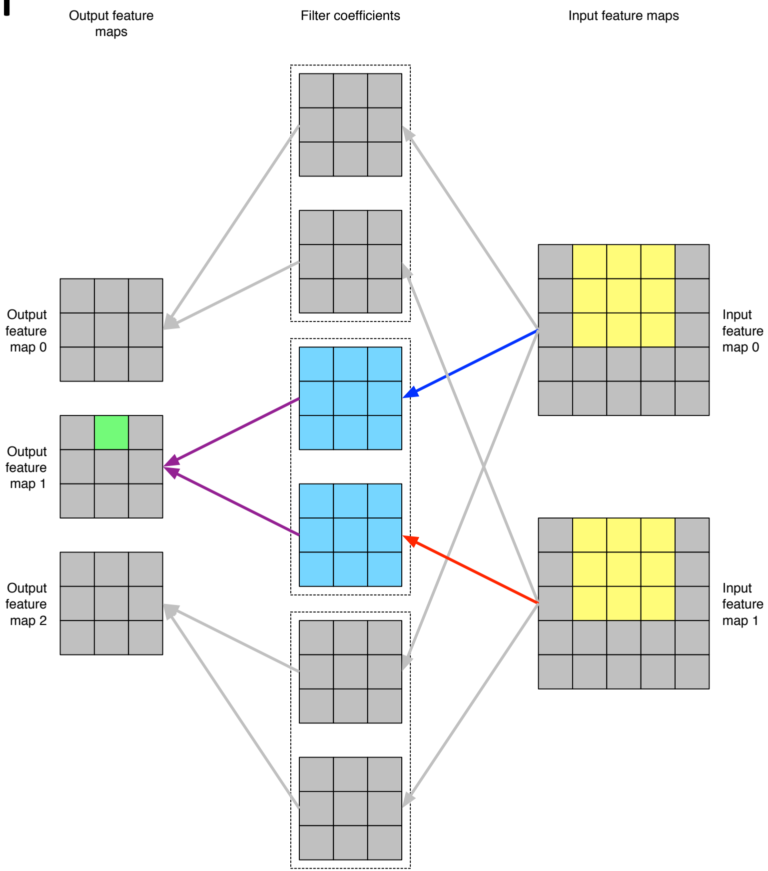

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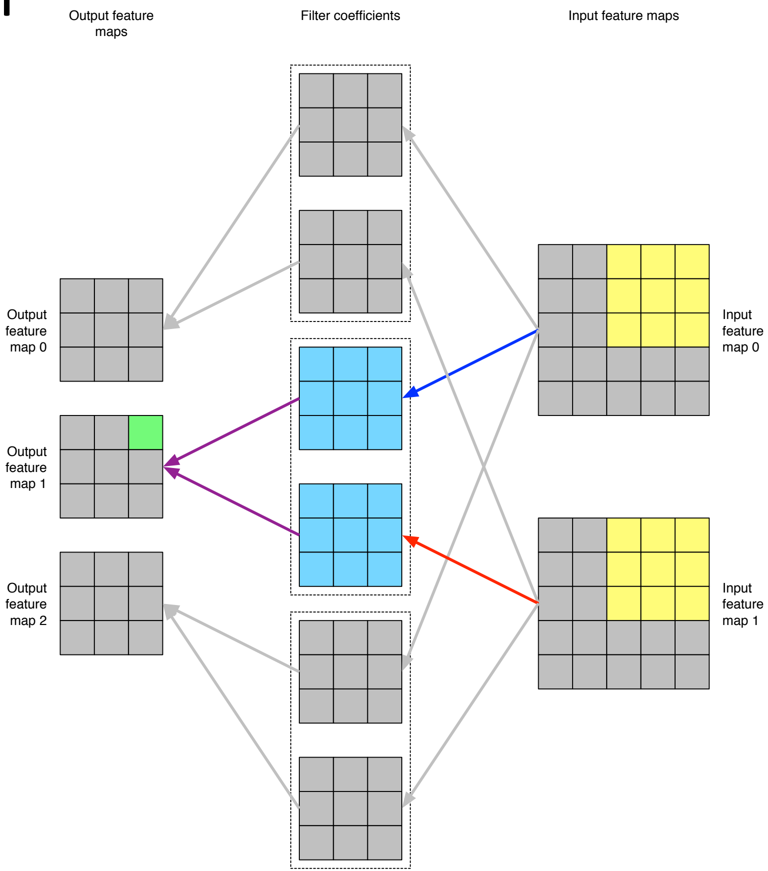

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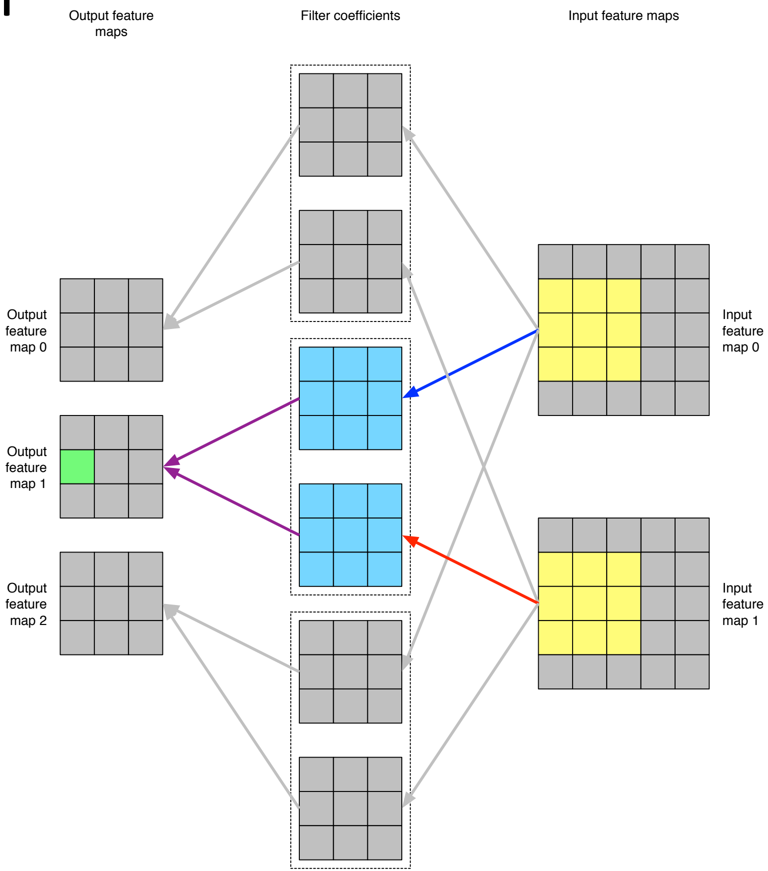

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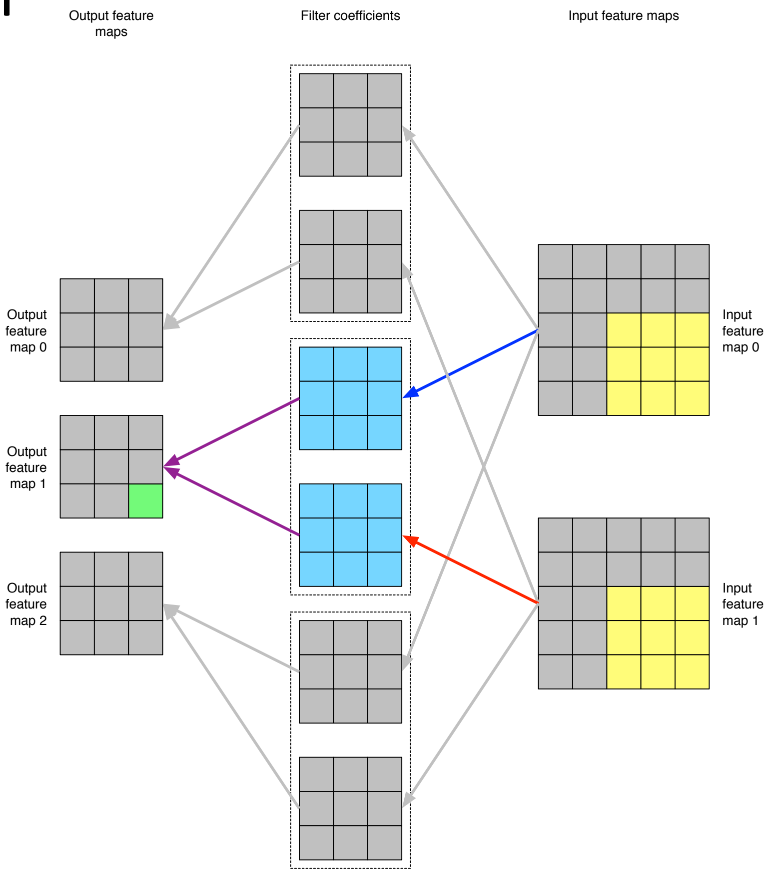

