DM587

Scientific Programming

Numerical Methods
LU Factorization

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[*Based on slides by Lieven Vandenberghe, UCLA*]

Outline

1. Operation Count

2. LU Factorization

3. Other Topics

In solving large scale-linear systems, Gaussian elimination and Gauss-Jordan elimination are not suitable because of:

- computer roundoff errors
- memory usage
- speed

Computer methods are based on LU decomposition.

Outline

1. Operation Count
2. LU Factorization
3. Other Topics

Complexity of matrix algorithms

- flop counts
- vector-vector operations
- matrix-vector product
- matrix-matrix product

Floating point numbers

$$x = m \cdot \beta^e \; ; \qquad l \leq e \leq u$$

with mantissa m, base β, and exponent e

$$m = \pm d_0.d_1 d_2 \cdots d_t \;\; , \quad 0 \leq d_i < \beta$$

	β	t	l	u
IEEE SP	2	23	-126	127
IEEE DP	2	52	-1022	1023
Cray	2	48	-16383	16384
HP calculator	10	12	-499	499
IBM mainframe	16	6	-64	63

Flop counts

floating-point operation (flop)

- one floating-point addition, subtraction, multiplication, or division
- other common definition: one multiplication followed by one addition

flop counts of matrix algorithm

- total number of flops is typically a polynomial of the problem dimensions
- usually simplified by ignoring lower-order terms

applications

- a simple, machine-independent measure of algorithm complexity
- not an accurate predictor of computation time on modern computers

Vector-vector operations

- inner product of two n-vectors

$$\boldsymbol{x}^T\boldsymbol{y} = x_1y_1 + x_2y_2 + \ldots + x_ny_n$$

n multiplications and $n-1$ additions $= 2n$ flops ($2n$ if $n \gg 1$)

- addition or subtraction of n-vectors: n flops
- scalar multiplication of n-vector : n flops

Matrix-vector product

matrix-vector product with $m \times n$-matrix A:

$$\boldsymbol{y} = A\boldsymbol{x}$$

m elements in y; each element requires an inner product of length n:

$$(2n-1)m \text{ flops}$$

approximately $2mn$ for large n special cases

- $m = n$, A diagonal: n flops
- $m = n$, A lower triangular: $n(n+1)$ flops
- A very sparse (lots of zero coefficients): $\#\mathit{flops} \ll 2mn$

Matrix-matrix product

product of $m \times n$-matrix A and $n \times p$-matrix B:

$$C = AB$$

mp elements in C; each element requires an inner product of length n:

$$mp(2n-1) flops$$

approximately $2mnp$ for large n.

Approximate Cost for an $n \times n$ Matrix A with Large n	
Algorithm	**Cost in Flops**
Gauss–Jordan elimination (forward phase)	$\approx \frac{2}{3}n^3$
Gauss–Jordan elimination (backward phase)	$\approx n^2$
LU-decomposition of A	$\approx \frac{2}{3}n^3$
Forward substitution to solve $L\mathbf{y} = \mathbf{b}$	$\approx n^2$
Backward substitution to solve $U\mathbf{x} = \mathbf{y}$	$\approx n^2$
A^{-1} by reducing $[A \mid I]$ to $[I \mid A^{-1}]$	$\approx 2n^3$
Compute $A^{-1}\mathbf{b}$	$\approx 2n^3$

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Overview

- factor-solve method
- LU factorization
- solving $Ax = b$ with A nonsingular
- the inverse of a nonsingular matrix
- LU factorization algorithm
- effect of rounding error
- sparse LU factorization

Definitions

Definition (Triangular Matrices)

An $n \times n$ matrix is said to be upper triangular if $a_{ij} = 0$ for $i > j$ and lower triangular if $a_{ij} = 0$ for $i < j$. Also A is said to be triangular if it is either upper triangular or lower triangular.

Example:

$$\begin{bmatrix} 3 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 4 & 3 \end{bmatrix} \qquad \begin{bmatrix} 3 & 5 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 7 \end{bmatrix}$$

Definition (Diagonal Matrices)

An $n \times n$ matrix is diagonal if $a_{ij} = 0$ whenever $i \neq j$.

