**Root-mean-square deviation**

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For the [bioinformatics](https://en.wikipedia.org/wiki/Bioinformatics) concept, see [Root-mean-square deviation of atomic positions](https://en.wikipedia.org/wiki/Root-mean-square_deviation_of_atomic_positions).

The **root-mean-square deviation (RMSD)** or **root-mean-square error (RMSE)** is a frequently used measure of the differences between values (sample and population values) predicted by a model or an estimator and the values actually observed. The RMSD represents the [sample standard deviation](https://en.wikipedia.org/wiki/Sample_standard_deviation) of the differences between predicted values and observed values. These individual differences are called [residuals](https://en.wikipedia.org/wiki/Errors_and_residuals_in_statistics) when the calculations are performed over the data sample that was used for estimation, and are called *prediction errors* when computed out-of-sample. The RMSD serves to aggregate the magnitudes of the errors in predictions for various times into a single measure of predictive power. RMSD is a good measure of [accuracy](https://en.wikipedia.org/wiki/Accuracy_and_precision), but only to compare forecasting errors of different models for a particular variable and not between variables, as it is scale-dependent.[[1]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-1)

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**Formula**

The RMSD of an [estimator](https://en.wikipedia.org/wiki/Estimator) θ ^ {\displaystyle {\hat {\theta }}} with respect to an estimated parameter θ {\displaystyle \theta } is defined as the square root of the [mean square error](https://en.wikipedia.org/wiki/Mean_square_error):

RMSD ⁡ ( θ ^ ) = MSE ⁡ ( θ ^ ) = E ⁡ ( ( θ ^ − θ ) 2 ) . {\displaystyle \operatorname {RMSD} ({\hat {\theta }})={\sqrt {\operatorname {MSE} ({\hat {\theta }})}}={\sqrt {\operatorname {E} (({\hat {\theta }}-\theta )^{2})}}.}

For an [unbiased estimator](https://en.wikipedia.org/wiki/Unbiased_estimator), the RMSD is the square root of the variance, known as the [standard deviation](https://en.wikipedia.org/wiki/Standard_deviation).

The RMSD of predicted values y ^ t {\displaystyle {\hat {y}}\_{t}} for times *t* of a [regression's](https://en.wikipedia.org/wiki/Regression_analysis) [dependent variable](https://en.wikipedia.org/wiki/Dependent_variable) y t {\displaystyle y\_{t}} is computed for *n* different predictions as the square root of the mean of the squares of the deviations:

RMSD = ∑ t = 1 n ( y ^ t − y t ) 2 n . {\displaystyle \operatorname {RMSD} ={\sqrt {\frac {\sum \_{t=1}^{n}({\hat {y}}\_{t}-y\_{t})^{2}}{n}}}.}

In some disciplines, the RMSD is used to compare differences between two things that may vary, neither of which is accepted as the "standard". For example, when measuring the average difference between two time series x 1 , t {\displaystyle x\_{1,t}} and x 2 , t {\displaystyle x\_{2,t}} , the formula becomes

RMSD = ∑ t = 1 n ( x 1 , t − x 2 , t ) 2 n . {\displaystyle \operatorname {RMSD} ={\sqrt {\frac {\sum \_{t=1}^{n}(x\_{1,t}-x\_{2,t})^{2}}{n}}}.}

**Normalized root-mean-square deviation**

Normalizing the RMSD facilitates the comparison between datasets or models with different scales. Though there is no consistent means of normalization in the literature, common choices are the mean or the range (defined as the maximum value minus the minimum value) of the measured data:[[2]](https://en.wikipedia.org/wiki/Root-mean-square_deviation" \l "cite_note-2)

N R M S D = R M S D y max − y min {\displaystyle \mathrm {NRMSD} ={\frac {\mathrm {RMSD} }{y\_{\max }-y\_{\min }}}} or N R M S D = R M S D y ¯ {\displaystyle \mathrm {NRMSD} ={\frac {\mathrm {RMSD} }{\bar {y}}}} .

This value is commonly referred to as the **normalized root-mean-square deviation** or **error** (**NRMSD** or **NRMSE**), and often expressed as a percentage, where lower values indicate less residual variance. In many cases, especially for smaller samples, the sample range is likely to be affected by the size of sample which would hamper comparisons.

When normalising by the mean value of the measurements, the term **coefficient of variation of the RMSD, CV(RMSD)** may be used to avoid ambiguity.[[3]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-3) This is analogous to the [coefficient of variation](https://en.wikipedia.org/wiki/Coefficient_of_variation) with the RMSD taking the place of the [standard deviation](https://en.wikipedia.org/wiki/Standard_deviation).