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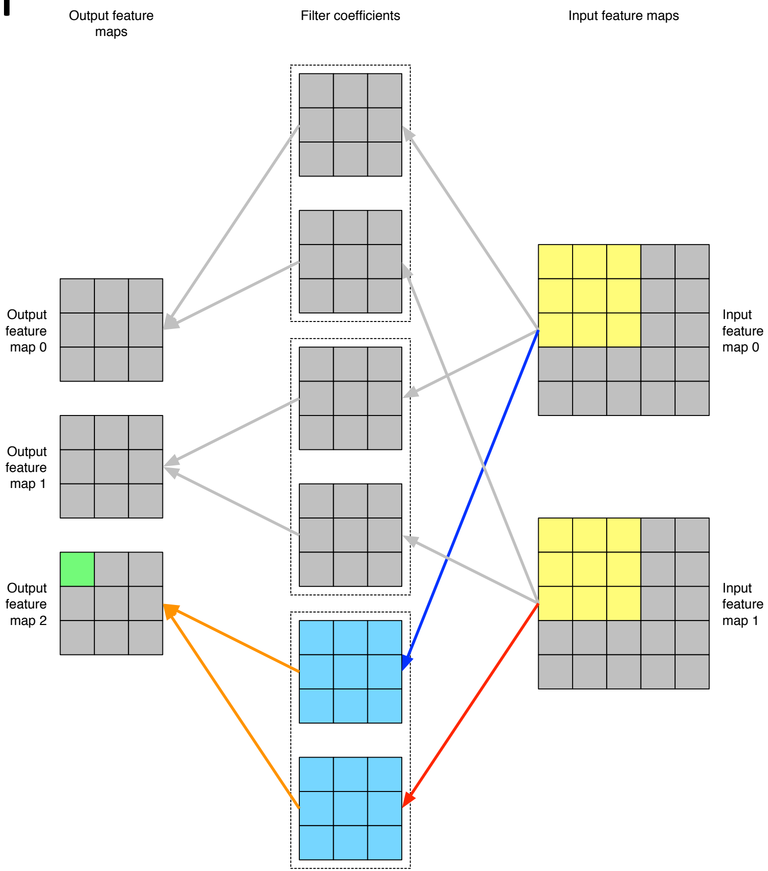

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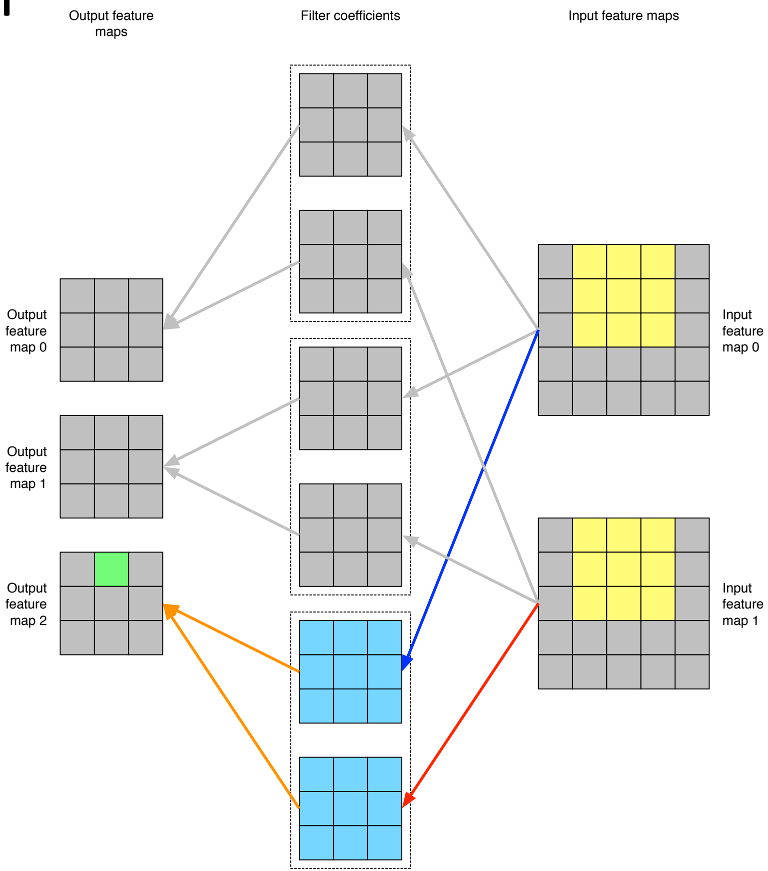

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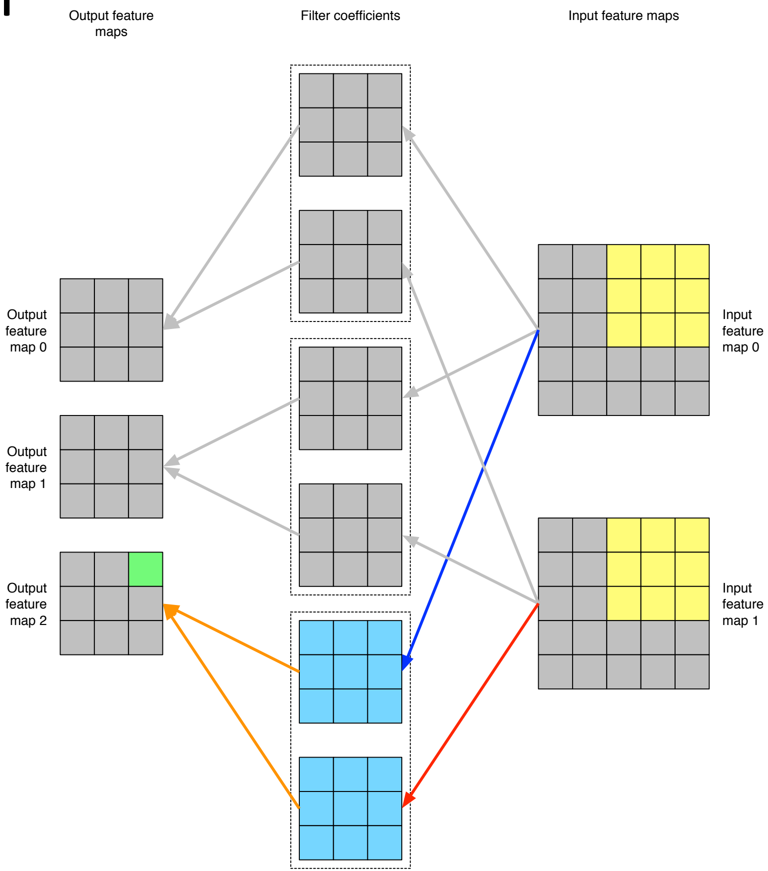