Example:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Multiple right-hand sides

two equations with the same matrix but different right-hand sides

$$Ax = b, \qquad A\tilde{x} = \tilde{b}$$

- factor A once (f flops)
- solve with right-hand side b (s flops)
- solve with right-hand side $\tilde{b}$ (s flops)

cost: $f + 2s$ instead of $2(f + s)$ if we solve second equation from scratch

conclusion: if $f \gg s$, we can solve the two equations at the cost of one

LU factorization

LU factorization without pivoting

$$A = LU$$

- L unit lower triangular, U upper triangular
- does not always exist (even if A is nonsingular)

LU factorization (with row pivoting)

$$A = PLU$$

- P permutation matrix, L unit lower triangular, U upper triangular
- exists if and only if A is nonsingular (see later)

cost: $(2/3)n^3$ if A has order n

Solving linear equations by LU factorization

solve $Ax = b$ with A nonsingular of order n

factor-solve method using LU factorization

1. factor A as $A = PLU$ ($(2/3)n^3$ flops)
2. solve $(PLU)x = b$ in three steps
   - permutation: $z_1 = P^T b$ (0 flops)
   - forward substitution: solve $Lz_2 = z_1$ (n^2 flops)
   - back substitution: solve $Ux = z_2$ (n^2 flops)

total cost: $(2/3)n^3 + 2n^2$ flops, or roughly $(2/3)n^3$

this is the standard method for solving $Ax = b$

Multiple right-hand sides

two equations with the same matrix A (nonsingular and $n \times n$):

$$Ax = b, \qquad A\tilde{x} = \tilde{b}$$

- factor A once
- forward/back substitution to get x
- forward/back substitution to get $\tilde{x}$

cost: $(2/3)n^3 + 4n^2$ or roughly $(2/3)n^3$

exercise: propose an efficient method for solving

$$Ax = b, \qquad A^T\tilde{x} = \tilde{b}$$

Inverse of a nonsingular matrix

suppose A is nonsingular of order n, with LU factorization

$$A = PLU$$

- inverse from LU factorization

$$A^{-1} = (PLU)^{-1} = U^{-1}L^{-1}P^T$$

- gives interpretation of solve step: evaluate

$$x = A^{-1}b = U^{-1}L^{-1}P^Tb$$

  in three steps

$$z_1 = P^Tb, \qquad z_2 = L^{-1}z_1, \qquad x = U^{-1}z_2$$

Computing the inverse

solve $AX = I$ by solving n equations

$$AX_1 = e_1, \qquad AX_2 = e_2, \qquad \ldots, \qquad AX_n = e_n$$

X_i is the ith column of X; e_i is the ith unit vector of size n

- one LU factorization of A: $2n^3/3$ flops
- n solve steps: $2n^3$ flops

total: $(8/3)n^3$ flops

conclusion: do not solve $Ax = b$ by multiplying A^{-1} with b

LU factorization without pivoting

partition A, L, U as block matrices:

$$A = \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad L = \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix}, \qquad U = \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

- a_{11} and u_{11} are scalars
- L_{22} unit lower-triangular, U_{22} upper triangular of order $n-1$

determine L and U from $A = LU$, *i.e.*,

$$\begin{aligned} \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} \\ &= \begin{bmatrix} u_{11} & U_{12} \\ u_{11}L_{21} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix} \end{aligned}$$

recursive algorithm:

- determine first row of U and first column of L

$$u_{11} = a_{11}, \qquad U_{12} = A_{12}, \qquad L_{21} = (1/a_{11})A_{21}$$

- factor the $(n-1) \times (n-1)$-matrix $A_{22} - L_{21}U_{12}$ as

  $$A_{22} - L_{21}U_{12} = L_{22}U_{22}$$

  this is an LU factorization (without pivoting) of order $n-1$

cost: $(2/3)n^3$ flops (no proof)

Example

LU factorization (without pivoting) of

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix}$$

write as $A = LU$ with L unit lower triangular, U upper triangular

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of U, first column of L:

$$\begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{bmatrix} 9 & 4 \\ 7 & 9 \end{bmatrix} - \begin{bmatrix} 1/2 \\ 3/4 \end{bmatrix} \begin{bmatrix} 2 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix}$$

$$\begin{bmatrix} 8 & -1/2 \\ 11/2 & 9/4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & -1/2 \\ 0 & u_{33} \end{bmatrix}$$

- third row of U: $u_{33} = 9/4 + 11/32 = 83/32$

conclusion:

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & 8 & -1/2 \\ 0 & 0 & 83/32 \end{bmatrix}$$

Not every nonsingular A can be factored as $A = LU$

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of U, first column of L:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{bmatrix} 0 & 2 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix}$$

$u_{22} = 0$, $u_{23} = 2$, $l_{32} \cdot 0 = 1$?