C V ( R M S D ) = R M S D y ¯ {\displaystyle \mathrm {CV(RMSD)} ={\frac {\mathrm {RMSD} }{\bar {y}}}}

**Applications**

* In [meteorology](https://en.wikipedia.org/wiki/Meteorology), to see how effectively a [mathematical](https://en.wikipedia.org/wiki/Mathematics) model predicts the behavior of the [atmosphere](https://en.wikipedia.org/wiki/Atmosphere).
* In [bioinformatics](https://en.wikipedia.org/wiki/Bioinformatics), the RMSD is the measure of the average distance between the atoms of [superimposed](https://en.wikipedia.org/wiki/Protein_structural_alignment) [proteins](https://en.wikipedia.org/wiki/Proteins).
* In [structure based drug design](https://en.wikipedia.org/wiki/Drug_design#Structure-based), the RMSD is a measure of the difference between a crystal conformation of the ligand [conformation](https://en.wikipedia.org/wiki/Conformer) and a [docking](https://en.wikipedia.org/wiki/Docking_%28molecular%29) prediction.
* In [economics](https://en.wikipedia.org/wiki/Economics), the RMSD is used to determine whether an economic model fits [economic indicators](https://en.wikipedia.org/wiki/Economic_indicator). Some experts have argued that RMSD is less reliable than Relative Absolute Error.[[4]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-4)
* In [experimental psychology](https://en.wikipedia.org/wiki/Experimental_psychology), the RMSD is used to assess how well mathematical or computational models of behavior explain the empirically observed behavior.
* In [GIS](https://en.wikipedia.org/wiki/GIS), the RMSD is one measure used to assess the accuracy of spatial analysis and remote sensing.
* In [hydrogeology](https://en.wikipedia.org/wiki/Hydrogeology), RMSD and NRMSD are used to evaluate the calibration of a groundwater model.[[5]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-5)
* In [imaging science](https://en.wikipedia.org/wiki/Imaging_science), the RMSD is part of the [peak signal-to-noise ratio](https://en.wikipedia.org/wiki/Peak_signal-to-noise_ratio), a measure used to assess how well a method to reconstruct an image performs relative to the original image.
* In [computational neuroscience](https://en.wikipedia.org/wiki/Computational_neuroscience), the RMSD is used to assess how well a system learns a given model.[[6]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-6)
* In [Protein nuclear magnetic resonance spectroscopy](https://en.wikipedia.org/wiki/Protein_nuclear_magnetic_resonance_spectroscopy), the RMSD is used as a measure to estimate the quality of the obtained bundle of structures.
* Submissions for the [Netflix Prize](https://en.wikipedia.org/wiki/Netflix_Prize) were judged using the RMSD from the test dataset's undisclosed "true" values.
* In simulation of energy consumption of buildings, the RMSE and CV(RMSE) are used to calibrate models to measured building performance.[[7]](https://en.wikipedia.org/wiki/Root-mean-square_deviation#cite_note-7)

**See also**

* [Root mean square](https://en.wikipedia.org/wiki/Root_mean_square)
* [Average absolute deviation](https://en.wikipedia.org/wiki/Average_absolute_deviation)
* [Mean signed deviation](https://en.wikipedia.org/wiki/Mean_signed_deviation)
* [Mean squared deviation](https://en.wikipedia.org/wiki/Mean_squared_deviation)
* [Squared deviations](https://en.wikipedia.org/wiki/Squared_deviations)
* [Errors and residuals in statistics](https://en.wikipedia.org/wiki/Errors_and_residuals_in_statistics)

**References**

 *Hyndman, Rob J. Koehler, Anne B.; Koehler (2006). "Another look at measures of forecast accuracy". International Journal of Forecasting* ***22*** *(4): 679–688.* [*doi*](https://en.wikipedia.org/wiki/Digital_object_identifier)*:*[*10.1016/j.ijforecast.2006.03.001*](https://dx.doi.org/10.1016%2Fj.ijforecast.2006.03.001)*.*

  [*"Coastal Inlets Research Program (CIRP) Wiki - Statistics"*](http://cirpwiki.info/wiki/Statistics#Normalization)*. Retrieved 4 February 2015.*

  [*"FAQ: What is the coefficient of variation?"*](http://www.ats.ucla.edu/stat/mult_pkg/faq/general/coefficient_of_variation.htm)*. Retrieved 4 February 2015.*

  *J. Scott Armstrong & Fred Collopy (1992).* [*"Error Measures For Generalizing About Forecasting Methods: Empirical Comparisons"*](http://faculty.weatherhead.case.edu/Fred-Collopy/researchArticles/ErrorMeasures.pdf) *(PDF). International Journal of Forecasting* ***8*** *(1): 69–80.* [*doi*](https://en.wikipedia.org/wiki/Digital_object_identifier)*:*[*10.1016/0169-2070(92)90008-w*](https://dx.doi.org/10.1016%2F0169-2070%2892%2990008-w)*.*

  *Anderson, M.P.; Woessner, W.W. (1992). Applied Groundwater Modeling: Simulation of Flow and Advective Transport (2nd ed.). Academic Press.*

  [Ensemble Neural Network Model](http://www.ocgy.ubc.ca/projects/clim.pred/NN/3.1/model.html)

1.  [ANSI/BPI-2400-S-2012: Standard Practice for Standardized Qualification of Whole-House Energy Savings Predictions by Calibration to Energy Use History](http://www.bpi.org/Web%20Download/BPI%20Standards/BPI-2400-S-2012_Standard_Practice_for_Standardized_Qualification_of_Whole-House%20Energy%20Savings_9-28-12_sg.pdf)

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