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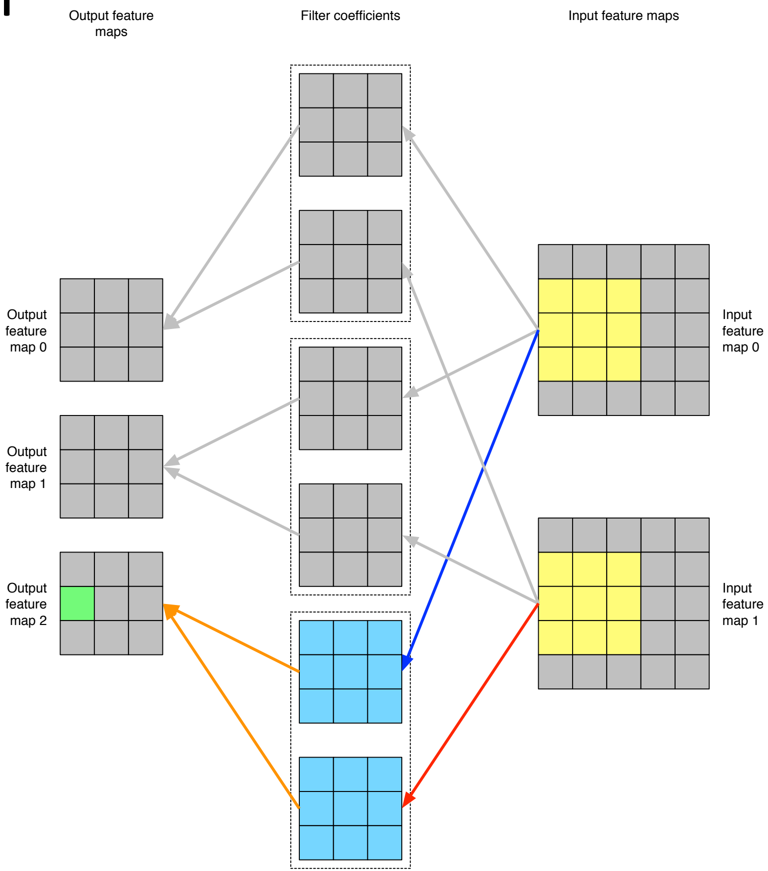

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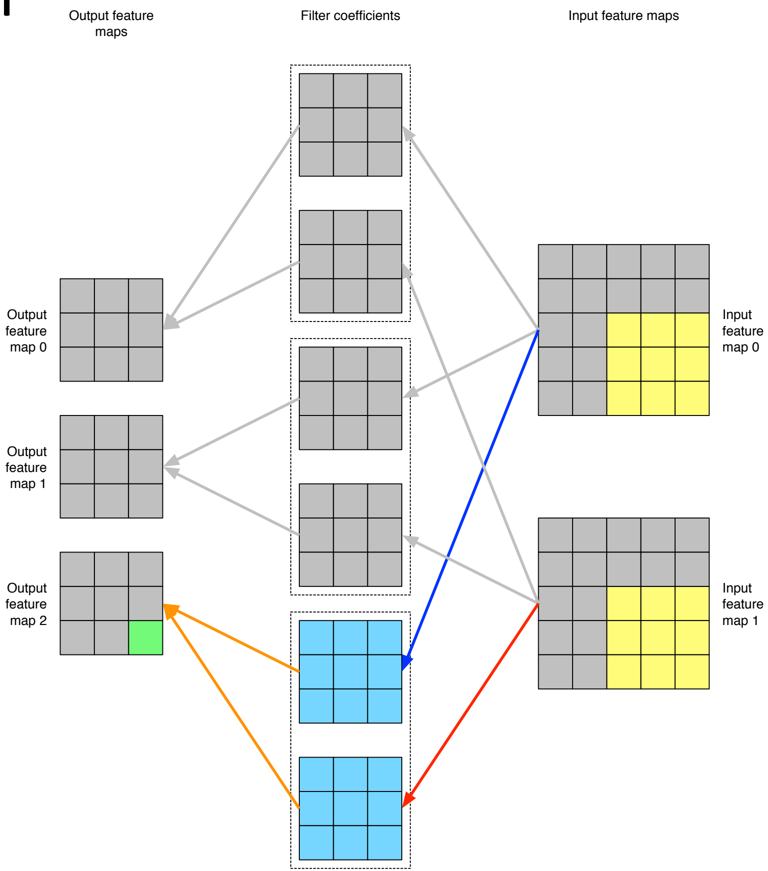


CNN Style 2D Convolution

- Note that 2D correlation is typically used instead of 2D convolution
  - Equivalent with a flip of the filter and indexing change
  - But will still refer to it at CNN style 2D convolution and not CNN style 2D correlation

- Mathematically it's 6 loops (listed from common outer to inner)
  - Output feature map channel $n_o = 0, \ldots, N_o – 1$
  - Output feature map row $m_r = 0, \ldots, L_r – F_r = M_r – 1$
  - Output feature map col $m_c = 0, \ldots, L_c – F_c = M_c – 1$
  - Input feature map channel $n_i = 0, \ldots, N_i – 1$
  - Filter row $f_r = 0, \ldots, F_r – 1$
  - Filter col $f_c = 0, \ldots, F_c – 1$

- For each n_o, m_r and m_c
  - $Y(n_o, m_r, m_c) = \Sigma_{ni}\, \Sigma_{fr}\, \Sigma_{fc}\, H(n_o, n_i, f_r, f_c)\, X(n_i, m_r + f_r, m_c + f_c)$

CNN Style 2D Convolution

- For each n_o, m_r and m_c
    - $Y(n_o, m_r, m_c) = \Sigma_{ni} \Sigma_{fr} \Sigma_{fc} H(n_o, n_i, f_r, f_c) X(n_i, m_r + f_r, m_c + f_c)$
- Can be viewed as an inner product (by expanding the summations)
    - Of a vector formed from N_i F_r F_c filter coefficients
    - With a vector formed from F_r F_c elements of each N_i input feature maps
    - To produce a single output at the corresponding row col of an output feature map
- Repeated
    - For all row col values of the output feature map using the same filter coefficients
    - For all output feature map channels using different filter coefficients for each output feature map channel

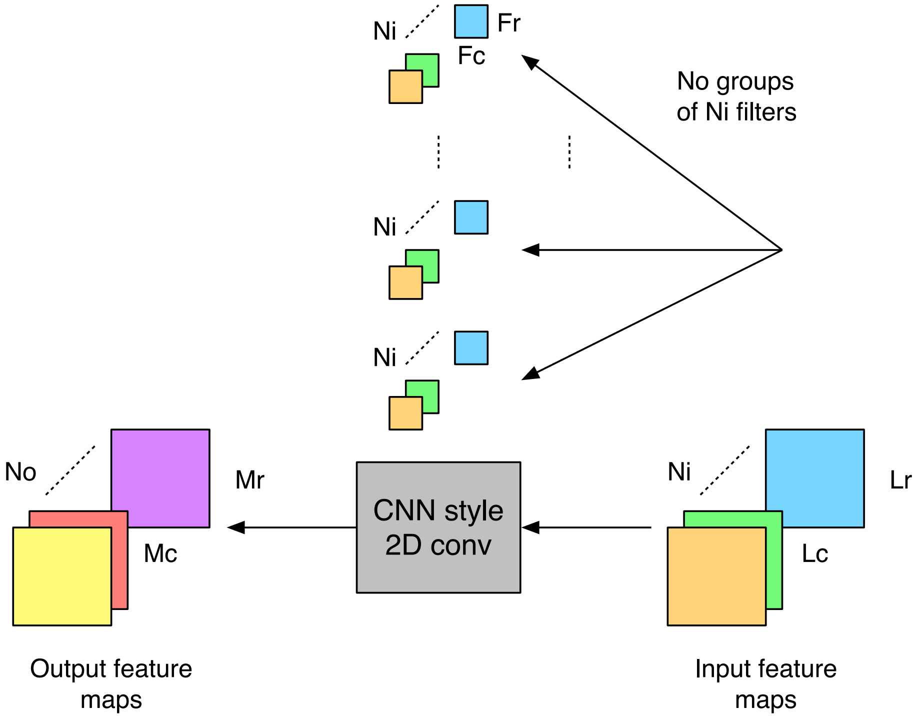
CNN Style 2D Convolution

- High performance implementations of CNN style 2D convolution do not explicitly use 6 loops (but compute the same thing)

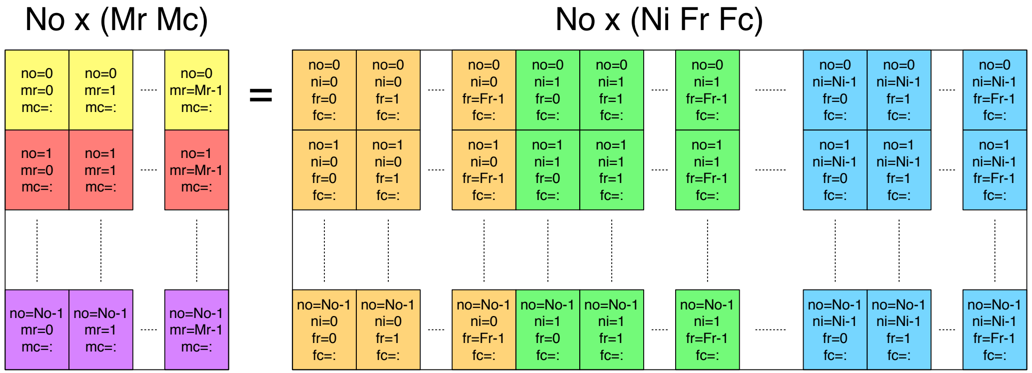
- The key realization is that CNN style 2D convolution can be written as matrix matrix multiplication: $Y^{2D} = H^{2D} X^{2D}$
  - H^{2D} = reshape 4D filter coefficient tensor to 2D matrix
    - Trivial, nothing actually needs to be reshaped in practice
  - X^{2D} = form 3D input feature map tensor into 2D Toeplitz style filtering matrix
    - This is the key
    - Will generate blocks of this on the fly as each input is repeated ~ F_r F_c times
  - Y^{2D} = compute 2D matrix of output feature maps
    - Matrix matrix multiplication is efficient in hardware
    - Trivial to reshape to 3D output feature map tensor, nothing actually needs to be done in practice