LU factorization (with row pivoting)

if A is $n \times n$ and nonsingular, then it can be factored as

$$A = PLU$$

P is a permutation matrix, L is unit lower triangular, U is upper triangular

- not unique; there may be several possible choices for P, L, U
- interpretation: permute the rows of A and factor $P^T A$ as $P^T A = LU$
- also known as *Gaussian elimination with partial pivoting* (GEPP)
- cost: $(2/3)n^3$ flops

we will skip the details of calculating P, L, U

Example

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 0 & 15/19 & 1 \end{bmatrix} \begin{bmatrix} 6 & 8 & 8 \\ 0 & 19/3 & -8/3 \\ 0 & 0 & 135/19 \end{bmatrix}$$

the factorization is not unique; the same matrix can be factored as

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & -19/5 & 1 \end{bmatrix} \begin{bmatrix} 2 & 9 & 0 \\ 0 & 5 & 5 \\ 0 & 0 & 27 \end{bmatrix}$$

Effect of rounding error

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

exact solution:

$$x_1 = \frac{-1}{1 - 10^{-5}}, \qquad x_2 = \frac{1}{1 - 10^{-5}}$$

let us solve the equations using LU factorization, rounding intermediate results to 4 significant decimal digits

we will do this for the two possible permutation matrices:

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

first choice of P: $P = I$ (no pivoting)

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} 10^{-5} & 1 \\ 0 & 1 - 10^5 \end{bmatrix}$$

L, U rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \Longrightarrow \qquad z_1 = 1, \quad z_2 = -10^5$$

back substitution

$$\begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^5 \end{bmatrix} \qquad \Longrightarrow \qquad x_1 = 0, \quad x_2 = 1$$

error in x_1 is 100%

second choice of P: interchange rows

$$\begin{bmatrix} 1 & 1 \\ 10^{-5} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1-10^{-5} \end{bmatrix}$$

L, U rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \Longrightarrow \qquad z_1 = 0, \quad z_2 = 1$$

backward substitution

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \Longrightarrow \qquad x_1 = -1, \quad x_2 = 1$$

error in x_1, x_2 is about 10^{-5}

conclusion:

- for some choices of P, small rounding errors in the algorithm cause very large errors in the solution
- this is called **numerical instability**: for the first choice of P, the algorithm is unstable; for the second choice of P, it is stable
- from numerical analysis: there is a simple rule for selecting a good (stable) permutation (we'll skip the details, since we skipped the details of the factorization algorithm)
- in the example, the second permutation is better because it permutes the largest element (in absolute value) of the first column of A to the 1,1-position

Sparse linear equations

if A is sparse, it is usually factored as

$$A = P_1 L U P_2$$

P_1 and P_2 are permutation matrices

- interpretation: permute rows and columns of A and factor $\tilde{A} = P_1^T A P_2^T$

$$\tilde{A} = LU$$

- choice of P_1 and P_2 greatly affects the sparsity of L and U: many heuristic methods exist for selecting good permutations

- in practice: #flops $\ll (2/3)n^3$; exact value is a complicated function of n, number of nonzero elements, sparsity pattern

Conclusion

different levels of understanding how linear equation solvers work:

highest level: `x = A\b` costs $(2/3)n^3$; more efficient than `x = inv(A)*b`

intermediate level: factorization step $A = PLU$ followed by solve step

lowest level: details of factorization $A = PLU$

- for most applications, level 1 is sufficient
- in some situations ($e.g.$, multiple right-hand sides) level 2 is useful
- level 3 is important only for experts who write numerical libraries

Theorem

If A is a square matrix that can be reduced to a row echelon form U by Gaussian elimination without row interchanges, then A can be factored as $A = LU$, where L is a lower triangular matrix.

We know that the Gaussian elimination operations can be accomplished by multiplying A on the left by an appropriate sequence of elementary matrices; that is, there exist elementary matrices $E_1, E_2, ..., E_k$ such that

$$E_k \cdots E_2 E_1 A = U$$

where U is an upper triangular matrix Since elementary matrices are invertible, we can solve for A as

$$A = E_1^{-1} E_2^{-1} \cdots E_k^{-1} U$$

$$A = LU$$

$$L = E_1^{-1} E_2^{-1} \cdots E_k^{-1}$$

L is lower triangular because:

- multiplying a row by a nonzero constant, and adding a scalar multiple of one row to another

