

Interpolation and approximation

Kristina Kislyakova

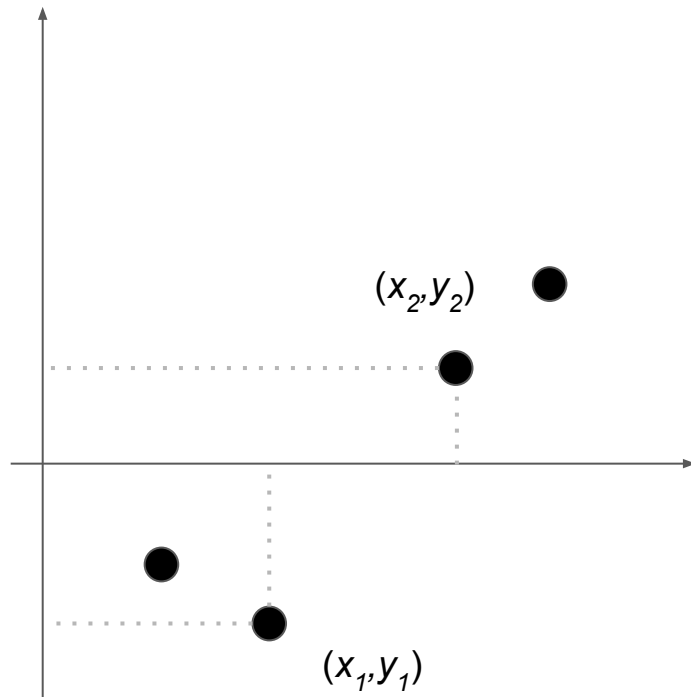
University of Vienna - 29.10.2025

Outline

- Concepts and common uses of **interpolation** and **approximation** schemes
- Linear interpolation methods
- Lagrange, Hermite and Taylor polynomial interpolation
- Cubic splines
- Multi-dimensional applications: Bilinear interpolation, Kriging
- Weighted approximation schemes, robust statistics, outlier filtering, GPR
- Cookbook for what to use, when and what to be aware of.

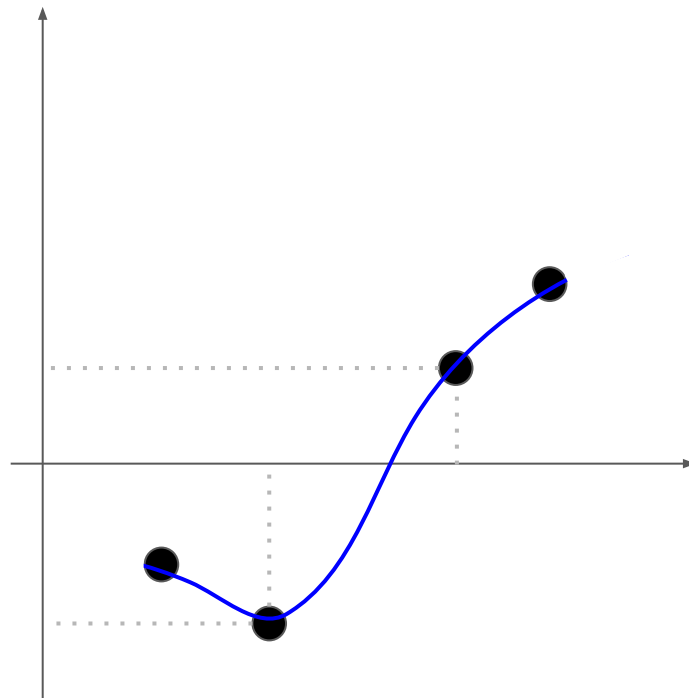
Discrete data representations

- Often have discrete data points for which you require an estimate at an intermediate value of (x,y)



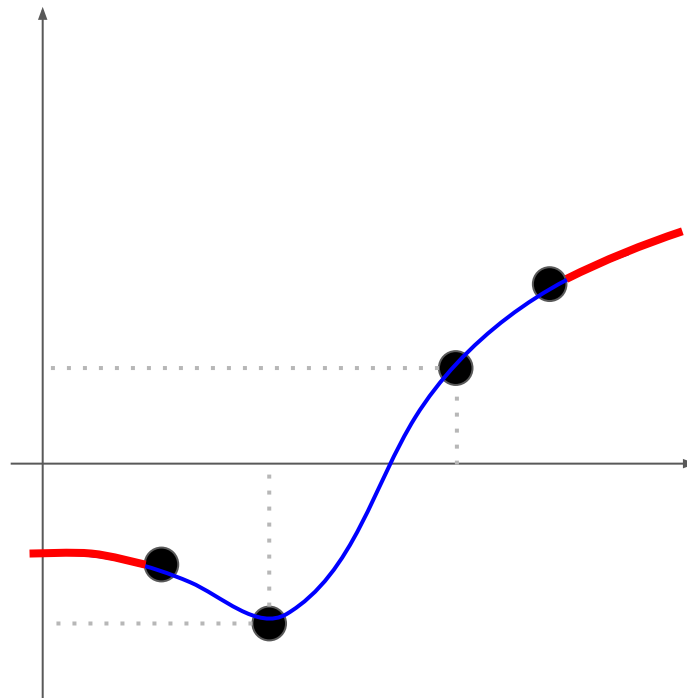
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- Functional representation of $y_i(x_i)$ allows sub-sampling/re-binning to intermediate values ([interpolation](#))



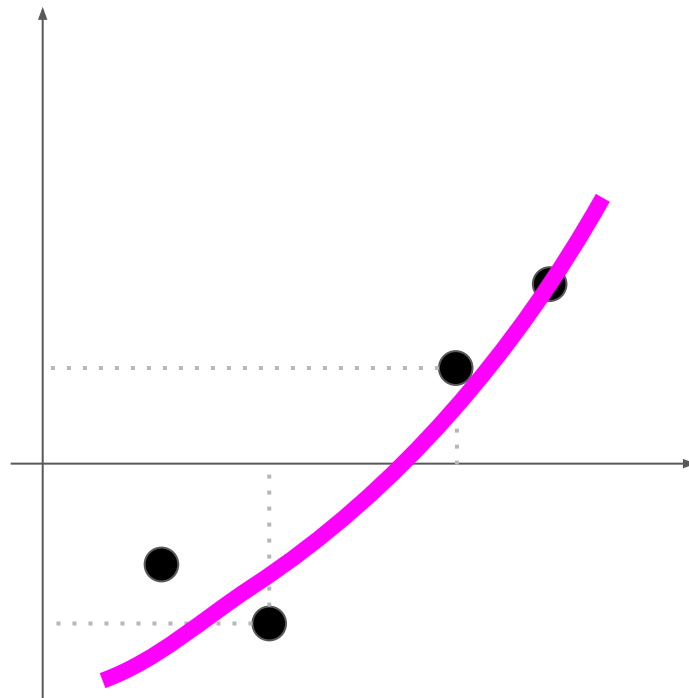
Discrete data representations

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- Functional representation of $y_i(x_i)$ allows sub-sampling/re-binning to intermediate values (**interpolation**)
- Sometimes **extrapolation** beyond $[x_{min}, x_{max}]$ is desired as well



Discrete data representations

- Often have discrete data points for which you require an estimate at an intermediate value of (x,y)
- Functional representation of $y_i(x_i)$ allows sub-sampling/re-binning to intermediate values (interpolation)
- Sometimes extrapolation beyond $[x_{min}, x_{max}]$ is desired as well
- Functions that do not pass through irregular points are approximations

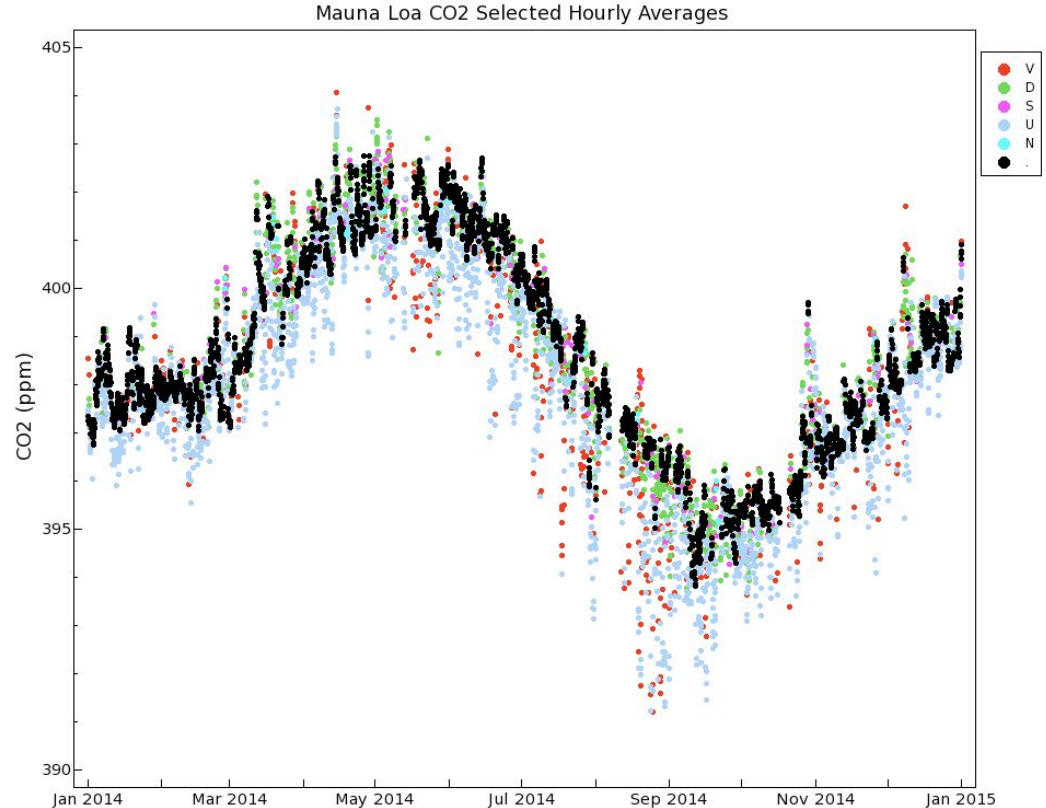


When is interpolation applicable? Useful?

- Missing data. For example, sparse data series in....

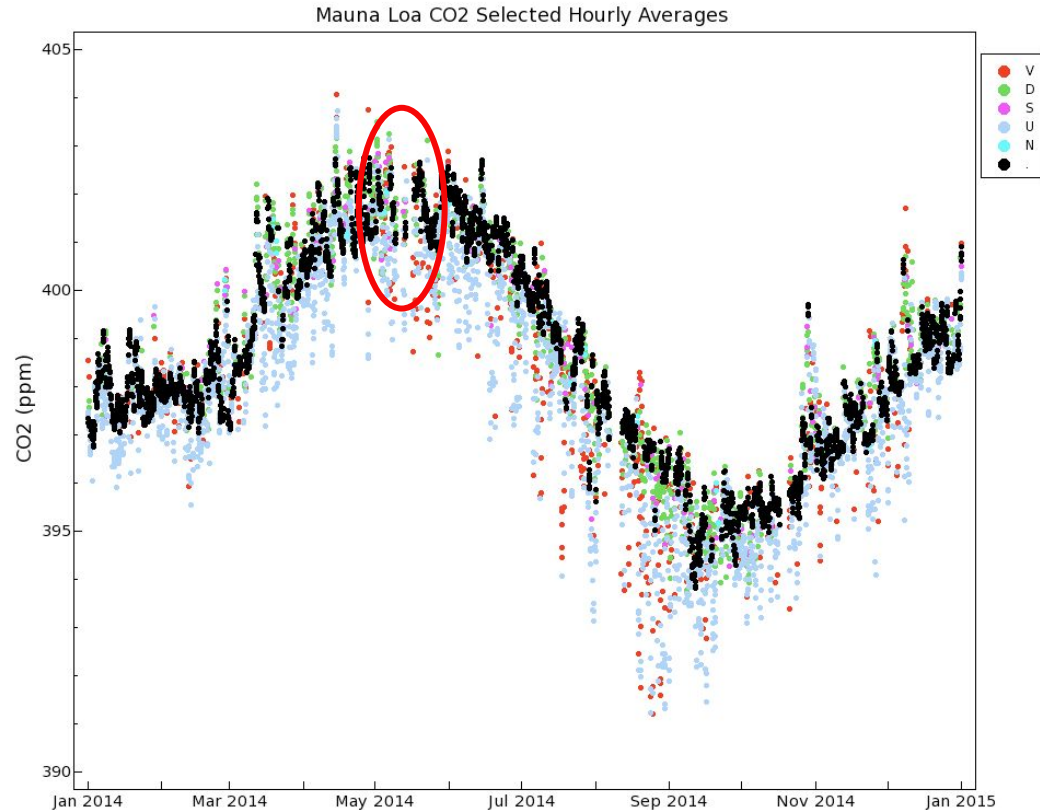
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- Historic climate records
- Could often have missing, or corrupted data to interpolate through



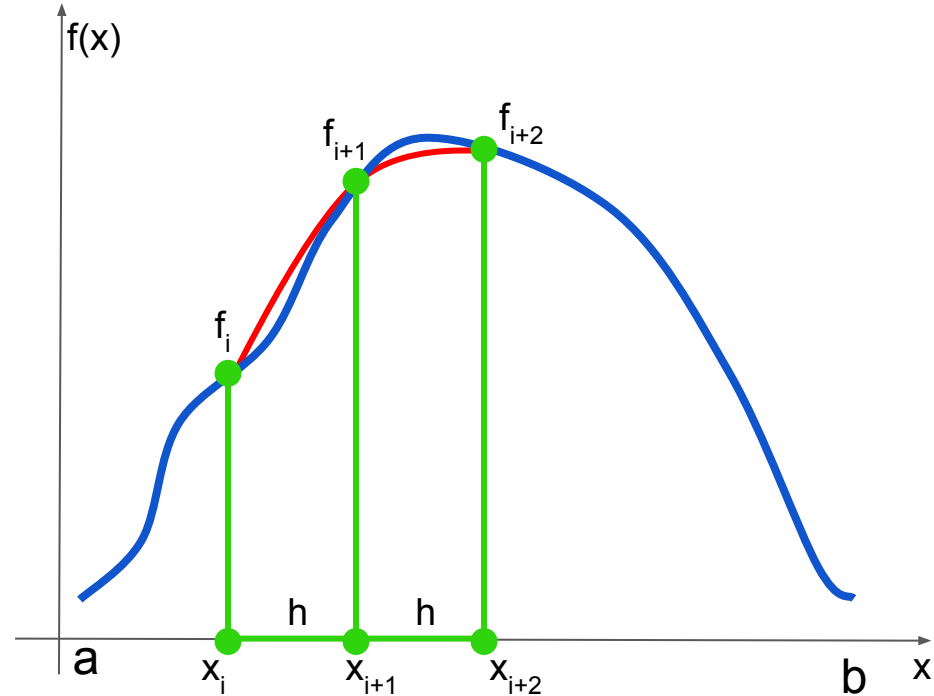
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When is interpolation applicable? Useful?

- Numerical integration...
- We will see in the next lectures how some interpolation schemes naturally allow for efficient numerical integration



Pitfalls in interpolation?