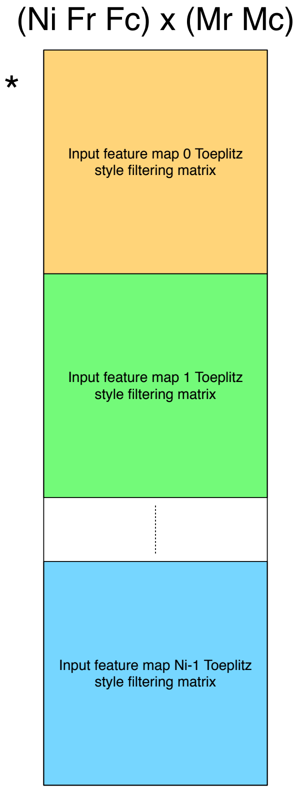
CNN Style 2D Convolution

- Starting point / reminder
- Input feature maps
  - 3D tensor
  - N_i inputs x L_r rows x L_c cols
- Filter coefficients
  - 4D tensor
  - N_o outputs x N_i inputs x F_r rows x F_c cols
- Output feature maps
  - 3D tensor
  - N_o outputs x M_r rows x M_c cols



CNN Style 2D Convolution

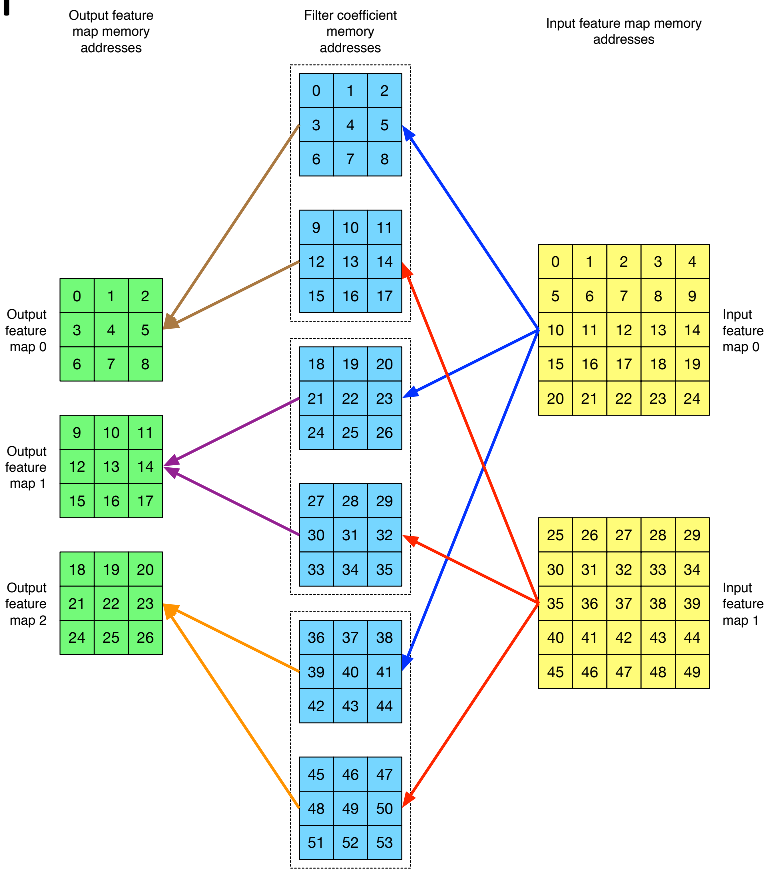




- CNN style 2D convolution written as matrix matrix multiplication
  - Output feature maps (each box is 1 x M_c elements)
  - Filter coefficients (each box is 1 x F_c elements)
  - Input feature maps (ordering not shown)

CNN Style 2D Convolution

- An example showing CNN style 2D convolution is matrix matrix multiplication using 2 x 5 x 5 input feature maps, 3 x 2 x 3 x 3 filters and 3 x 3 x 3 output feature maps
- This figure illustrates memory addresses (specifically offsets to the initial pointer for each array)
- The next page shows where the memory addresses go in matrix matrix multiplication



CNN Style 2D Convolution

0	1	2	3	4	5	6	7	8
9	10	11	12	13	14	15	16	17
18	19	20	21	22	23	24	25	26

Output feature map memory addresses
(note vectorization)

=

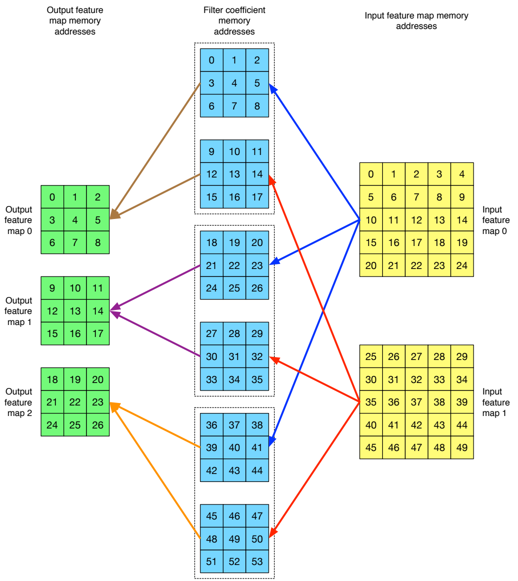
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53

Filter coefficient memory addresses
(note vectorization)

0	1	2	5	6	7	10	11	12
1	2	3	6	7	8	11	12	13
2	3	4	7	8	9	12	13	14
5	6	7	10	11	12	15	16	17
6	7	8	11	12	13	16	17	18
7	8	9	12	13	14	17	18	19
10	11	12	15	16	17	20	21	22
11	12	13	16	17	18	21	22	23
12	13	14	17	18	19	22	23	24
25	26	27	30	31	32	35	36	37
26	27	28	31	32	33	36	37	38
27	28	29	32	33	34	37	38	39
30	31	32	35	36	37	40	41	42
31	32	33	36	37	38	41	42	43
32	33	34	37	38	39	42	43	44
35	36	37	40	41	42	45	46	47
36	37	38	41	42	43	46	47	48
37	38	39	42	43	44	47	48	49

Input feature map memory addresses (note Toeplitz filtering matrix structure)

- Main figure is matrix form
- Small figure is convolution form from previous page for reference



CNN Style 2D Convolution

- Limiting cases illustrated via depth wise separable convolution that splits CNN style 2D convolution into 2 layers
  - Traditional 2D convolution followed by CNN style 2D convolution with 1 x 1 filters
  - Less generality of either vs original, but 1 extra level of depth

- Traditional 2D convolution to mix across space ($N_i = N_o = 1$)
  - Can also get small values of N_i and N_o via grouping
  - Equivalent to vector matrix multiplication
  - Note that K dimension reduces from ($N_i F_r F_c$) to ($F_r F_c$)

- CNN style 2D convolution with 1 x 1 filters to mix across channel
  - Equivalent to standard matrix matrix multiplication
  - Note that K dimension reduces from ($N_i F_r F_c$) to N_i