- If A is an invertible matrix that can be reduced to row echelon form without row interchanges, then A can be factored uniquely as

  $$A = LDU$$

  where L is a lower triangular matrix with 1's on the main diagonal, D is a diagonal matrix, and U is an upper triangular matrix with 1's on the main diagonal. This is called the LDU-decomposition (or LDU-factorization) of A.
  "shift" the diagonal entries of U (or of L) to a diagonal matrix D and write U as $U = U'D$

- If desired, the diagonal matrix and the lower triangular matrix in the LU-decomposition can be multiplied to produce an LU-decomposition in which the 1's are on the main diagonal of U rather than L. (This is yet another example that LU decompositions are not unique)

Note that the columns of L' are obtained by dividing each entry in the corresponding column of L by the diagonal entry in the column. Thus, for example, we can rewrite
In general, LU-decompositions are not unique.

$$A = LU = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}$$

Software

- In 1979 an important library of machine-independent linear algebra programs called LINPACK was developed at Argonne National Laboratories.
- Many of the programs in that library use the LU and other decomposition methods (SVD, Schur's decomposition, Cholesky decomposition, etc).
- Variations of the LINPACK routines in Fortran are used in many computer programs, including Scipy, MATLAB, Mathematica, and Maple.

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Numerical Solutions

- A matrix A is said to be ill conditioned if relatively small changes in the entries of A can cause relatively large changes in the solutions of $A\boldsymbol{x} = \boldsymbol{b}$.
- A is said to be well conditioned if relatively small changes in the entries of A result in relatively small changes in the solutions of $A\boldsymbol{x} = \boldsymbol{b}$.
- reaching RREF as in Gauss-Jordan requires more computation and more numerical instability hence disadvantageous.
- Gauss elimination is a direct method: the amount of operations can be specified in advance. Indirect or Iterative methods work by iteratively improving approximate solutions until a desired accuracy is reached. Amount of operations depend on the accuracy required. (way to go if the matrix is sparse)

Gauss-Seidel Iterative Method

Example

$$\begin{array}{rcrcrcrcl} x_1 & - & 0.25x_2 & - & 0.25x_3 & & & = & 50 \\ -0.25x_1 & + & x_2 & & & - & 0.25x_4 & = & 50 \\ -0.25x_1 & & & + & x_3 & - & 0.25x_4 & = & 25 \\ & - & 0.25x_2 & - & 0.25x_3 & + & x_4 & = & 25 \end{array}$$

$$\begin{array}{rclcrcrcrcl} x_1 & = & & & 0.25x_2 & + & 0.25x_3 & & & + & 50 \\ x_2 & = & 0.25x_1 & & & & & + & 0.25x_4 & + & 50 \\ x_3 & = & 0.25x_1 & & & & & + & 0.25x_4 & + & 25 \\ x_4 & = & & & 0.25x_2 & + & 0.25x_3 & & & + & 25 \end{array}$$

We start from an approximation, eg, $x_1^{(0)} = 100, x_2^{(0)} = 100, x_3^{(0)} = 100, x_4^{(0)} = 100$, and use the equatiuons above to find a perhaps better approximation:

$$\begin{array}{rclcrcrcrcrcr} x_1^{(1)} & = & & & 0.25x_2^{(0)} & + & 0.25x_3^{(0)} & & & + & 50.00 & = & 100.00 \\ x_2^{(1)} & = & 0.25x_1^{(1)} & & & & & + & 0.25x_4^{(0)} & + & 50.00 & = & 100.00 \\ x_3^{(1)} & = & 0.25x_1^{(1)} & & & & & + & 0.25x_4^{(0)} & + & 25.00 & = & 75.00 \\ x_4^{(1)} & = & & & 0.25x_2^{(1)} & + & 0.25x_3^{(1)} & & & + & 25.00 & = & 68.75 \end{array}$$

$$
\begin{aligned}
x_1^{(2)} &= & & 0.25x_2^{(1)} &+& 0.25x_3^{(1)} & & &+& 50.00 &=& 93.750 \\
x_2^{(2)} &= 0.25x_1^{(2)} & & & & & + & 0.25x_4^{(1)} &+& 50.00 &=& 90.625 \\
x_3^{(2)} &= 0.25x_1^{(2)} & & & & & + & 0.25x_4^{(1)} &+& 25.00 &=& 65.625 \\
x_4^{(2)} &= & & 0.25x_2^{(2)} &+& 0.25x_3^{(2)} & & &+& 25.00 &=& 64.062
\end{aligned}
$$