- There are subjective decisions in the type of adopted interpolation schemes.
- Need to consider your application, known biases in observations and how the error in interpolating some underlying behaviour affects your end goal

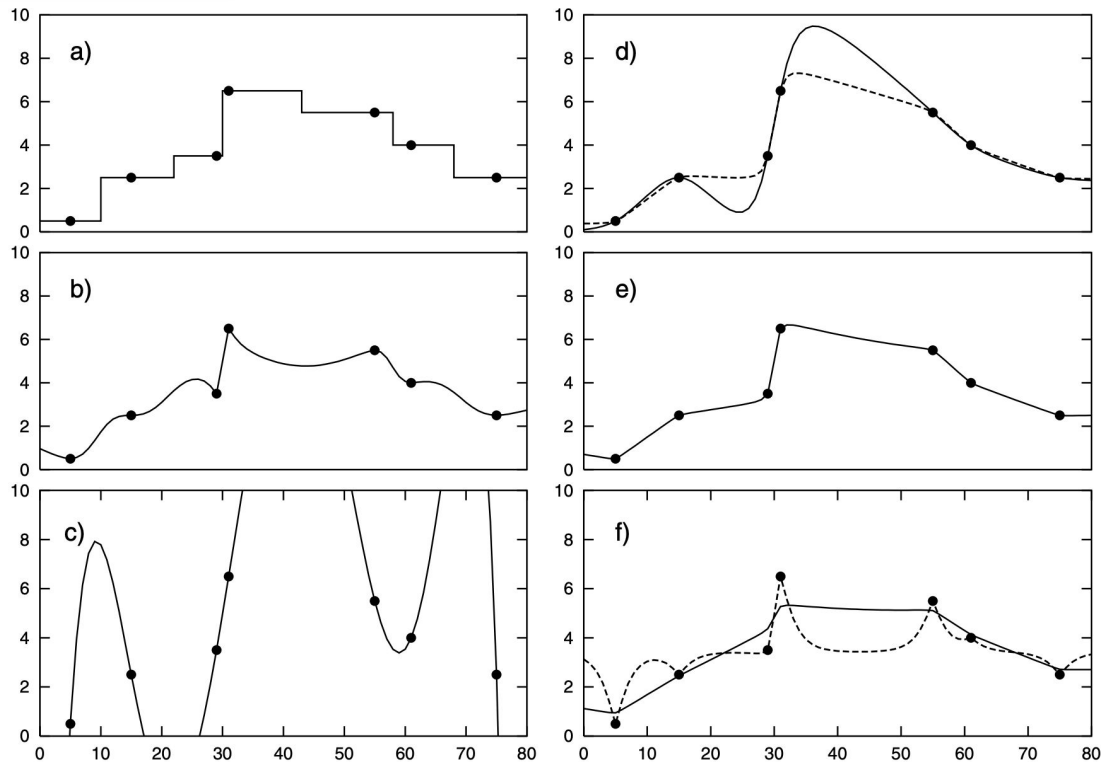
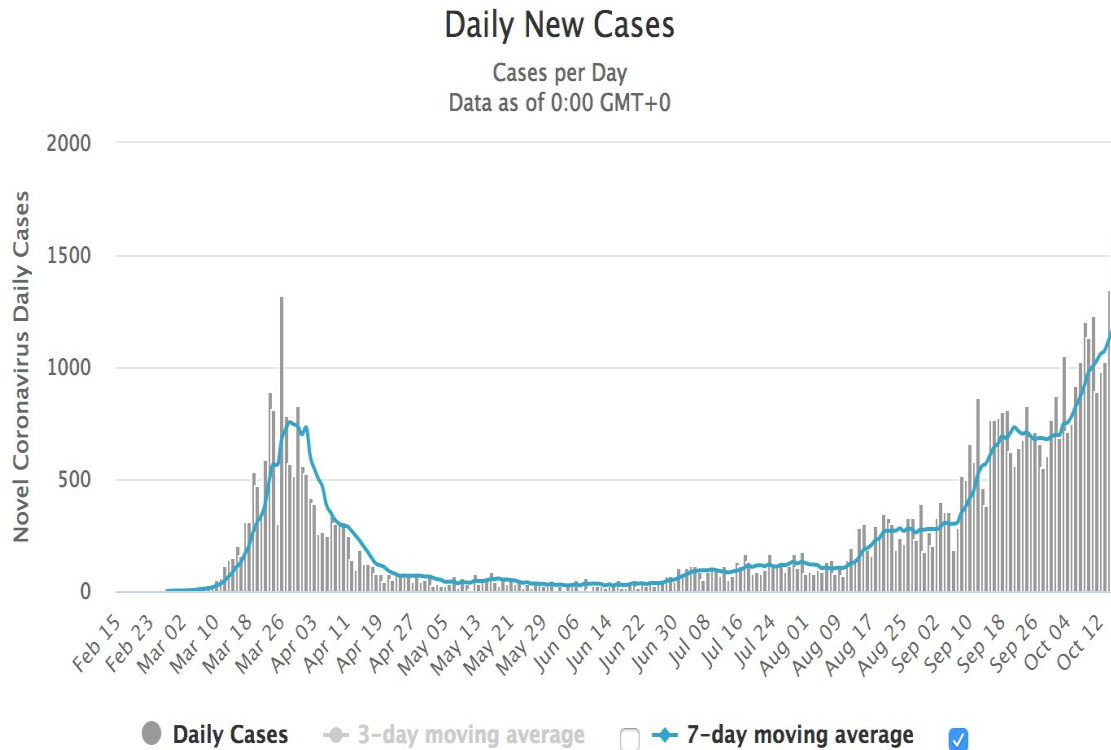


Figure 2.4. Comparison of interpolation methods for a one-dimensional example: (a) Thiessen method; (b) inverse distance squared; (c) example of overfitting using a sixth-order polynomial; (d) thin plate splines with different tension parameters; (e) kriging (zero nugget, large range); (f) kriging (solid line: large nugget, large range; dashed line: zero nugget, very short range).

What about approximations?

- Running averages, confidence intervals can give us a sense of the general trend without reproducing exact values
- For example daily case rates of infections
- Force of infection often specified in terms of per-capita infection rate over a 7 day window



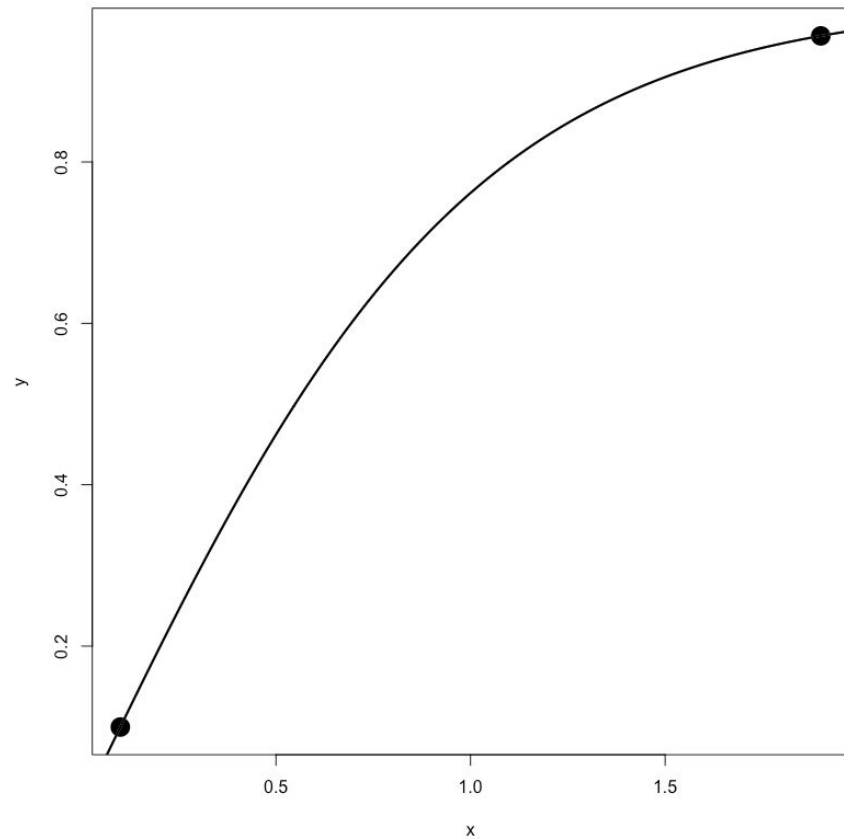
Distinction from other tools

- Important to keep in mind that **interpolation** and **approximations** are **non-physical**, and subject to some arbitrary choices
- They are fundamentally **different than fitting models** (analytic, numerical) to data (later lectures will cover this)
- In those cases you are using physical models to infer something from the dataset, and try to ascertain which model parameters are reproducing the data well.
- The tools we will discuss today are either numerically representing the data in places where your observations/simulations don't exist, or refining model grids in a way that can help you further analyze or characterize a problem.

Interpolation Methods:

Linear interpolation

- Simplest form to interpolate a function between two end points will be to create a linear fit.

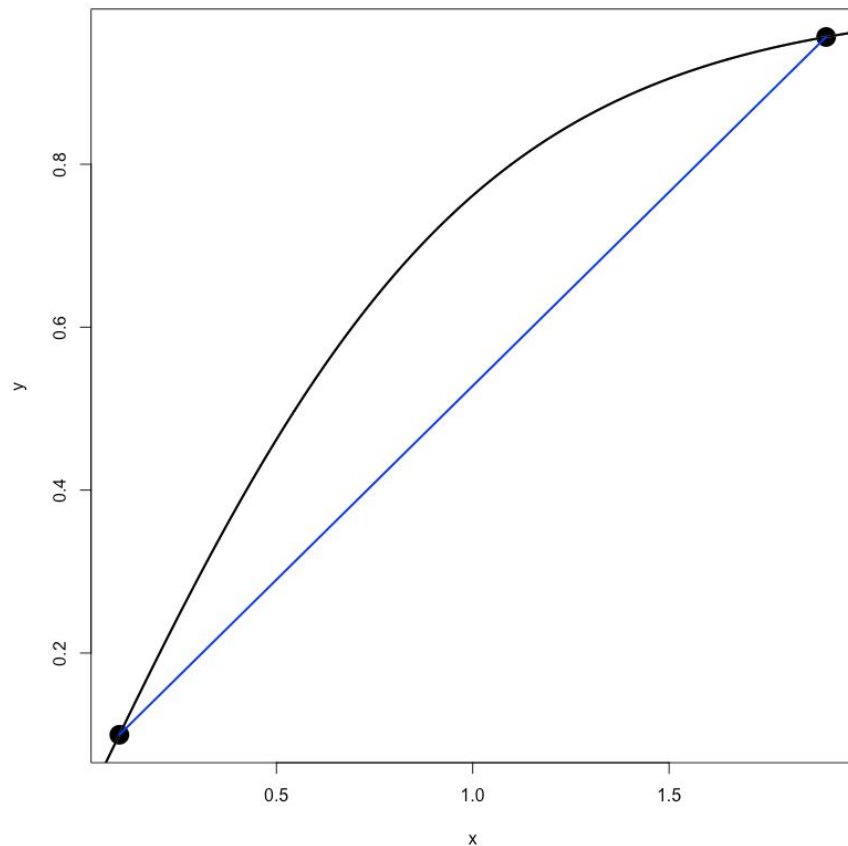


Interpolation Methods:

Linear interpolation

- Simplest form to interpolate a function between two end points will be to create a linear fit.
- Value at arbitrary x is:

$$y \equiv f(x) = \frac{y_2 - y_1}{x_2 - x_1}(x - x_1) + y_1$$



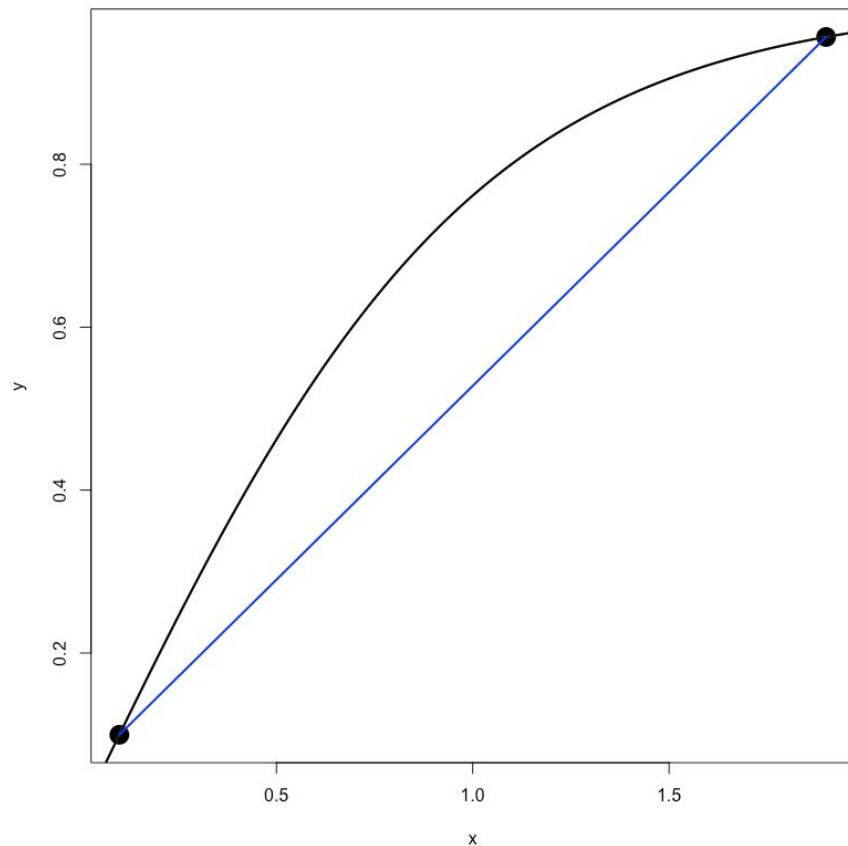
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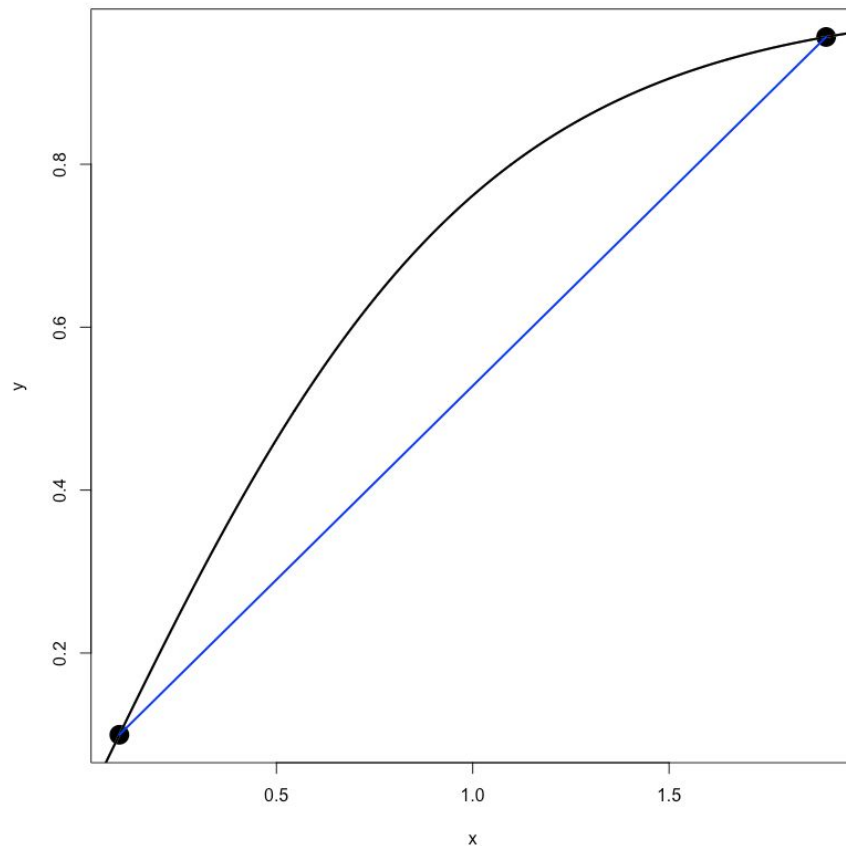
- Regardless of the form of $f(x)$, the error will approximately scale of order $(x_{i+1} - x_i)^2$