CNN Style 2D Convolution

0	1	2	3	4	5	6	7	8
9	10	11	12	13	14	15	16	17
18	19	20	21	22	23	24	25	26

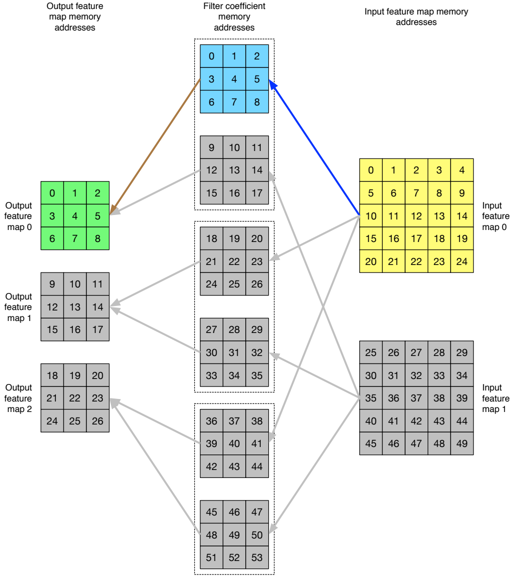
Output feature map memory addresses
(note vectorization)

=

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35
36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53

Filter coefficient memory addresses
(note vectorization)

- Traditional convolution
- Equivalent to vector matrix multiplication



Input feature map memory addresses (note Toeplitz filtering matrix structure)

0	1	2	5	6	7	10	11	12
1	2	3	6	7	8	11	12	13
2	3	4	7	8	9	12	13	14
5	6	7	10	11	12	15	16	17
6	7	8	11	12	13	16	17	18
7	8	9	12	13	14	17	18	19
10	11	12	15	16	17	20	21	22
11	12	13	16	17	18	21	22	23
12	13	14	17	18	19	22	23	24
25	26	27	30	31	32	35	36	37
26	27	28	31	32	33	36	37	38
27	28	29	32	33	34	37	38	39
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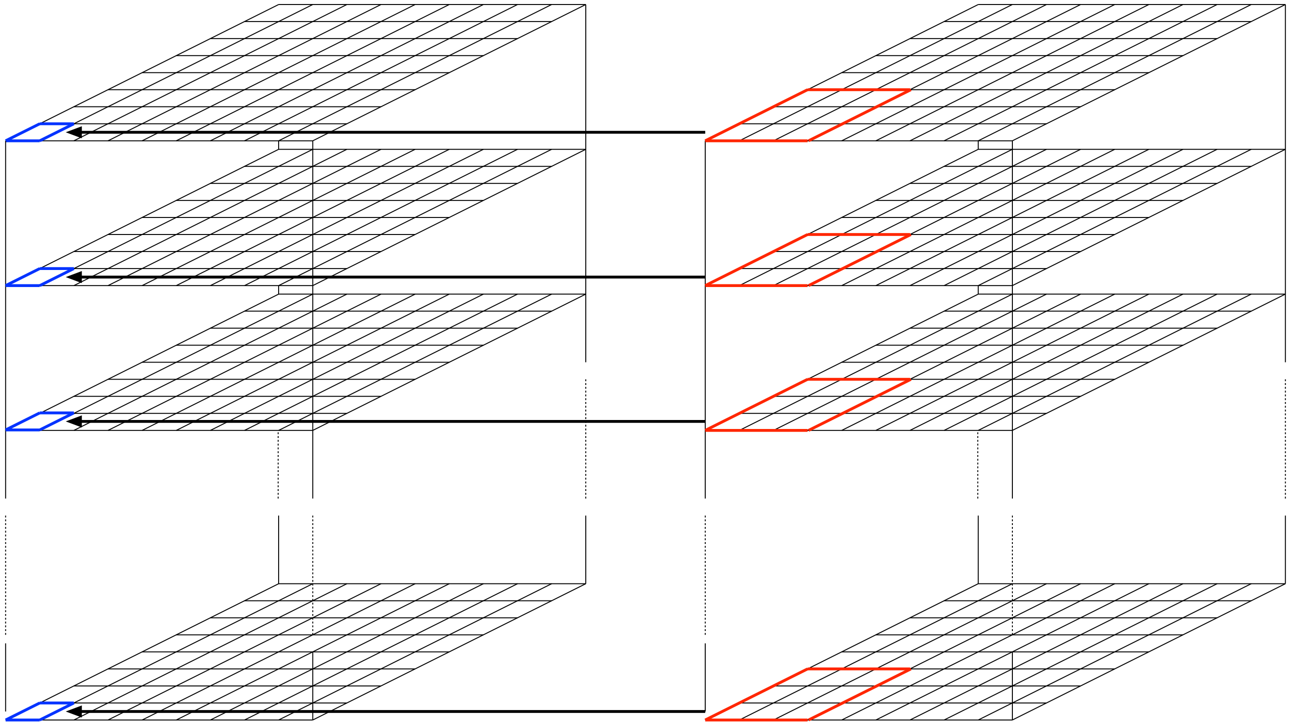
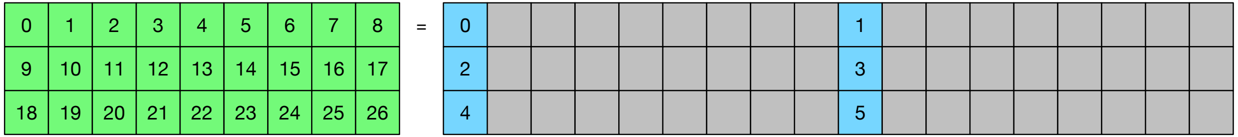
35	36	37	40	41	42	45	46	47
36	37	38	41	42	43	46	47	48
37	38	39	42	43	44	47	48	49

CNN Style 2D Convolution

An illustration of the input features used by traditional 2D convolution with 3x3 filters (equivalent to fully grouped CNN style 2D convolution with 3x3 filters) to produce each output feature

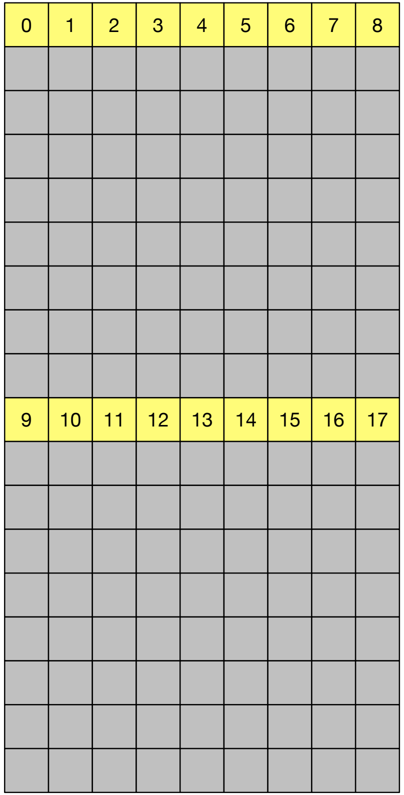


CNN Style 2D Convolution



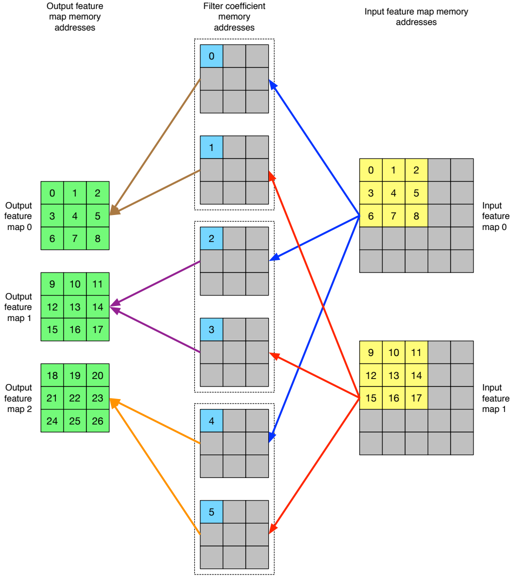
Output feature map memory addresses
(note vectorization)

Filter coefficient memory addresses
(note vectorization)



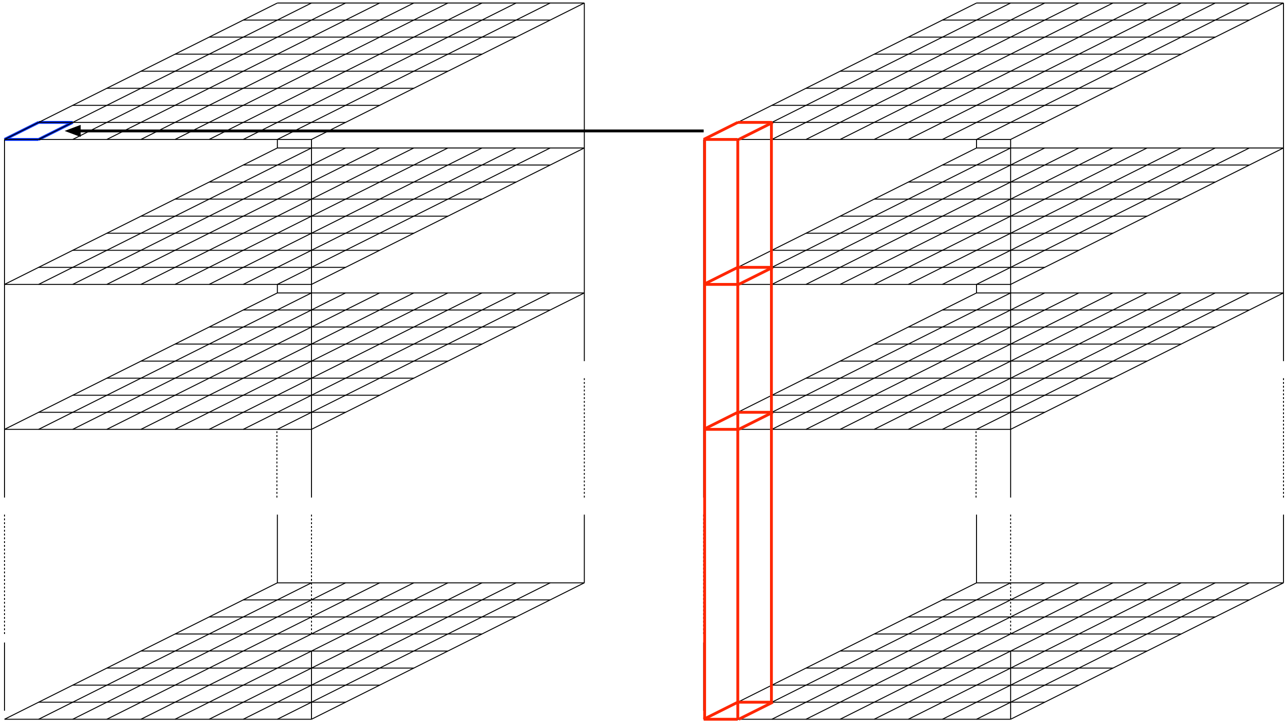
Input feature map memory addresses (note Toeplitz filtering matrix structure)

- CNN style 2D convolution with 1x1 filters
- Equivalent to pure matrix matrix multiplication



CNN Style 2D Convolution

An illustration of the input features used by CNN style 2D convolution with 1x1 filters to produce each output feature



CNN Style 2D Convolution

- Memory
  - Formulas
    - Input feature maps: $N_i \, L_r \, L_c$
    - Output feature maps: $N_o \, M_r \, M_c$
    - Filter coefficients: $N_i \, N_o \, F_r \, F_c$
  - Early in the network feature map memory tends to dominate
  - Deeper in the network filter coefficient memory tends to dominate

- Compute
  - Formula for MACs
    - $(N_o)\,(M_r\,M_c)\,(N_i\,F_r\,F_c) = (N_o\,M_r\,M_c)\,(N_i\,F_r\,F_c)$
      = (number of outputs) (number of input MACs per output)
  - Tends to be highest in the beginning of the network
    - If $(M_r\,M_c)$ is more aggressively reduced than $(N_i\,N_o)$ is increased
  - Scaling the input size by 1/2 in rows and cols ~ reduces compute by 1/4

CNN Style 2D Convolution

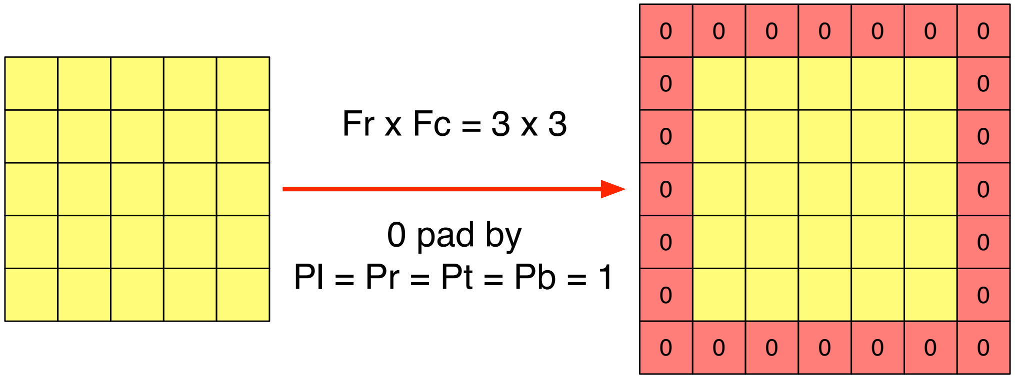
- Arithmetic intensity
  - Compute = $N_i N_o F_r F_c M_r M_c$ (MACs)
  - Data movement = $N_i L_r L_c + N_o M_r M_c + N_i N_o F_r F_c$ (elements)
  - Ratio = compute / data movement

CNN Style 2D Convolution

- Alternate view of CNN style 2D convolution
  - Add together Fr x Fc CNN style 2D convolutions with 1x1 filter size
    - Reminder: CNN style convolution with 1x1 filters is pure matrix matrix multiplication
    - Input size is reduced to Mr x Mc for each with an appropriate shift / offset of the original input
  - Tradeoffs
    - Advantage of simpler input feature map matrix structure and associated data movement logic
    - Drawback of additional input feature map memory movement
  - Side benefit: useful for understanding back propagation through a CNN style 2D convolution layer

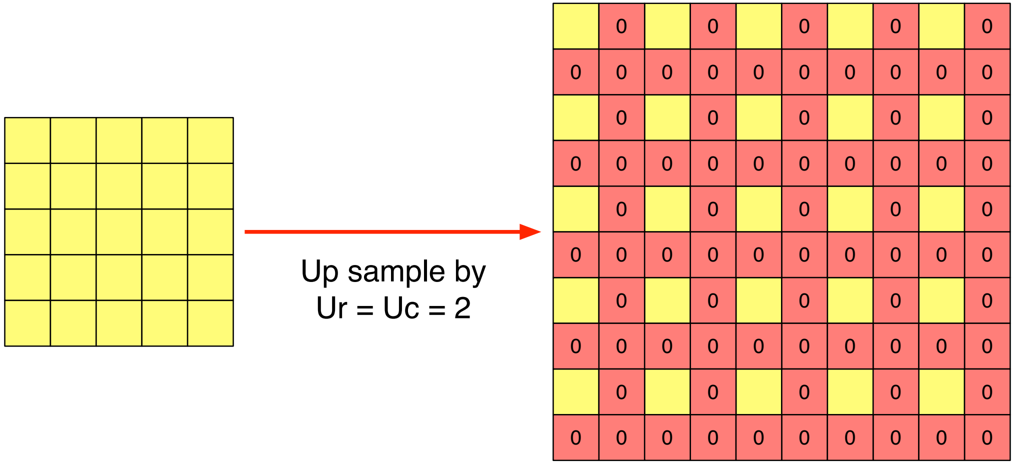
CNN Style 2D Convolution

- Variant: input feature map 0 padding
  - P_l left, P_r right, P_t top, P_b bottom
  - Typically $P_l + P_r = F_c - 1$ and $P_t + P_b = F_r - 1$
  - Used for same size input / output feature maps
  - Implementation key is efficient 0 insert



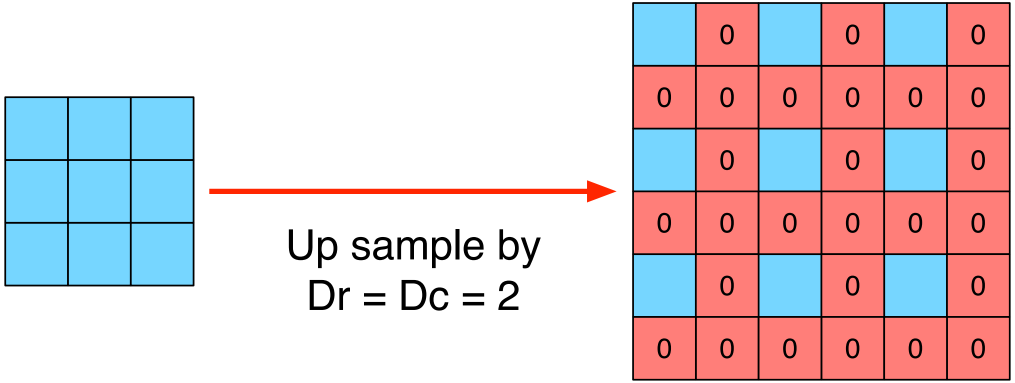
CNN Style 2D Convolution

- Variants: input feature map up sampling
  - U_r rows, U_c cols
  - Typically called transposed convolution, fractionally strided convolution or deconvolution
  - Used in decoder style head designs
  - Implementation key is input memory reuse
  - Alternatives are bilinear and nearest neighbor interpolation