Interpolation Methods:

Polynomial interpolation

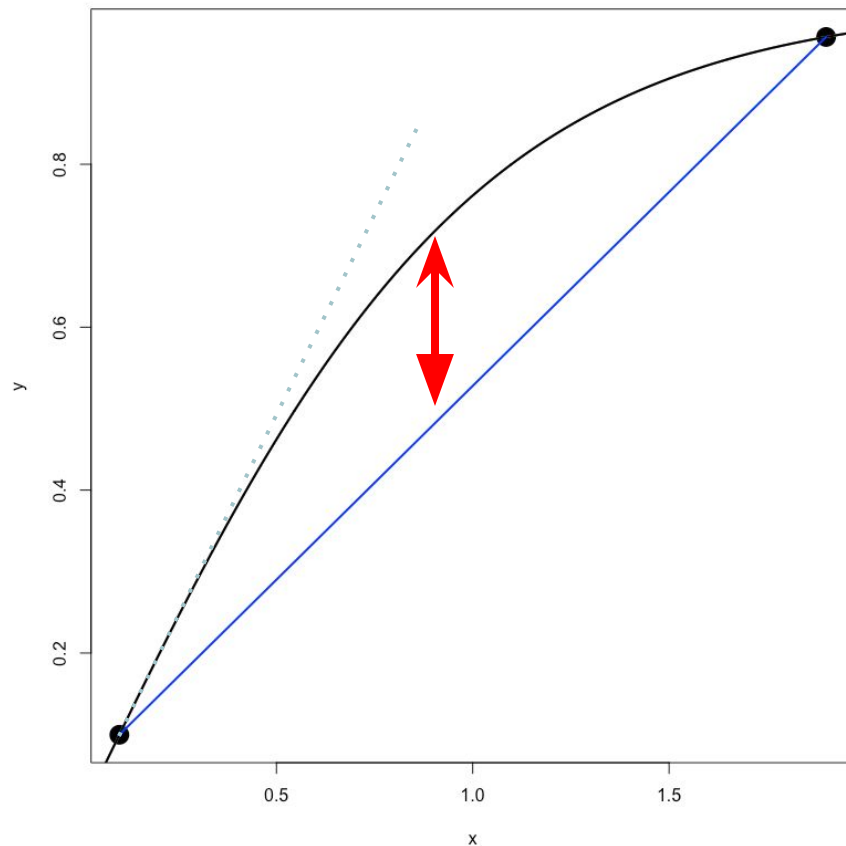
- Higher accuracy than linear, but requires a small interval.



Interpolation Methods:

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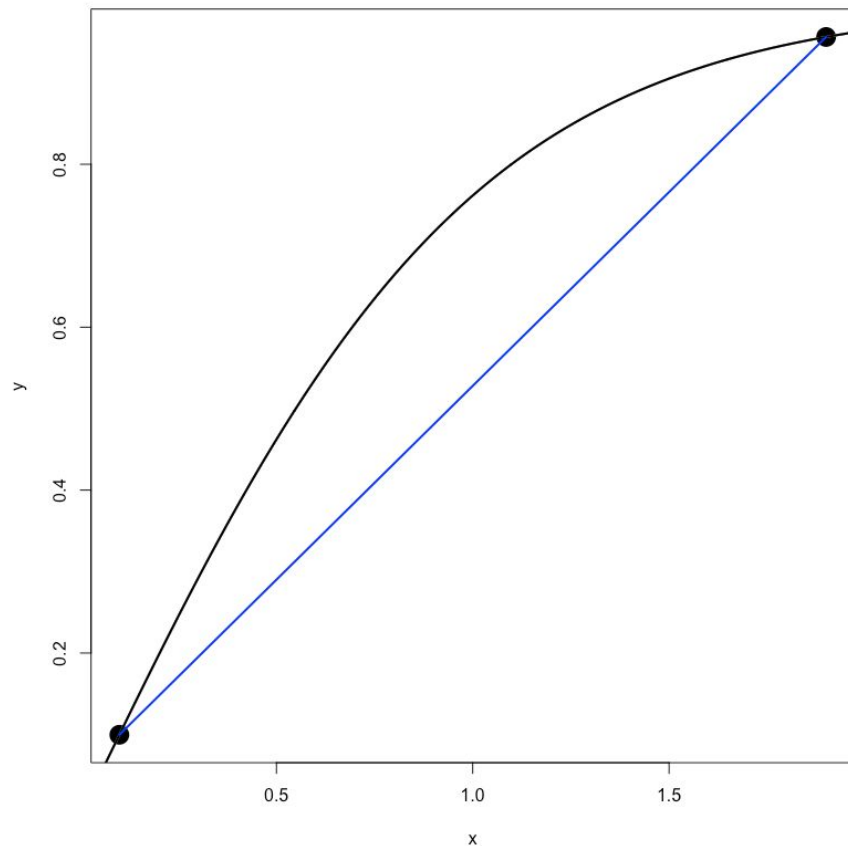
- Higher accuracy than linear, but requires a small interval
- This can potentially grow computation time



Interpolation Methods:

Polynomial interpolation

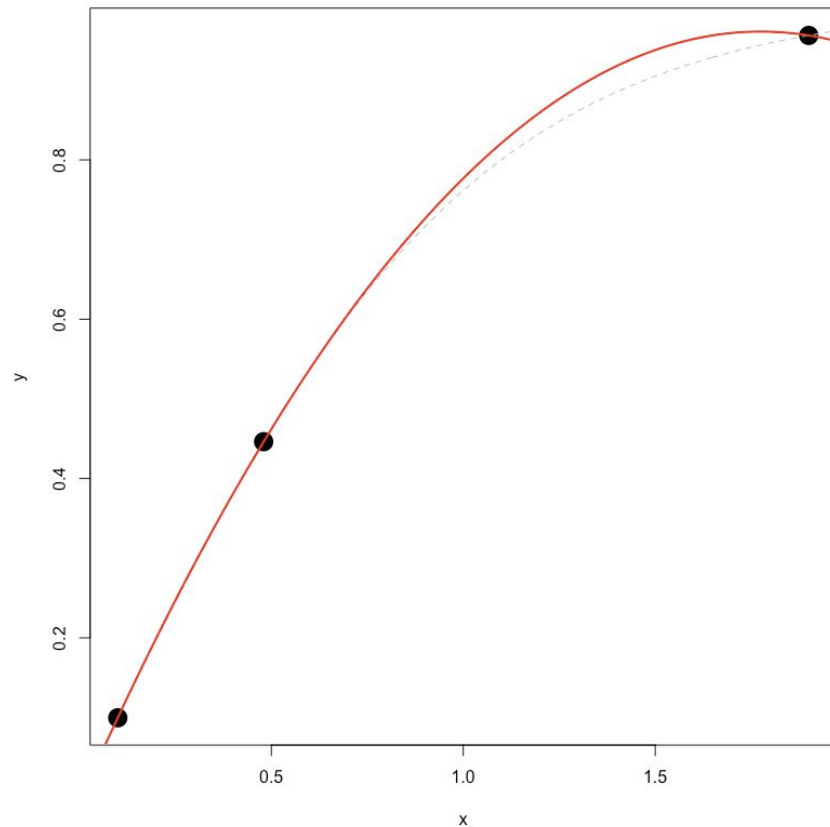
- Higher accuracy than linear, but requires a small interval
- This can potentially grow computation time
- Consider instead a polynomial function which passes through several points.



Interpolation Methods:

Polynomial interpolation

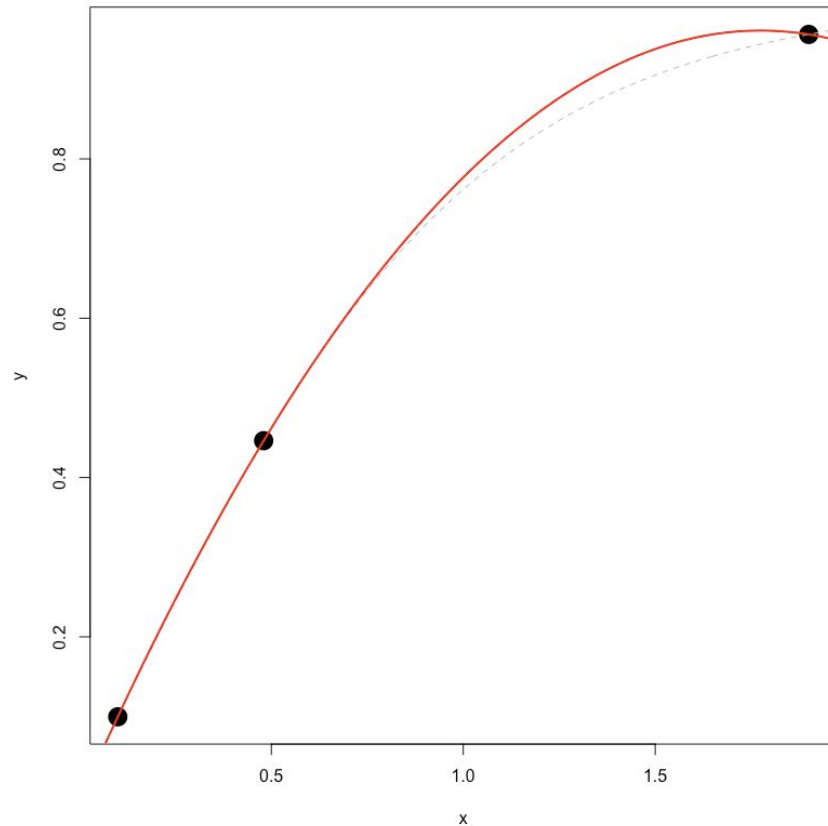
- Simplest extension would be quadratic, however let us look at general forms for polynomial interpolation.



Interpolation Methods:

Polynomial interpolation

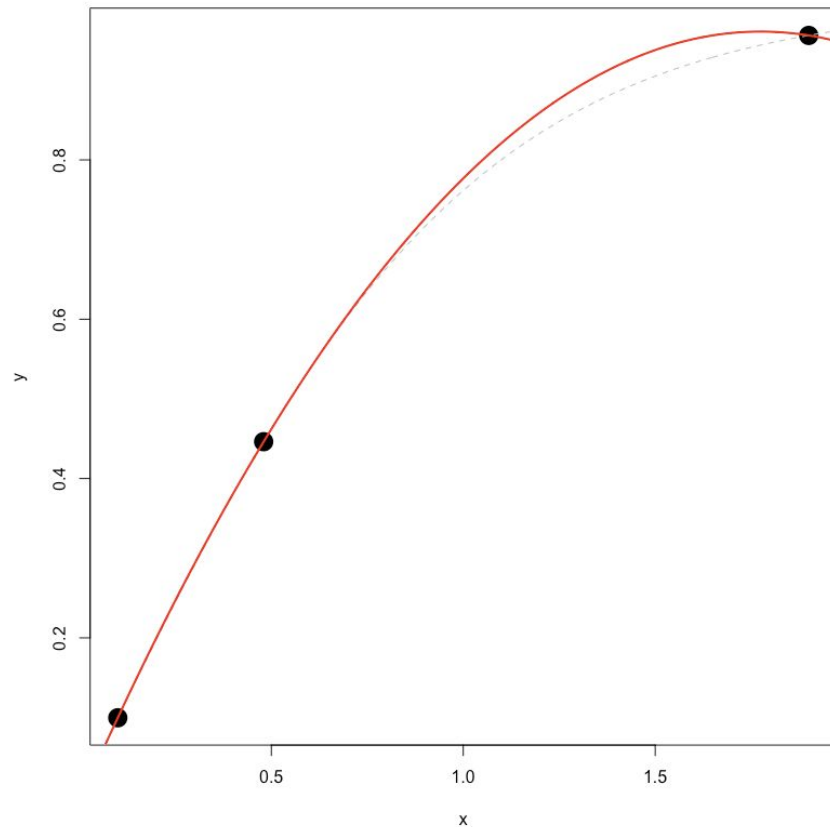
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- Allows you to interpolate generally, for arbitrary number of data points (x_i, y_i)



Interpolation Methods:

Polynomial interpolation

- Simplest extension would be quadratic, however let us look at general forms for polynomial interpolation.
- Allows you to interpolate generally, for arbitrary number of data points (x_i, y_i)
- Does not require evenly spaced data.



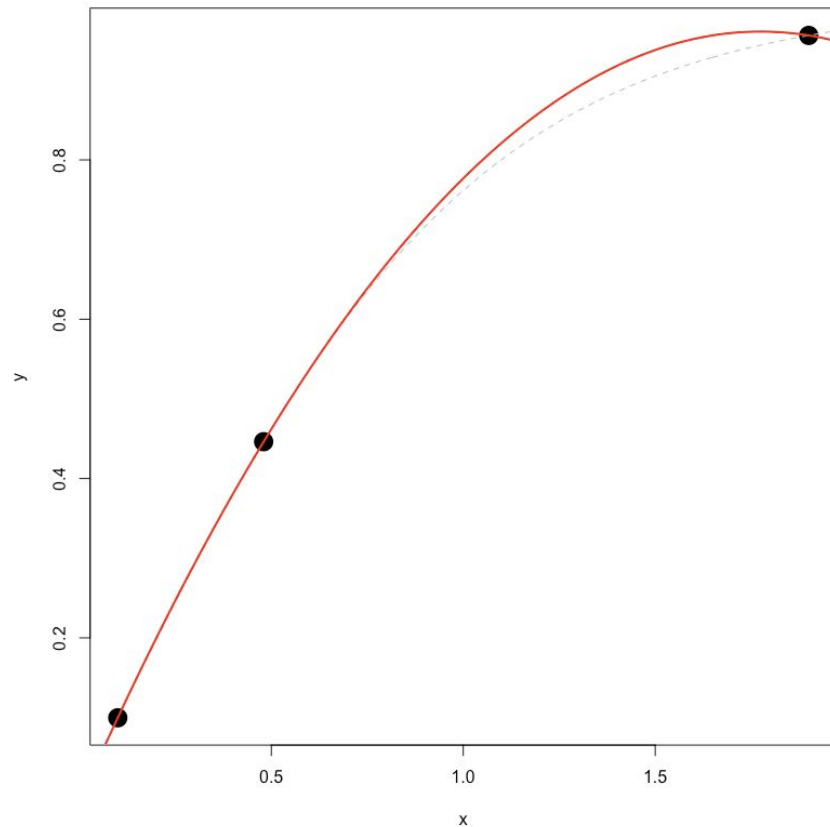
Interpolation Methods:

Polynomial interpolation

- A common and flexible implementation is **Lagrange interpolation**
- Basic idea: with n data points, can construct polynomial of order $n-1$

$$y \equiv f(x) = c_0x^2 + c_1x + c_2$$

- System of equations can be solved for the *coefficients* c_i

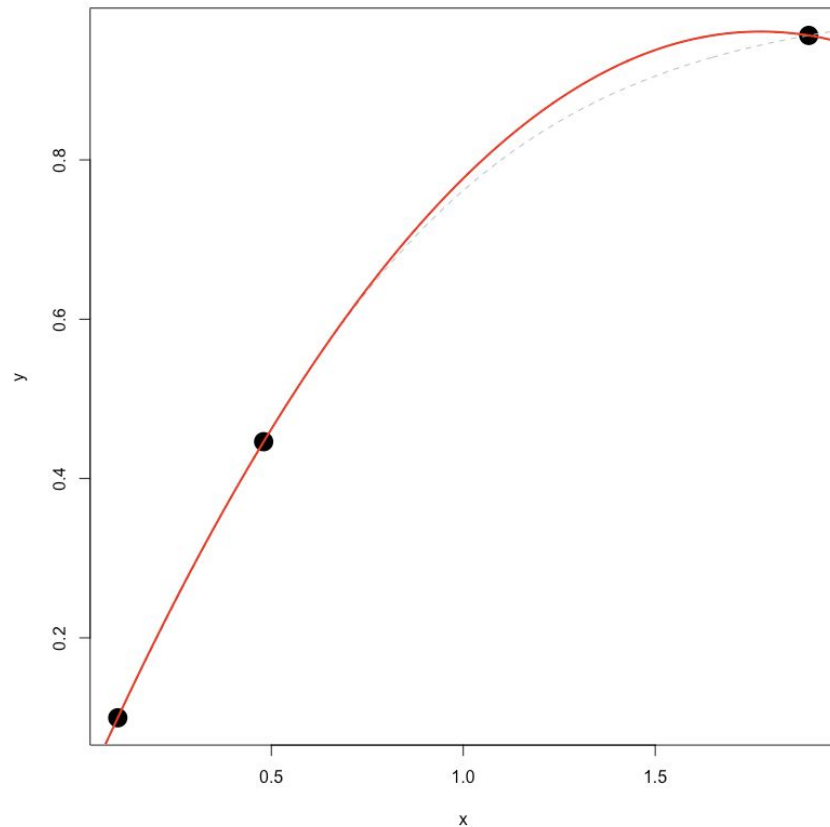


Interpolation Methods:

Polynomial interpolation

- Lagrange generalized a form of solutions so that extension to larger n is not unwieldy
- Basis functions L_i represent the *coefficients* in terms of the data x_i

$$L_i(x) = \prod_{j=0, j \neq i}^{n-1} \frac{x - x_j}{x_i - x_j}$$

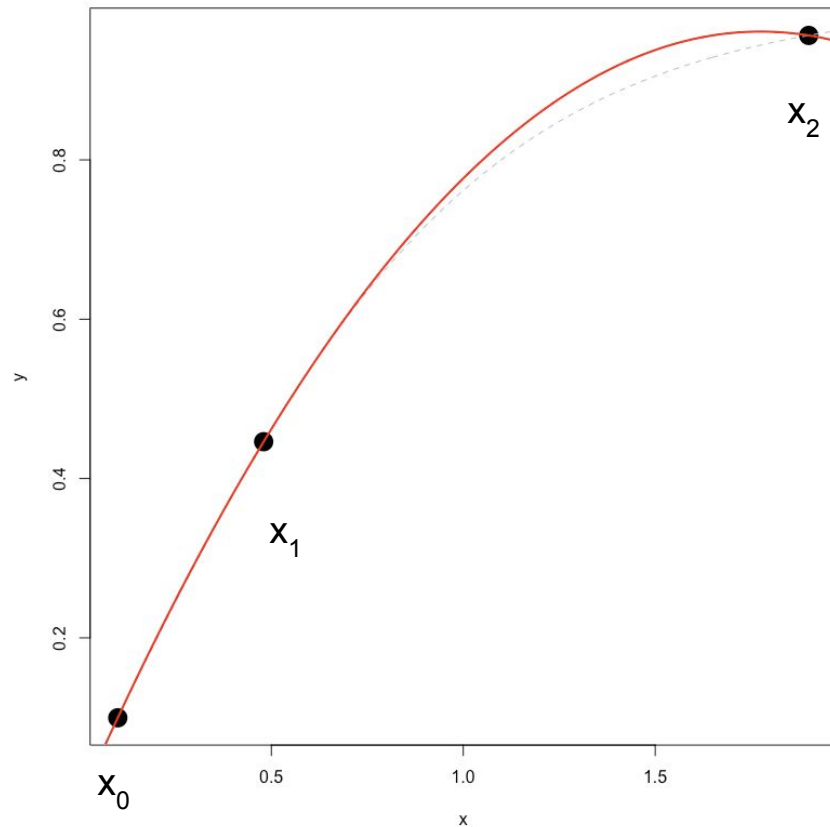


Interpolation Methods:

Polynomial interpolation

- For example with $n=3$ data points:

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Interpolation Methods:

Polynomial interpolation

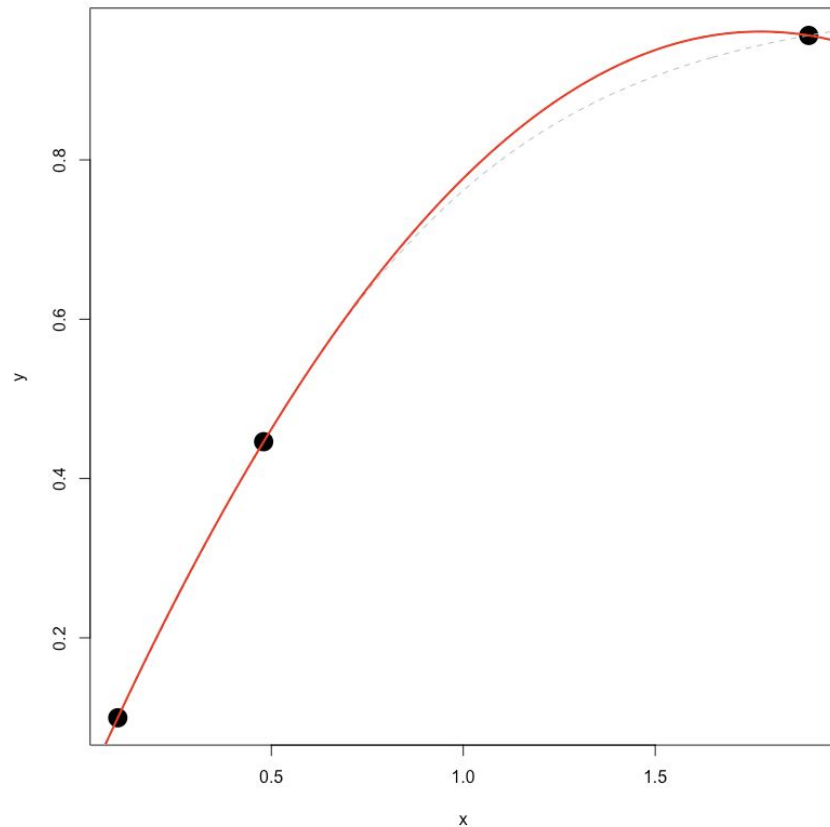
- For example with $n=3$ data points:

$$L_i(x) = \prod_{j=0, j \neq i}^{n-1} \frac{x - x_j}{x_i - x_j}$$

$$(x-x_1)/(x_0-x_1) * (x-x_2)/(x_0-x_2)$$

$$(x-x_0)/(x_1-x_0) * (x-x_2)/(x_1-x_2)$$

$$(x-x_0)/(x_2-x_0) * (x-x_1)/(x_2-x_1)$$



Interpolation Methods:

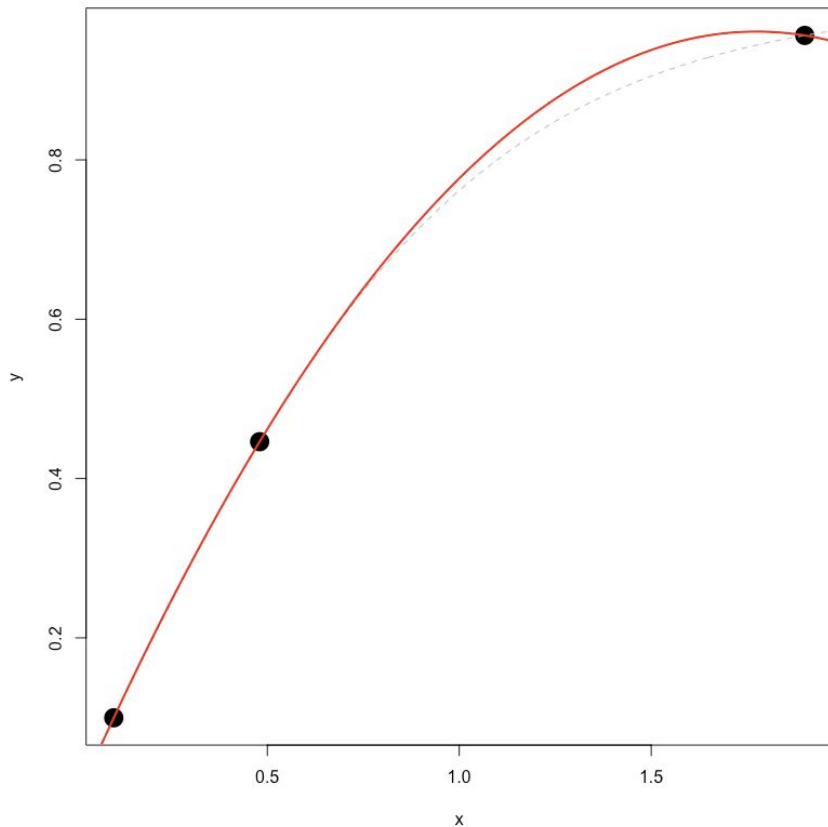
Polynomial interpolation

- For example with $n=3$ data points:

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \times \frac{x - x_2}{x_0 - x_2}$$

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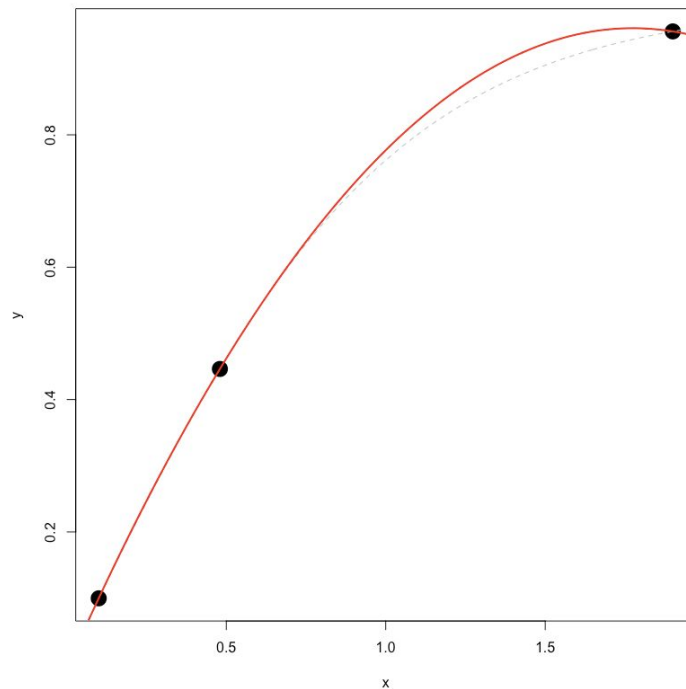
$$L_2(x) = \frac{x - x_0}{x_2 - x_0} \times \frac{x - x_1}{x_2 - x_1}$$



Interpolation Methods:

Polynomial interpolation

$$p(x) = \sum_{i=0}^{n-1} L_i(x) f_i(x)$$



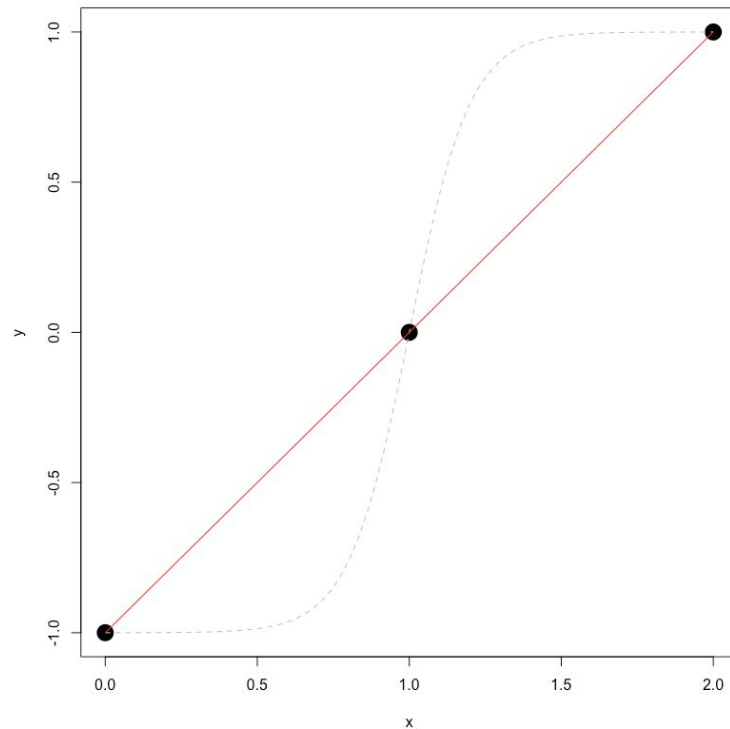
If equal spacings of Δx then this simplifies to:

$$p(x) = \frac{(x-x_1)(x-x_2)}{2\Delta x^2} f_0 - \frac{(x-x_0)(x-x_2)}{\Delta x^2} f_1 + \frac{(x-x_0)(x-x_1)}{2\Delta x^2} f_2$$

Interpolation Methods:

Polynomial interpolation

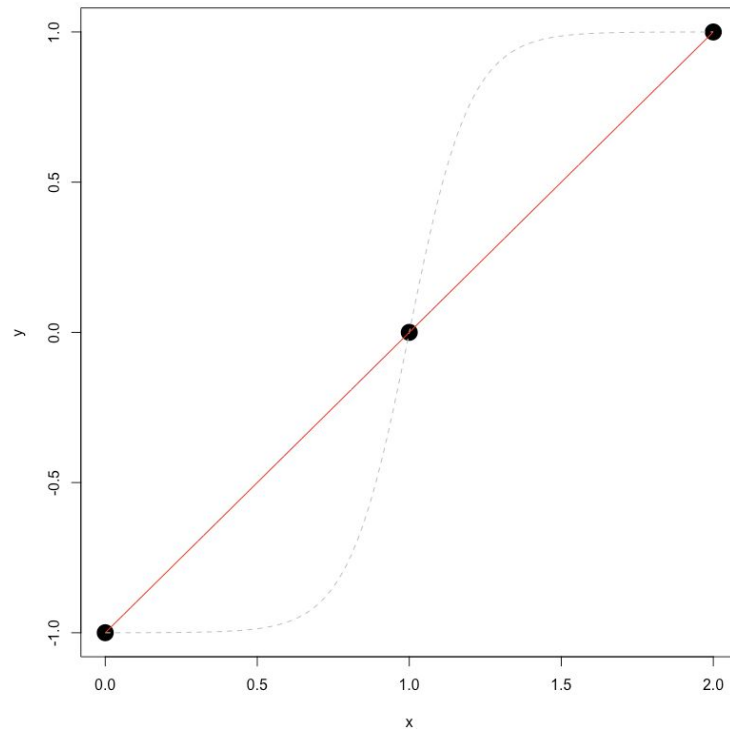
- **Pros:**
 - Easy to code and/or built-in to most languages (R, python, IDL)
 - Always finds a solution



Interpolation Methods:

Polynomial interpolation

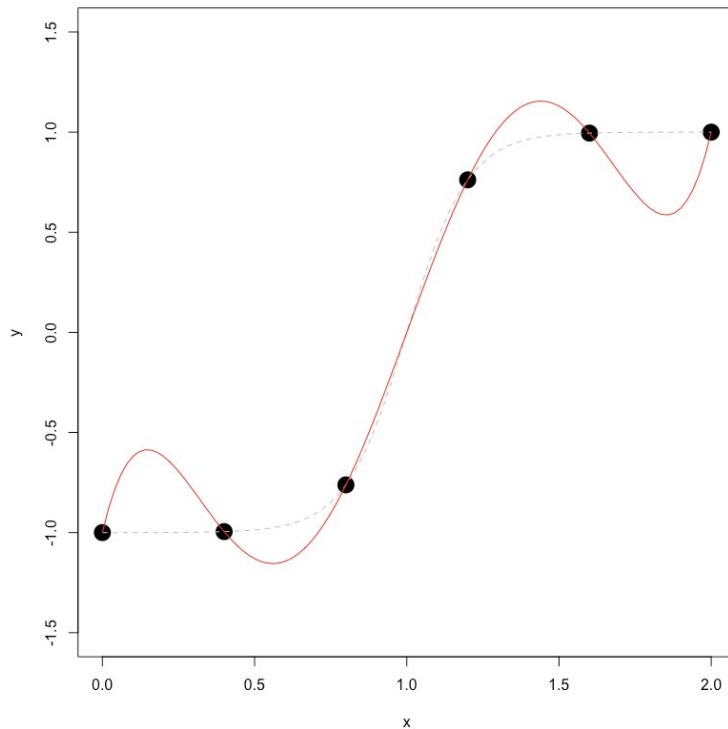
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 - As the number of points rise, some spacings will produce oscillations with large deviations



Interpolation Methods:

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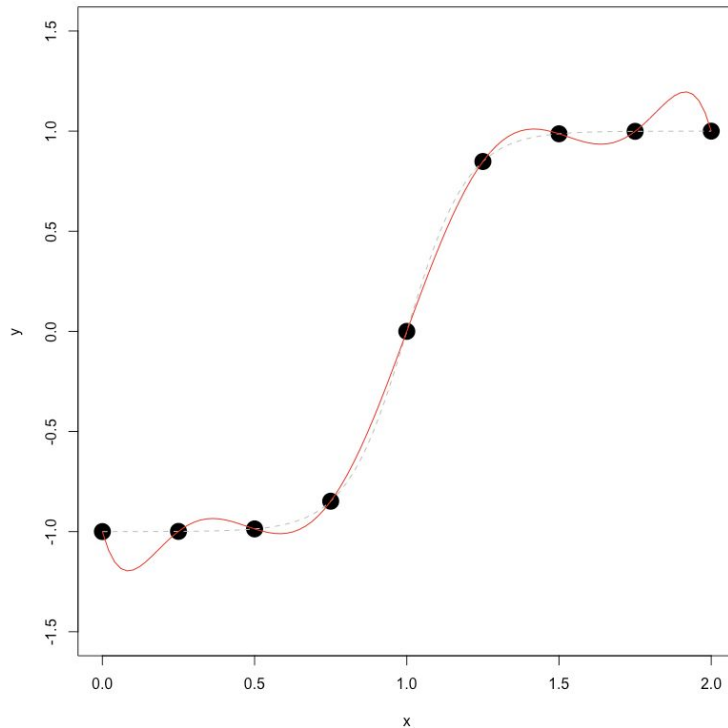
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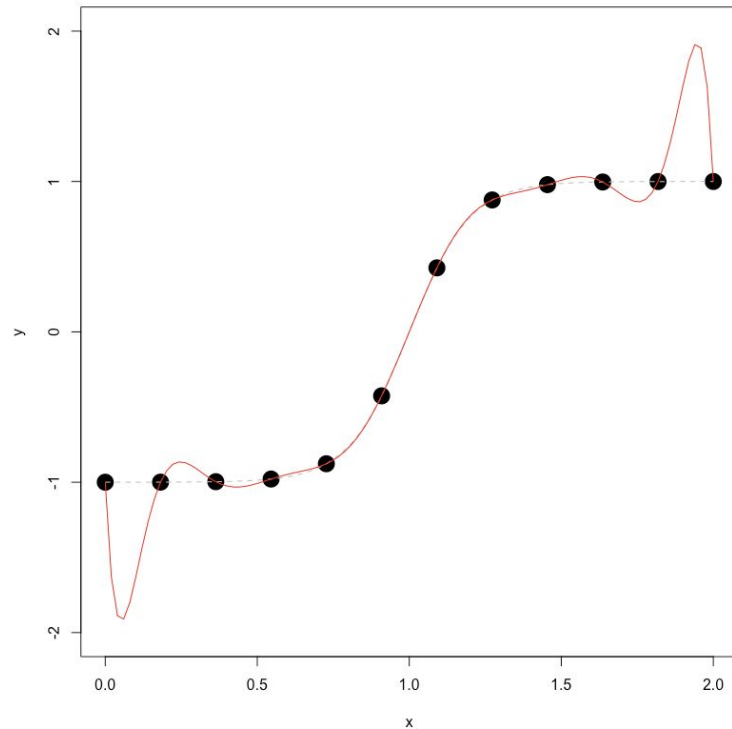
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Interpolation Methods:

Polynomial interpolation

- **Pros:**
 - Easy to code up, built-in to most languages (R, python, IDL)
 - Always finds a solution
- **Cons:**
 - As the number of points rise, some spacings will produce oscillations with large deviations
- Can be overcome if you can tailor the spacing of the points (*Chebyshev polynomial spacing*)



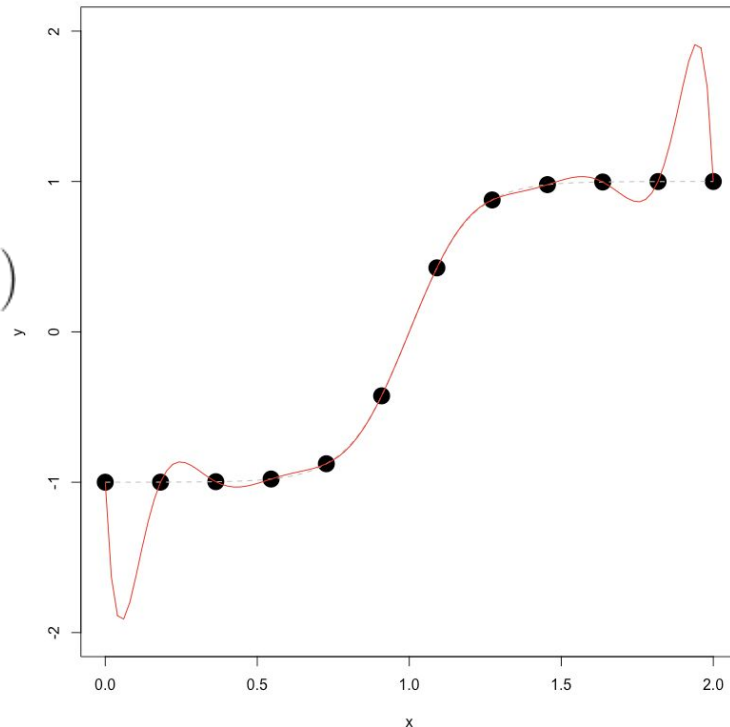
Interpolation Methods:

Aside: Assessing errors

- Formally consider the error of the interpolating polynomial bounded by:

$$f(x) - p(x) = \frac{f^{(n+1)}(u)}{(n+1)!} (x - x_0) \dots (x - x_n)$$

- Numerator is $(n+1)^{th}$ derivative of f at some point u within the interval of interest [at most over, $(a,b) = (x_0, x_n)$]



Interpolation Methods:

Aside: Assessing errors

- Often care about the maximum over an interval, so can consider:

$$E(x) = |f(x) - p(x)| \leq \max_{[a,b]} \left| \frac{f^{(n+1)}(u)}{(n+1)!} \right| \max_{[a,b]} \left| \prod_{i=0}^n (x - x_i) \right|$$

- Can revisit the statement about why linear approximation error goes as order $\sim (\Delta x)^2$

Interpolation Methods:

Aside: Assessing errors

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- In linear approximation case, for an unknown true function f , the approximation between x_i and x_{i+1} depends on the maximal curvature (f'') and the product of $|(x-x_0)(x-x_1)|$

Interpolation Methods:

Aside: Assessing errors

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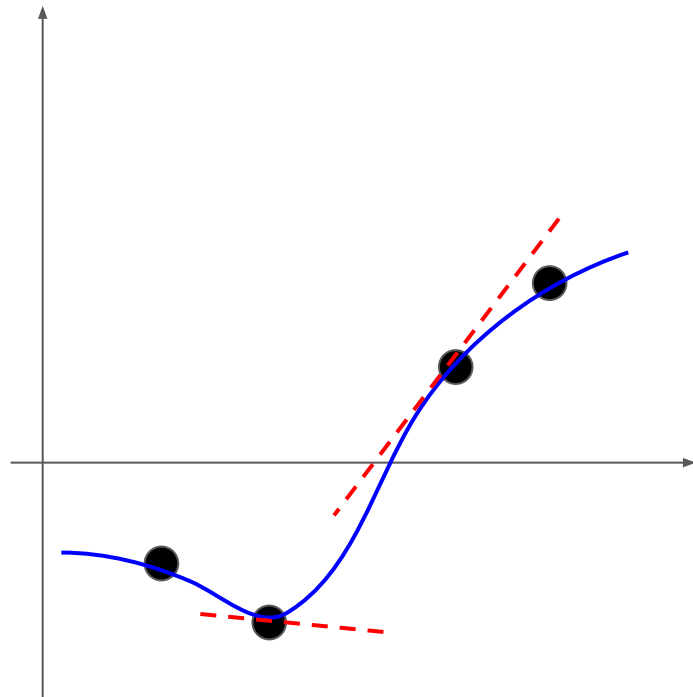
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- For generic interpolating functions we practically would want to then:
 - - if possible estimate maximum of $f^{(n+1)}(a < u < b)$
 - - compute maximum of $(x-x_0)(x-x_1)\dots(x-x_n)$ over all $(a < x < b)$

Interpolation Methods:

Hermite interpolation

- Can also include information on local derivative to improve accuracy.



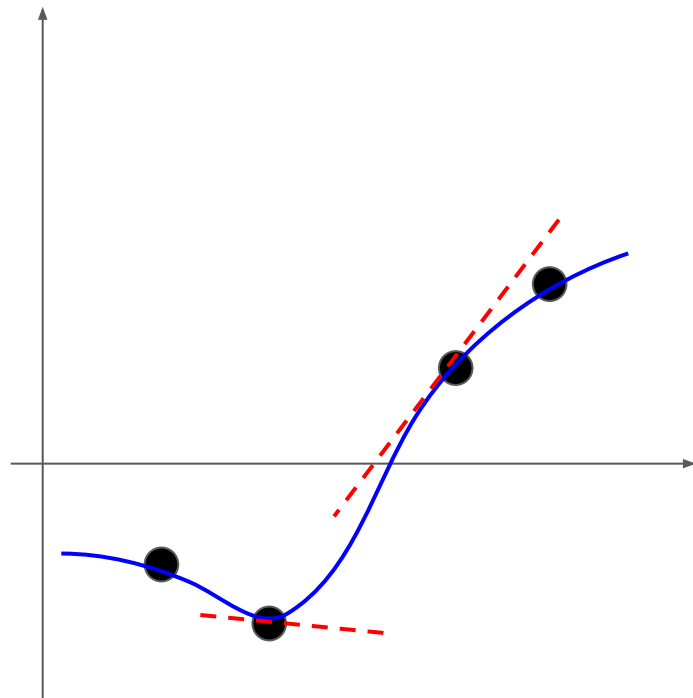
Interpolation Methods:

Hermite interpolation

- Can also include information on local derivative to improve accuracy.
- Polynomial of order n is:

$$f(x) = \sum_{i=0}^{n-1} A_i(x) f_i + \sum_{i=0}^{n-1} B_i(x) f'_i$$

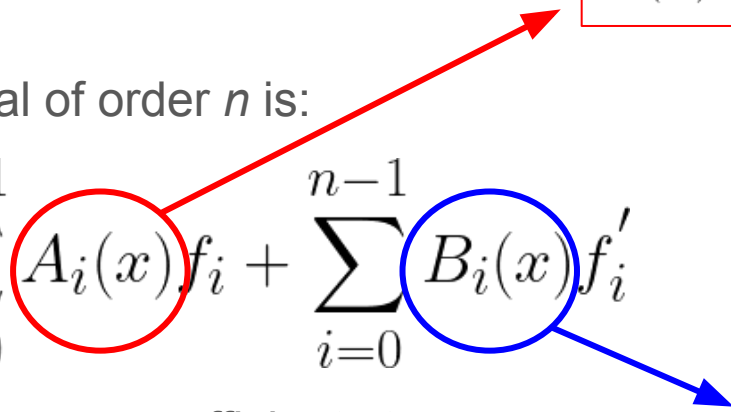
- Computes new coefficients to use with local derivatives and derivatives of Lagrange coefficients



Interpolation Methods:

Hermite interpolation

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- Polynomial of order n is:

$$f(x) = \sum_{i=0}^{n-1} A_i(x) f_i + \sum_{i=0}^{n-1} B_i(x) f'_i$$


$$A_i(x) = \left(1 - 2(x - x_i)L'_i(x_i)\right) \times L_i^2(x)$$

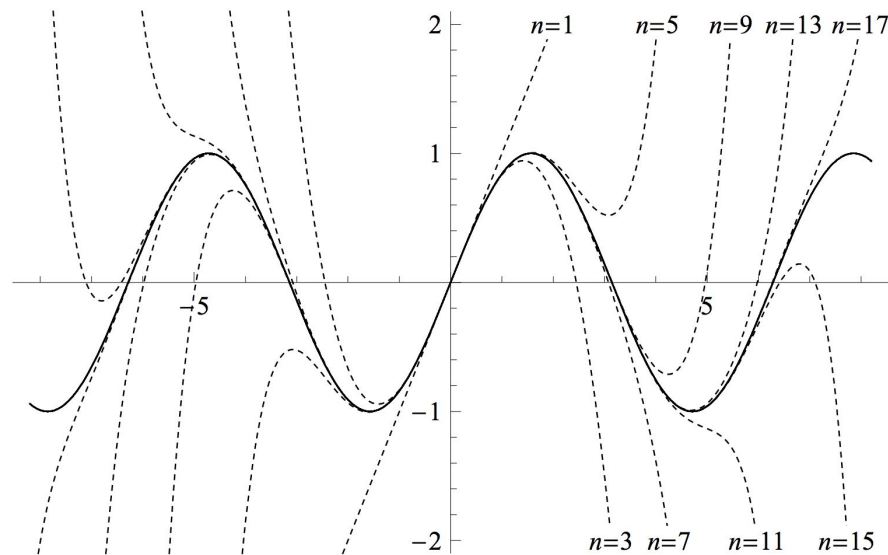
- Computes new coefficients to use with local derivative and derivative of Lagrange coefficients

$$B_i(x) = (x - x_i)L_i(x)^2$$

Interpolation Methods:

Taylor interpolation

- Hermite polynomials match the function and its first derivative at a set of particular points