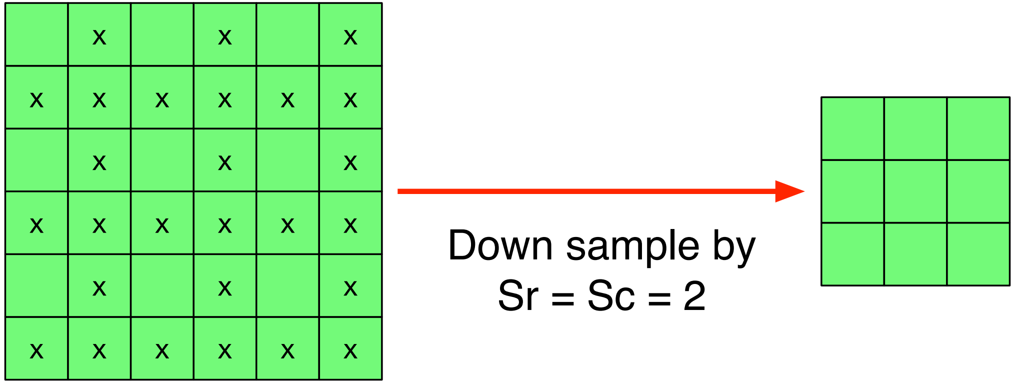
CNN Style 2D Convolution

- Variants: filter coefficient up sampling
  - D_r rows, D_c cols
  - Typically called dilated or Atrous convolution
  - Used to maintain spatial resolution with large receptive field
  - Implementation key is input feature map filtering matrix row removal



CNN Style 2D Convolution

- Variants: output feature map down sampling
  - S_r rows, S_c cols
  - Typically called strided convolution
  - Used to reduce spatial resolution
  - Implementation key is input feature map filtering matrix column removal
  - Alternative is pooling



Layers Built From Linear Transforms

Purpose

- You design a network to accomplish a goal
  - Don't ever lose sight of this
  - Network design is not arbitrary
  - So it always makes sense to stop and think how the operations you're including help you accomplish the goal you're trying to achieve
- Ask yourself
  - Why do xNNs include these layers?
  - How do these layers map from data to features to predictions?
  - Pay attention to how the input features are combined to generate output features
- The purpose of the next few slides is to introduce layers which include linear transformations and help build intuition on how they map from data to features to classes

Densely Connected Layer

- Densely connected or fully connected layer
  - **y** = f(**H x** + **v**)
  - **H x** is multiplication of a M x K matrix **H** with a K x 1 input vector **x** (batching will add a dim to **x**)
  - **v** is a M x 1 bias vector
  - f is a (sub) differential pointwise nonlinearity
    - ReLU: 0 out the negative values and pass the positive unchanged
    - Sigmoid: monotonic nonlinear map to (0, 1)
    - Tanh: monotonic nonlinear map to (-1, 1)
    - ...: many other options possible
  - **y** is a M x 1 output vector (batching will add a dim to **y**)

- A traditional neural network is composed of multiple densely connected layers
  - Transform from data to weak features
  - Transform from weak features to strong features
  - Transform from strong features to classes

Densely Connected Layer

- Some intuition of feature extraction and prediction for a densely connected layer
  - Sometimes linear classification is viewed as template matching where each row is a different template and the predicted class is the maximum output
- The inner product depends on magnitude and angle
  - Inner product definition reminder: $\langle \mathbf{a}, \mathbf{b} \rangle = ||\mathbf{a}||_2 \, ||\mathbf{b}||_2 \cos(\theta)$
- Each linearly extracted output feature is the inner product of a row of **H** and the input **x**
  - $z(m) = \mathbf{H}(m, :)\, \mathbf{x}$
  - $z(m)$ is the extracted feature or prediction
  - $\mathbf{H}(m, :)$ is the feature extractor or predictor
  - $\mathbf{x}$ is the input

Densely Connected Layer

- How strong or important is a feature extractor? $||\mathbf{H}(m, :)||_2$
  - Note that the input mag contributes the same to each extracted feature $||\mathbf{x}||_2$
  - So here input magnitude only matters relative to bias
  - But input magnitude will also matter for network structures with branches that come together
  - Input magnitude will also matter when the same feature extractor is applied to different inputs

- How aligned is the feature extractor with the input? θ
  - In same direction: positive feature
  - Orthogonal: 0 feature
  - In opposite direction: negative feature

Densely Connected Layer

- Intuition of bias
  - Affine transformation
  - Allows the dividing line to shift
  - Implementation as a rank 1 outer product
  - Will use bias in a constructive variant of the universal approximation proof
- Intuition of ReLU
  - Removes negatively aligned features or predictions
  - Allows depth
  - Subsequent layers combine positively aligned extracted features
- Intuition of other nonlinearities
  - Also allow depth
  - Sigmoid acts as a gate
  - Tanh acts as a positive / negative map

Densely Connected Layer

- Intuition of the size of K (input length) and M (output length)
  - Small K to large M
    - Different combinations of a small number of features to predict a large number of classes
  - Large K to small M
    - 1 feature or a combination of features to predict a small number of classes is now possible
  - Example: ImageNet classification and final fully connected layer size
  - Example: the game of 20 questions

Densely Connected Layer

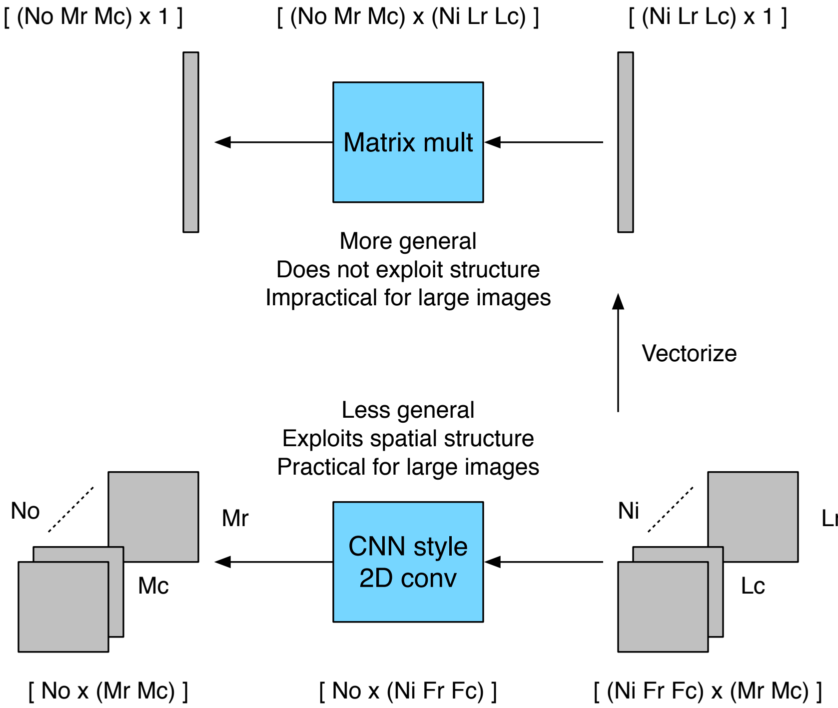
- In general, for the final classification layer, it's better to have K > M
  - Classification goal is to create matrix and bias that takes K features and makes the correct 1 of the M elements at the output much larger (closer to + ∞) than all the others
  - To get a feel for this consider 2 extreme cases
    - 2 features K linearly combined + bias then ReLU to predict 200 classes M
    - 200 features K linearly combined + bias then ReLU to predict 2 classes M
  - Create example features, matrices and biases for both cases
  - Look at sensitivity of the prediction to errors in the features for each
    - Can relate to matrix condition number
    - Show the condition number of K > M is always less than that of K < M
    - Now vary K and M and show diminishing returns after some point too
    - Generalize to considerations in a hierarchical head design

CNN Style 2D Convolution Layer

- CNN style 2D convolution layer
  - $\mathbf{Y}^{3D} = f(\mathbf{H}^{4D} \circledast \mathbf{X}^{3D} + \mathbf{V}^{3D})$
  - $\mathbf{H}^{4D} \circledast \mathbf{X}^{3D}$ is CNN style 2D convolution of a N_o x N_i x F_r x F_c tensor $\mathbf{H}^{4D}$ with a N_i x L_r x L_c input vec $\mathbf{X}^{3D}$
  - $\mathbf{V}^{3D}$ is a N_o x M_r x M_c bias tensor that is a constant for each output feature map
  - f is a pointwise nonlinearity as in the case of a densely connected layer with ReLU being common
  - $\mathbf{Y}^{3D}$ is a N_o x M_r x M_c output tensor
  - Batching can be thought of as adding a loop that applies this layer to multiple input / output pairs resulting in the addition of a dimension to X and Y after concatenation
    - $\mathbf{X}^{4D}$ is a B x N_o x M_r x M_c output tensor
    - $\mathbf{Y}^{4D}$ is a B x N_o x M_r x M_c output tensor
- A traditional CNN is composed of CNN style 2D convolution layers (in addition to other layer types and branching structures)
  - Transform from data to weak features
  - Transform from weak features to strong features

CNN Style 2D Convolution Layer

- Why use CNN style 2D convolution instead of vectorizing the input?
- Consider applying a standard neural network to an image
  - Dimensions / memory / arithmetic intensity make it unreasonable to apply normal neural network linear layer to large images
- Use CNN style 2D convolution layer instead
  - It's a less general transformations but if the input / problem has translational invariance then perhaps the loss of generality is ok
  - Very high (but not unreasonable) memory and compute for modern hardware



CNN Style 2D Convolution Layer

- Intuition of feature extraction
  - CNN style 2D convolution is a linear transformation
  - Output feature maps matrix = filter coefficient matrix * input feature maps filtering matrix
  - Matrix vector multiplication as used in a fully connected layer of a neural network had the intuition of matching features to inputs over channel
  - For CNN style 2D convolution it has the intuition of matching features to inputs over channel and space
    - How far can it see in space? For 1 layer? For repeated layers?
    - How many features does it work over?

CNN Style 2D Convolution Layer

- Intuition of bias
    - Add a constant to all elements in an output feature map
    - Can be a different constant for each output feature map
    - Affine transformation
    - Allows the dividing line to shift
    - Implementation using a rank 1 outer product

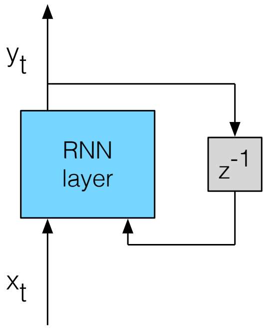
- Intuition of ReLU
    - Removes negatively aligned features or predictions
    - Allows depth
    - Subsequent layers combine positively aligned extracted features

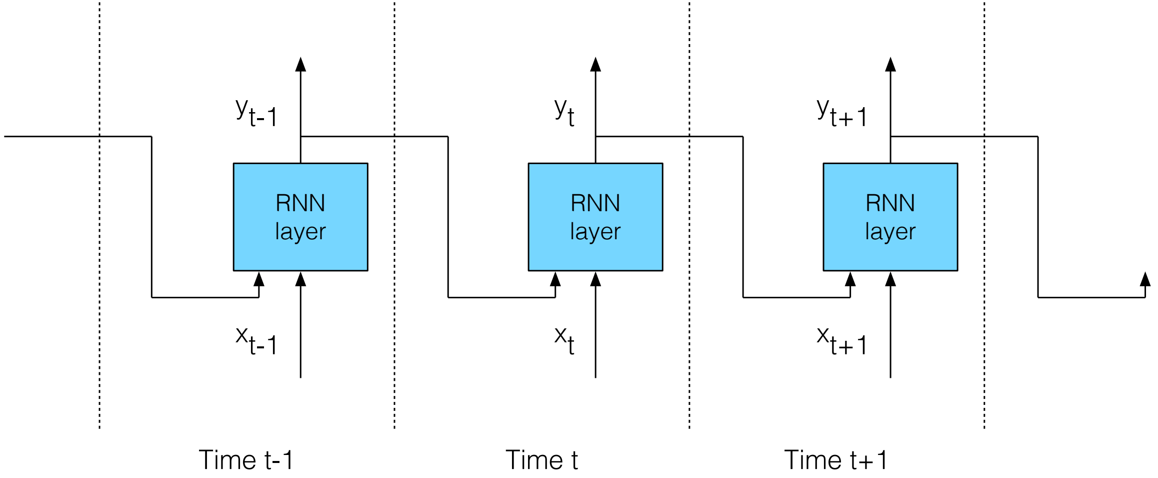
RNN Layer

- RNN layer
  - $\mathbf{y}_t = f(\mathbf{H}\,\mathbf{x}_t + \mathbf{G}\,\mathbf{y}_{t-1} + \mathbf{v})$
  - t is the current time step, t – 1 is the previous time step
  - $\mathbf{H}\,\mathbf{x}_t$ is multiplication of a M x K matrix **H** with a K x 1 input vector $\mathbf{x}_t$
  - $\mathbf{G}\,\mathbf{y}_{t-1}$ is multiplication of a M x M matrix **G** with a M x 1 previous output vector $\mathbf{y}_{t-1}$
  - **v** is a M x 1 bias vector
  - f is a pointwise nonlinearity as in the case of a densely connected layer
  - $\mathbf{y}_t$ is a M x 1 current output vector
- A traditional RNN is composed of multiple RNN layers
  - Transform from data to weak features to strong features
  - All sorts of structural configurations: stacked, bi directional, pyramidal
  - All sorts of variants to improve memory: GRU, LSTM
  - These will be discussed in later lectures in the context of speech and language

RNN Layer

A RNN layer illustrated with feedback (left) and unwrapped in time (right)





RNN Layer

- RNN intuition
  - Current output features are dependent on features extracted from the input and features extracted from the previous output
  - So it’s like a densely connected layer with the addition of a term that depends on the previous output
  - This allows for information to flow sequentially

Attention Based Layer

- Attention layer
  - $\mathbf{X}$ is a K x N input and $\mathbf{h}_m$ is a K x 1 key at position m
  - $\mathbf{a}_m^T = \mathbf{h}_m^T \mathbf{X}$ is a 1 x N attention score for position m
  - $\boldsymbol{\alpha}_m = \text{softmax}(\mathbf{a}_m)$ is a N x 1 attention distribution for position m
  - $\mathbf{y}_m = \mathbf{X} \boldsymbol{\alpha}_m$ is a K x 1 output

For now think of softmax() as a function that input vectors to a probability mass function (a vector whose elements are non negative and sum to 1)

More details will be given in the calculus and probability lectures

- This is just scratching the surface of attention and there are many possibilities
  - Different scoring functions (dot product shown above)
  - Different input windows (global / soft, local / hard fixed and adaptive)
  - Breaking the input into separate values and queries for use with the key
  - Single and multi head
  - Choice of key and binding location for the output
- An attention layer frequently connects an encoder and decoder or is used in self attention for feature encoding

Attention Based Layer

- Attention intuition
  - Depending on what you're interested in you focus on different things
    - Different parts of an image for captioning
    - Different parts of a sound waveform for speech to text transduction
    - Different parts of a sentence for language to language translation
  - Attention provides a way of doing this
  - The output is a weighted combination of inputs based on a key (what you're interested in)

Average Pooling

- Average pooling maps a region of an input feature map to a single value that's the average of the elements in that region
  - Local average pooling repeats this process across the whole input feature map in a periodic pattern
    - Implicitly a down sampling mechanism
    - Occasionally used between convolutional building blocks (though max pooling is more common)
  - Global average pooling averages a whole input feature map to a single value
    - Frequently used between convolutional layers and a final densely connected layer in a classification network
    - Aggregates all spatial information, loses all spatial resolution

32	36	68	56	72	48
8	40	64	84	80	12
28	96	92	76	16	4
52	88	44	20	60	24

Local avg pool ↓ 2x2 / 2

29	68	53
66	58	26

References

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