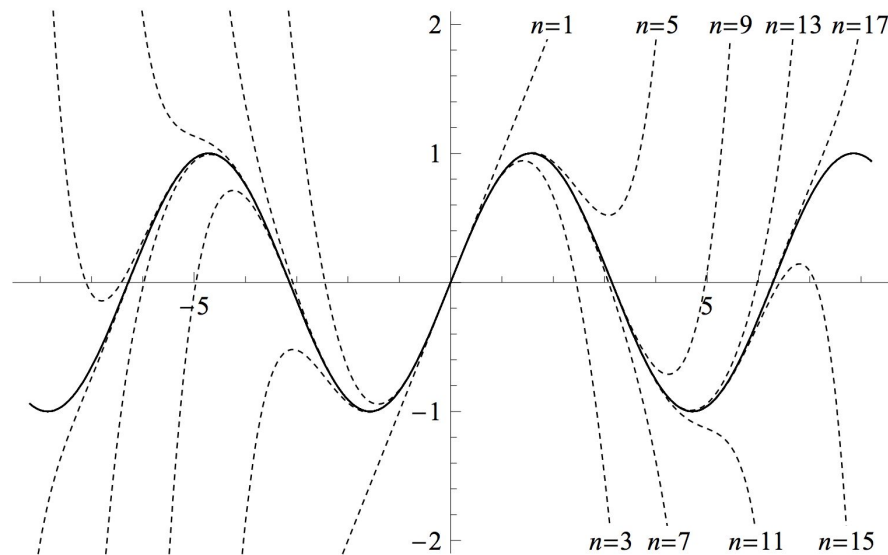


Taylor polynomials for different orders at the origin of $y = \sin(x)$

Interpolation Methods:

Taylor interpolation

- Hermite polynomials match the function and its first derivative at a set of particular points
- Taylor polynomial methods extend this to make the j^{th} derivative match at the same point x_i
[e.g., $p^{(j)}(x_i) = f^{(j)}(x_i)$]

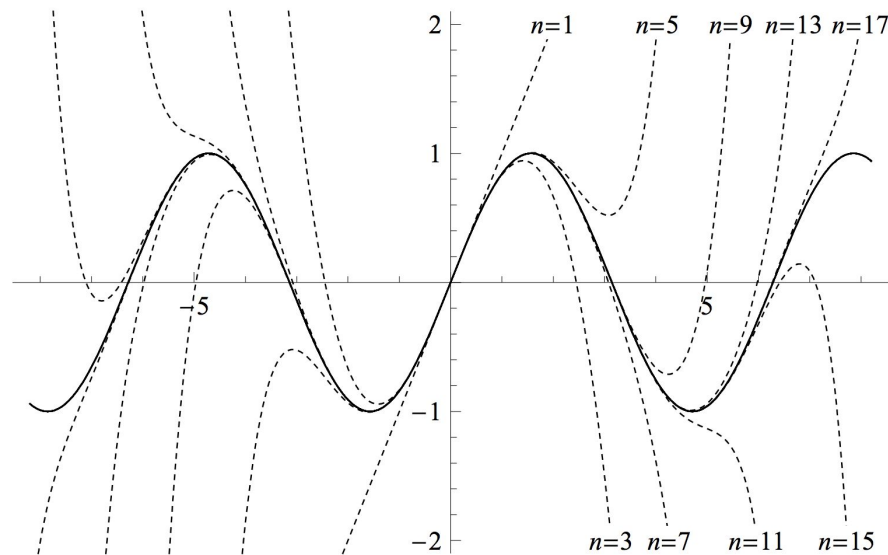


Taylor polynomials for different orders at the origin of $y = \sin(x)$

Interpolation Methods:

Taylor interpolation

$$p_j(f; a)(x) = \sum_{j=0}^m \frac{f^{(j)}(a)}{j!} (x - a)^j$$



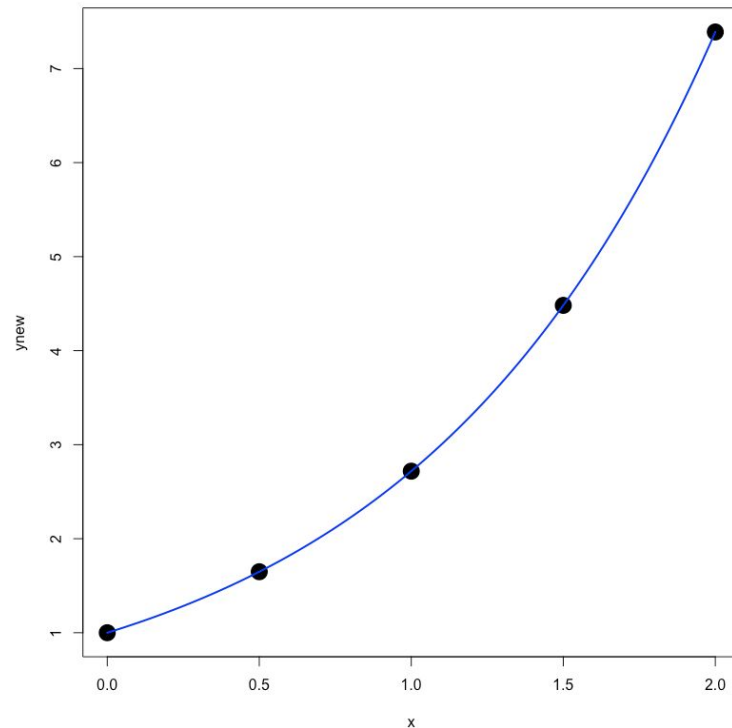
Taylor polynomials for different orders at the origin of
 $y = \sin(x)$

Interpolation Methods:

Taylor interpolation

- Simple Example: Approximate $y = e^x$ expanding about $a=0$

$$p_j(f; a)(x) = \sum_{j=0}^m \frac{f^{(j)}(a)}{j!} (x - a)^j$$

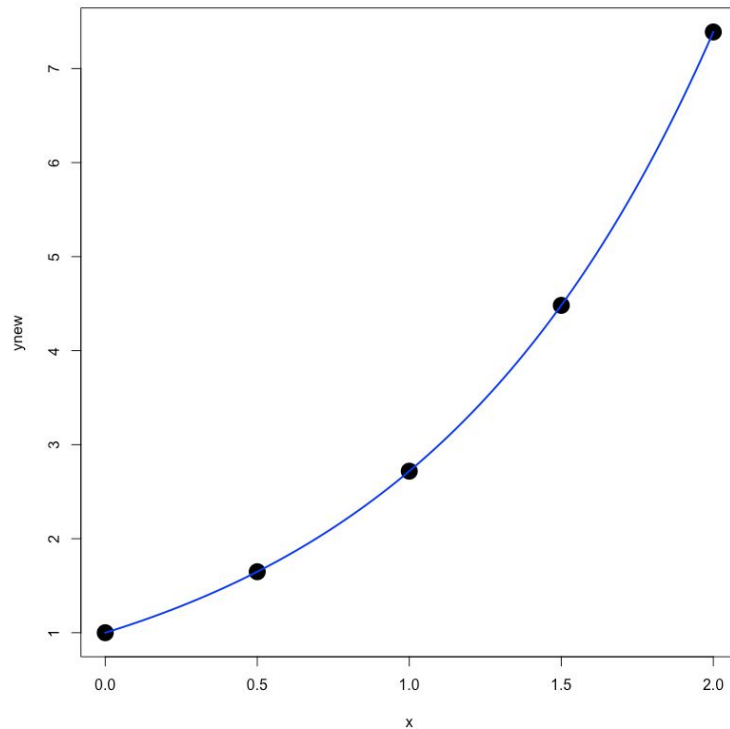


Interpolation Methods:

Taylor interpolation

- Error bound in Taylor polynomial typically cares about what order (j) you are using for the approximation

$$E(x) = p(x) - f(x) = \frac{(x - a)^{j+1}}{(j + 1)!} f^{(j+1)}(u)$$



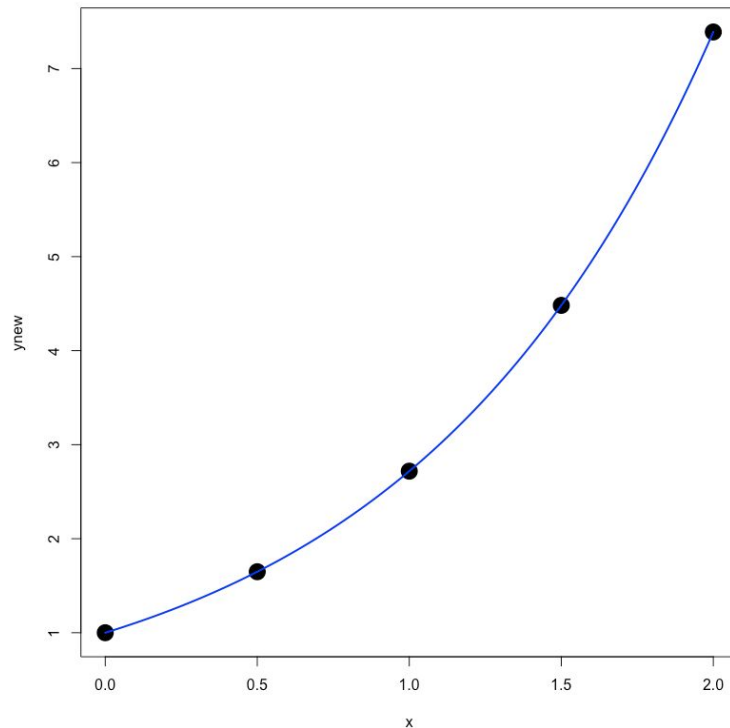
Interpolation Methods:

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$$E(x) = p(x) - f(x) = \frac{(x - a)^{j+1}}{(j + 1)!} f^{(j+1)}(u)$$

- Continuing our example - how precise do we approximate $f = e^x$ at $x=1$ with $p_5(f; a=0)(x)$?



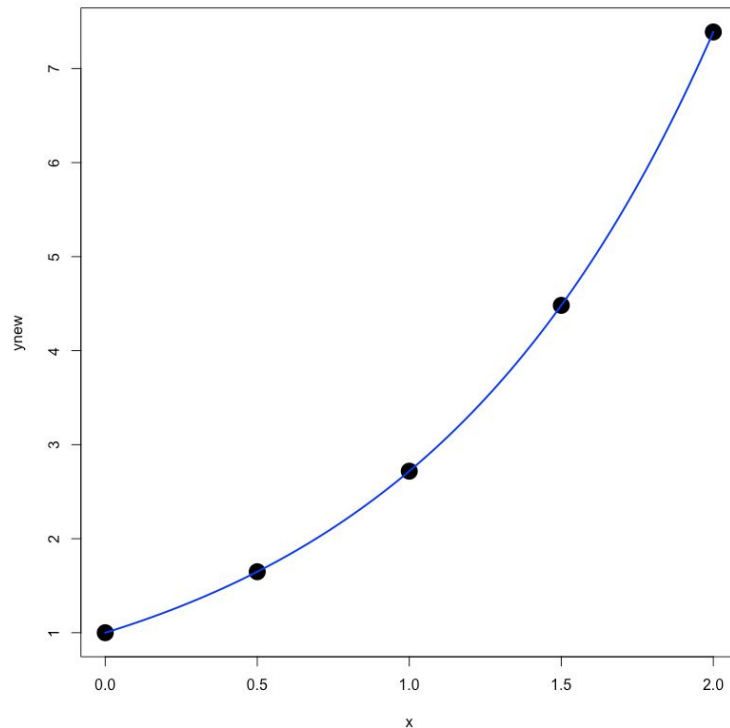
Interpolation Methods:

Taylor interpolation

- **First term** reduces to $1/(6!)$

(for $a=0, x=1, j=5$)

$$E(x) = \frac{(x - a)^{j+1}}{(j + 1)!} f^{(j+1)}(u)$$

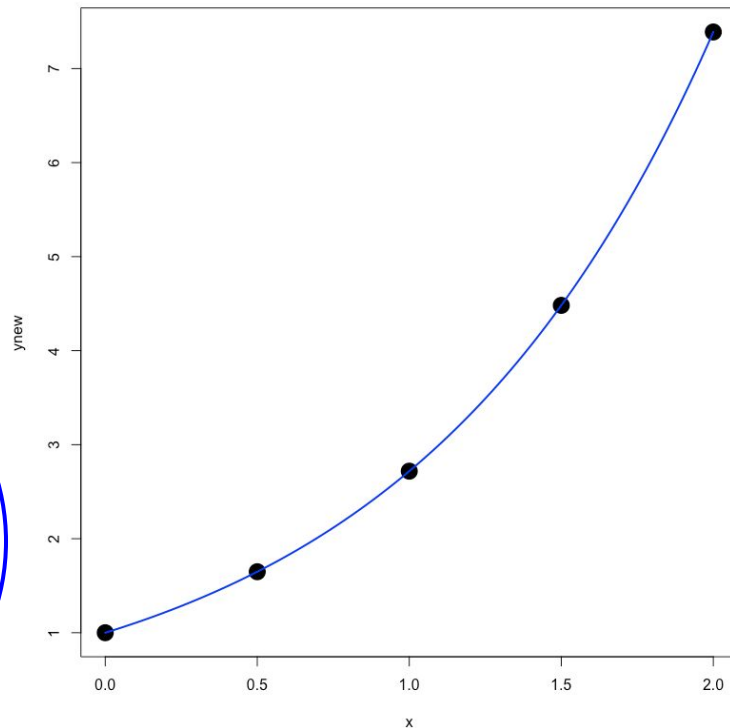


Interpolation Methods:

Taylor interpolation

- **Second term** is asking what the j^{th} derivative of the function is at some value u .

$$E(x) = \frac{(x - a)^{j+1}}{(j + 1)!} f^{(j+1)}(u)$$

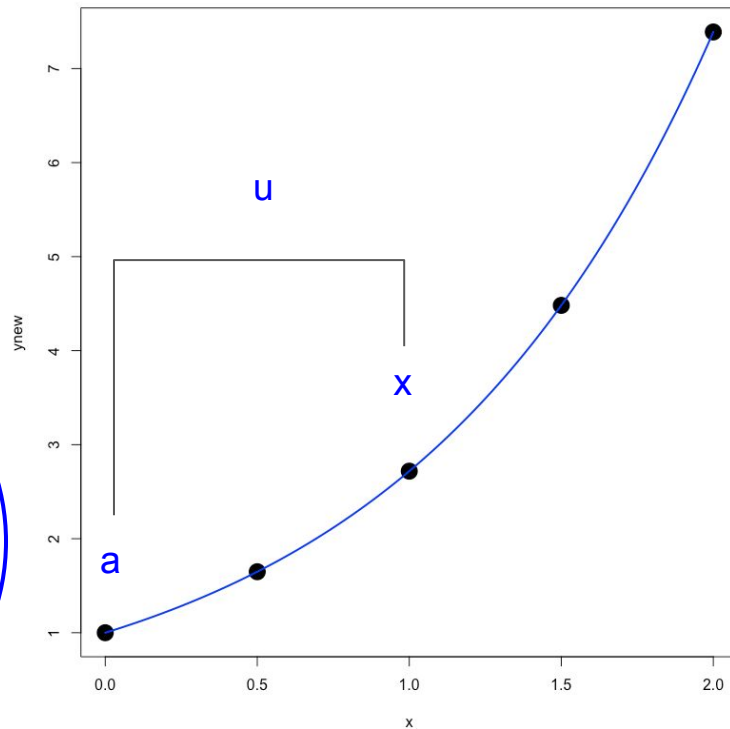


Interpolation Methods:

Taylor interpolation

- **Second term** is asking what the j^{th} derivative of the function is at some value u .
- We know that $a < u < x$ in this example

$$E(x) = \frac{(x - a)^{j+1}}{(j + 1)!} f^{(j+1)}(u)$$



Interpolation Methods:

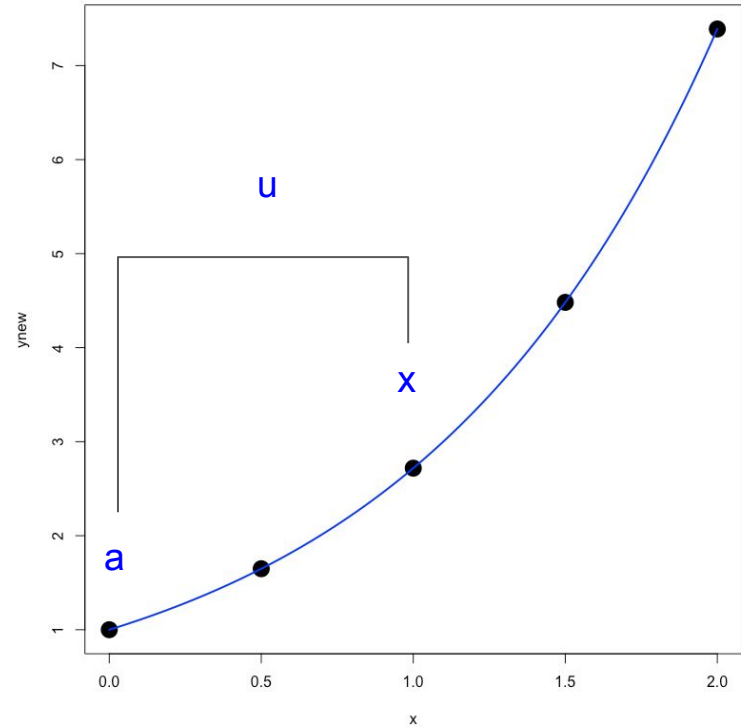
Taylor interpolation

- Expected error reduces to

$$E_5(x) = \frac{1}{6!} f^{(6)}(u \in [0, 1])$$

- Given that $f(x) = e^x$ and $u < 1$ we can bound maximum absolute error:

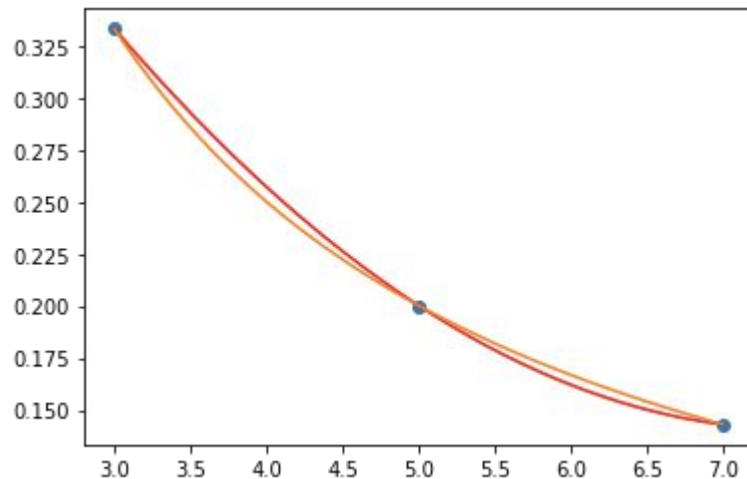
$$E_5(x) = \frac{1}{6!} f^{(6)}(u) \leq \frac{e^u}{6!} \leq \frac{e^1}{6!} \sim 0.00378$$



Interpolation Methods:

More ill-behaved examples

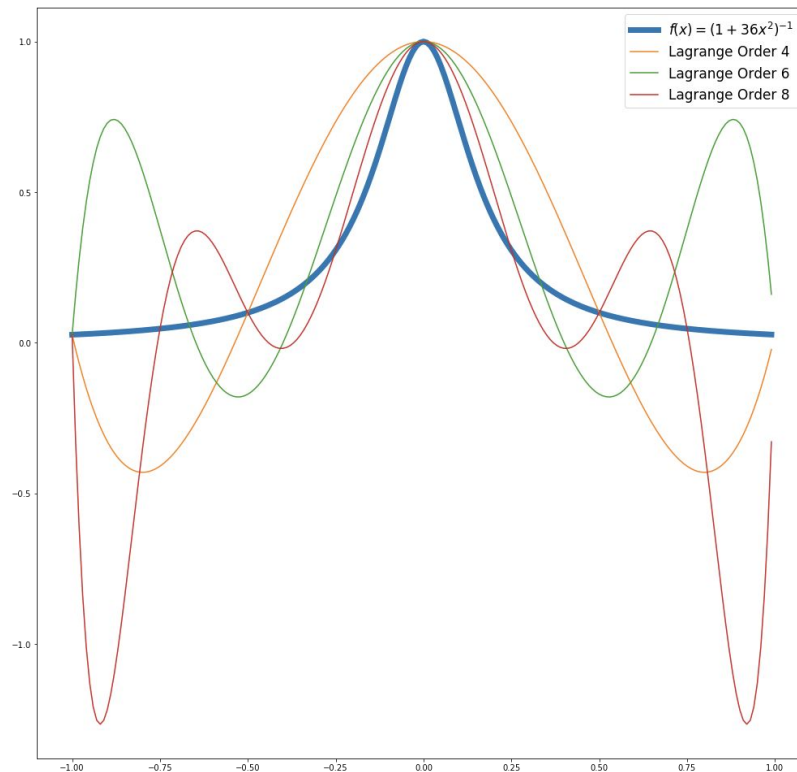
- What is guaranteed in these simple interpolation schemes, is that there **is a polynomial of some order n** which will pass through the points, **and reproduce the function to within a maximal interpolation error, $E_{n,\max}$**
- It is ***not guaranteed*** that the maximum error $E_{\max} \rightarrow 0$ as $n \rightarrow$ becomes large!



Interpolation Methods:

More ill-behaved examples

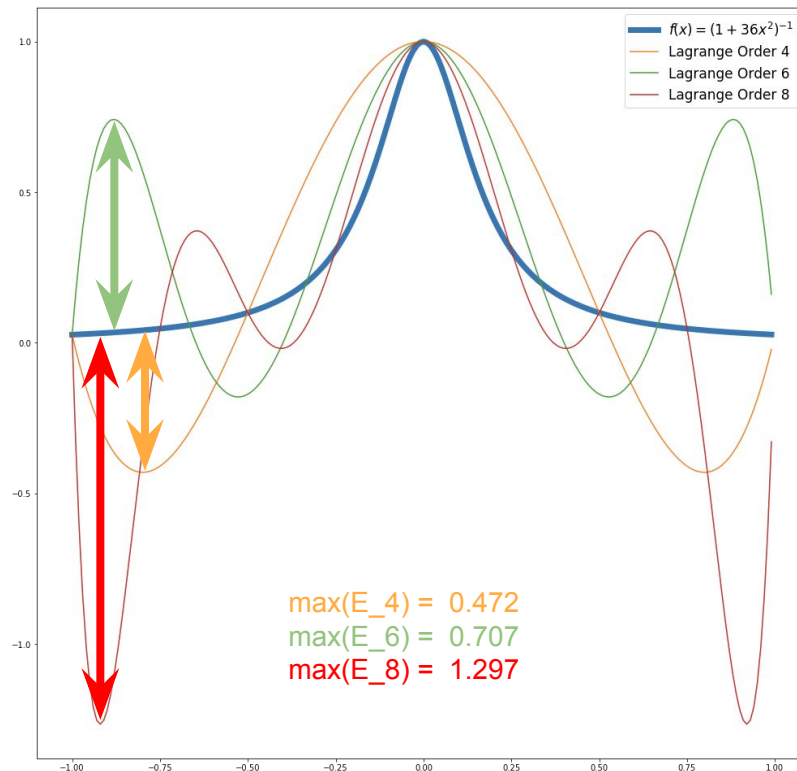
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Interpolation Methods:

More ill-behaved examples

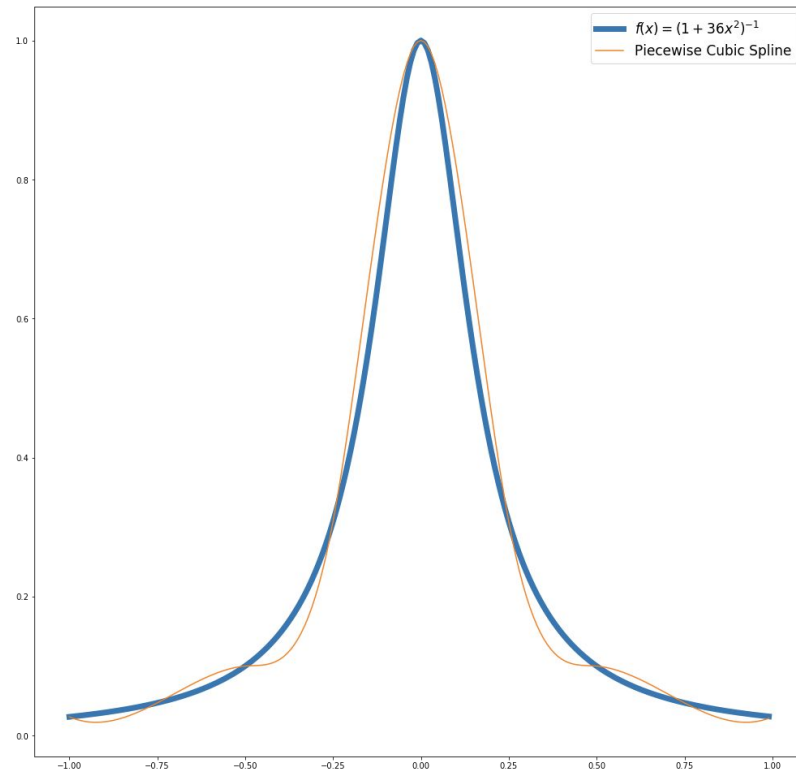
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Interpolation Methods:

More ill-behaved examples

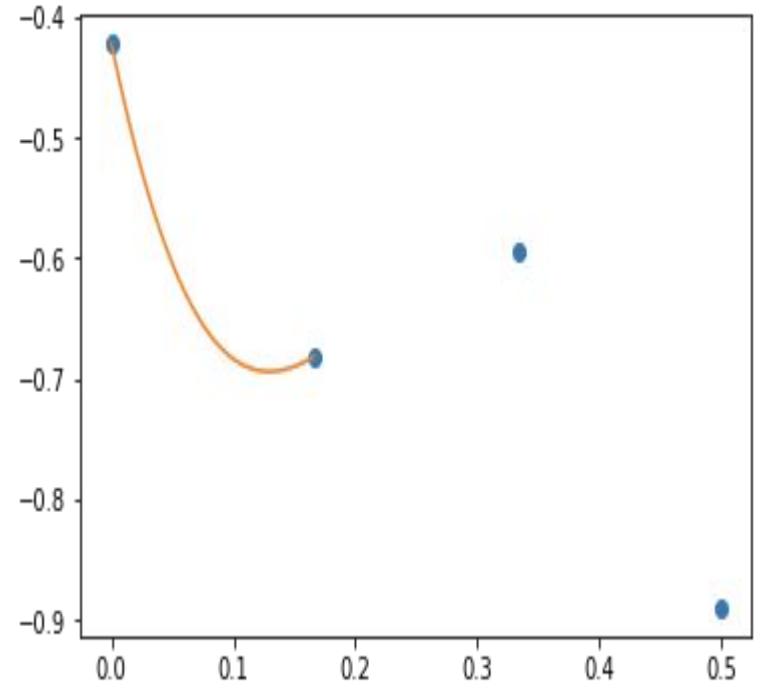
- We can try to improve this behaviour by considering *piecewise* interpolating functions.
- These divide the function into segments and impose boundary conditions for how interpolants must behave and inter-connect.



Interpolation Methods:

Spline interpolation

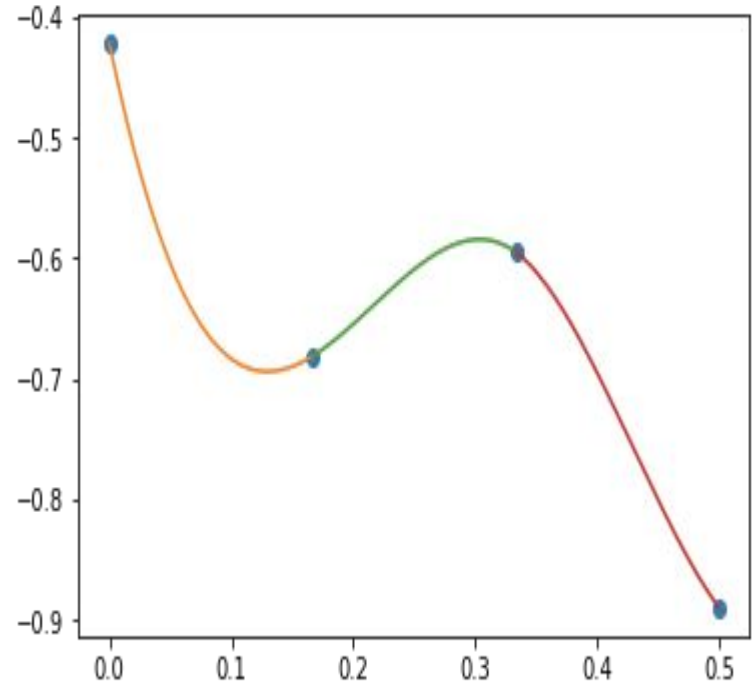
- To avoid errors with large number of points, we can break apart the data set into piecewise segments.



Interpolation Methods:

Spline interpolation

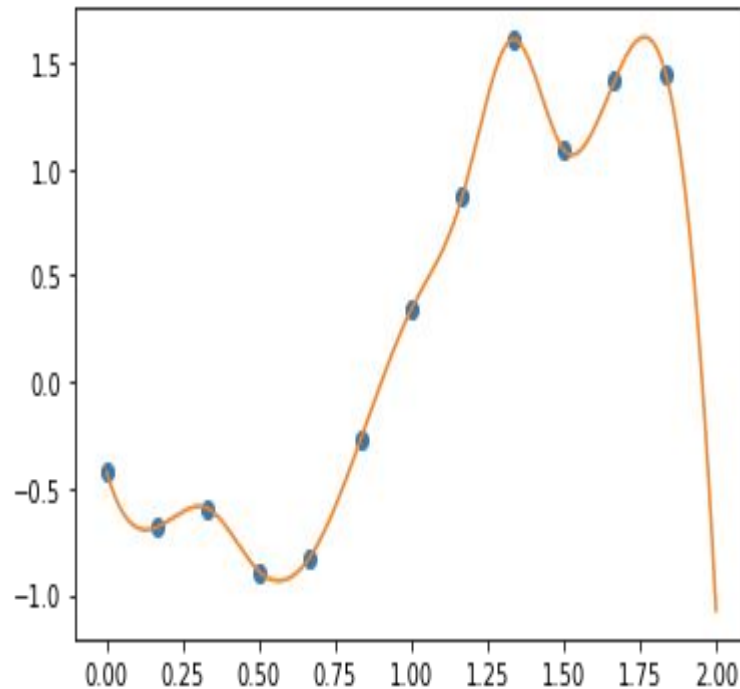
- To avoid errors with large number of points, we can break apart the data set into piecewise segments.
- Find flexible polynomials which reproduce continuity (slope and curvature) with the next segment



Interpolation Methods:

Spline interpolation

- To avoid errors with large number of points, we can break apart the data set into piecewise segments.
- Find flexible polynomials which reproduce continuity (slope and curvature) with the next segment
- Formally we require the first and second derivatives of each endpoint to match for each cubic polynomial constructed for a segment.

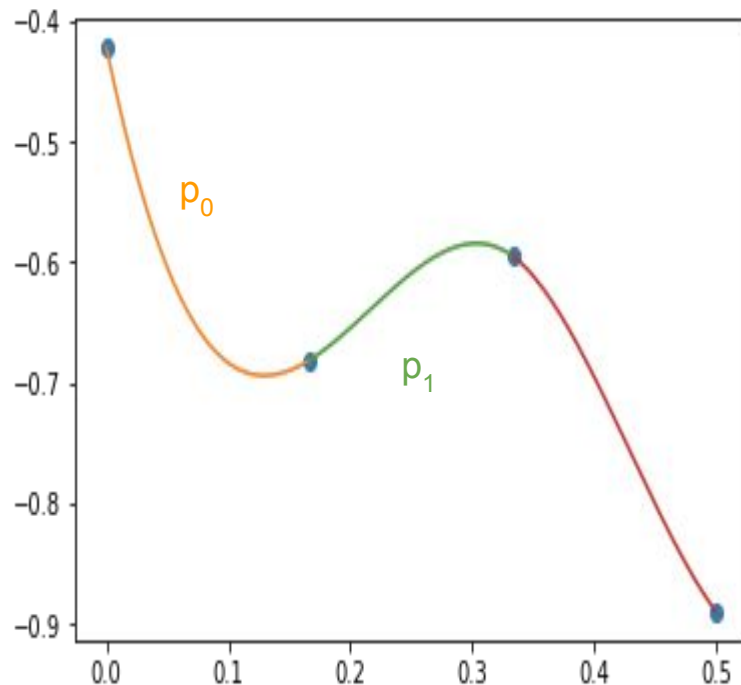


Interpolation Methods:

Spline interpolation

- In brief, for cubic splines ($m=3$), for each interval you have a polynomial which reproduces those points

$$p_i(x) = \sum_{k=0}^{m=3} c_{i,k} x^k$$

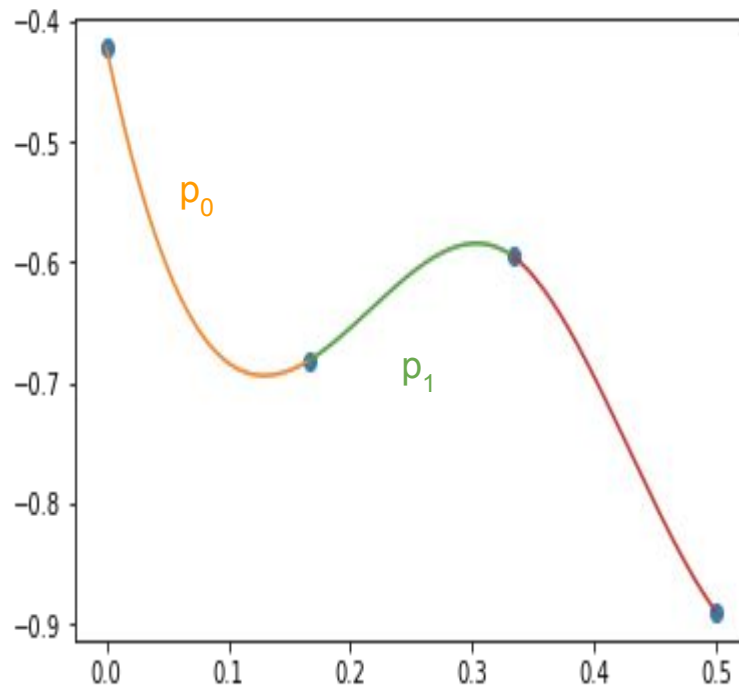


Interpolation Methods:

Spline interpolation

- Also require $j=0,\dots,m-1$ derivatives to match at interval transition points

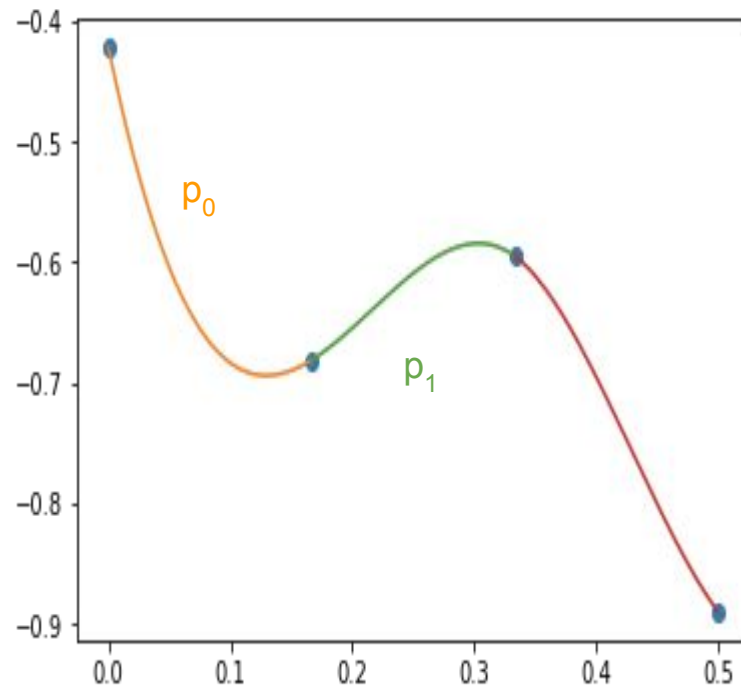
$$p_i^j(x_{i+1}) = p_{i+1}^j(x_{i+1})$$



Interpolation Methods:

Spline interpolation

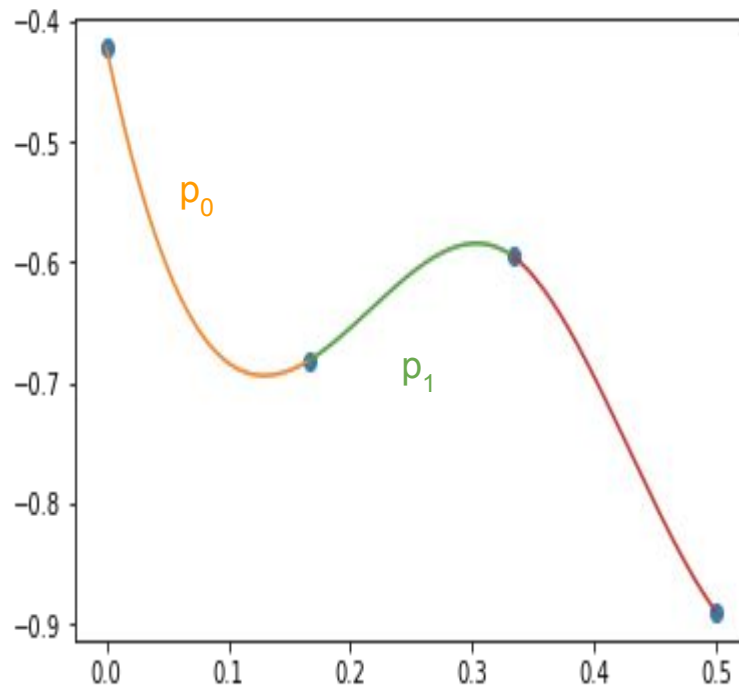
- If you have n data points, there are **$n-1$** intervals of $[x_i, x_{i+1}]$



Interpolation Methods:

Spline interpolation

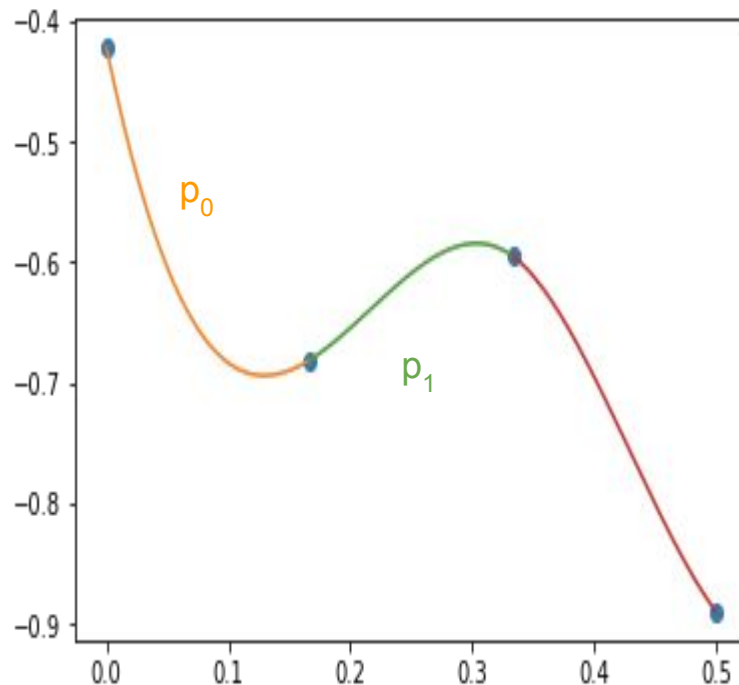
- If you have n data points, there are **$n-1$** intervals of $[x_i, x_{i+1}]$
- In each interval you have a polynomial that has order j with **$j+1$** coefficients



Interpolation Methods:

Spline interpolation

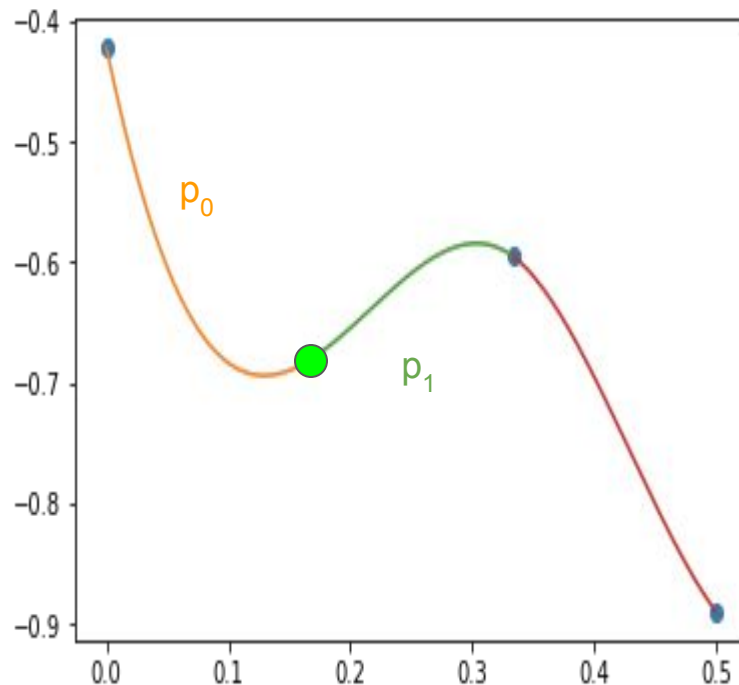
- If you have n data points, there are **$n-1$** intervals of $[x_i, x_{i+1}]$
- In each interval you have a polynomial that has order j with **$j+1$** coefficients
- Need to jointly solve for coefficients of all polynomials together →
Need **$(j+1)(n-1)$** (*= 12 constraints, in this example*)



Interpolation Methods:

Spline interpolation

- For all **middle points** you get continuity constraints between $p_i^j(x_i) = p_{i+1}^j(x_i)$ up to $j=m-1$



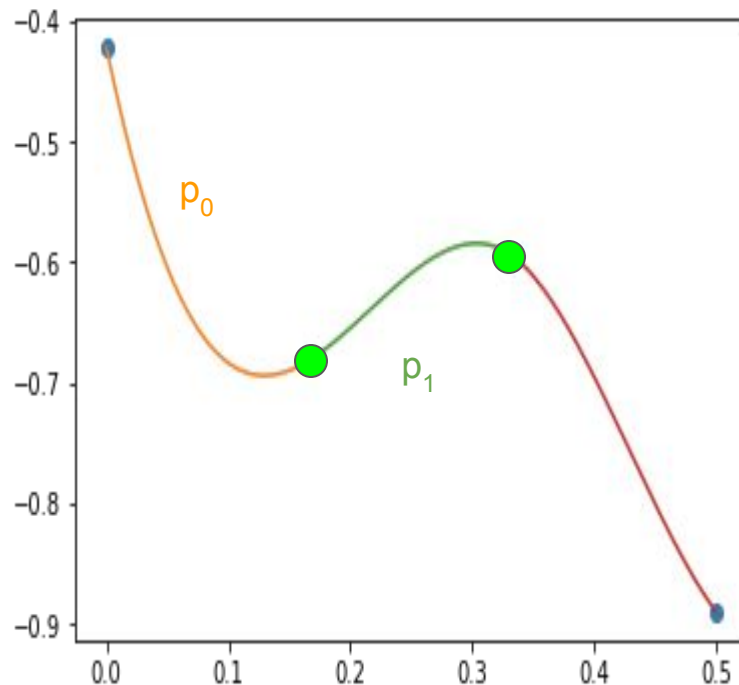
Interpolation Methods:

Spline interpolation

- For all **middle points** you get continuity constraints between $p_i^j(x_i) = p_{i+1}^j(x_i)$ up to $j=m-1$
- E.g.,

$$\begin{aligned}p_0(x_1) &= p_1(x_1) = y_1 \\p_0'(x_1) &= p_1'(x_1) \\p_0''(x_1) &= p_1''(x_1)\end{aligned}$$

- Same for other middle point... so **8** constraints so far

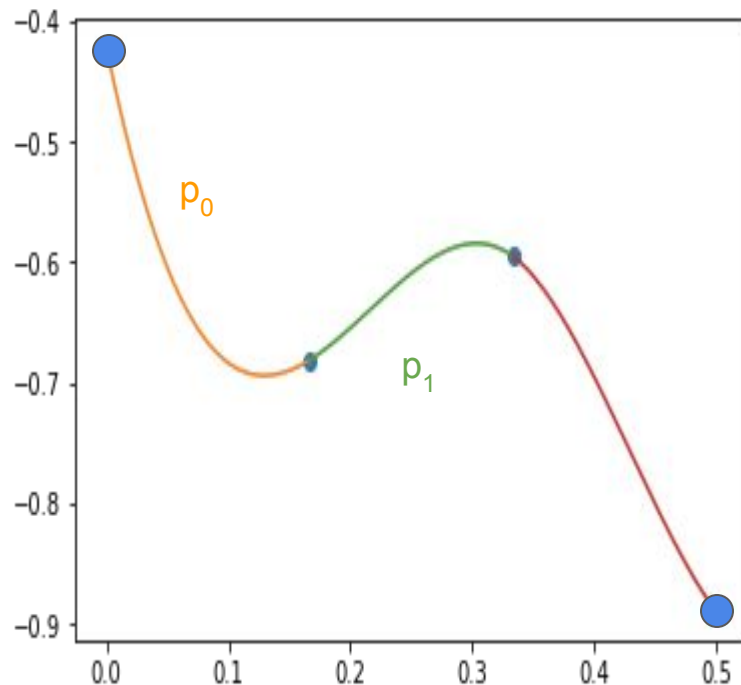


Interpolation Methods:

Spline interpolation

- **First and last point** must trivially satisfy the value of the data

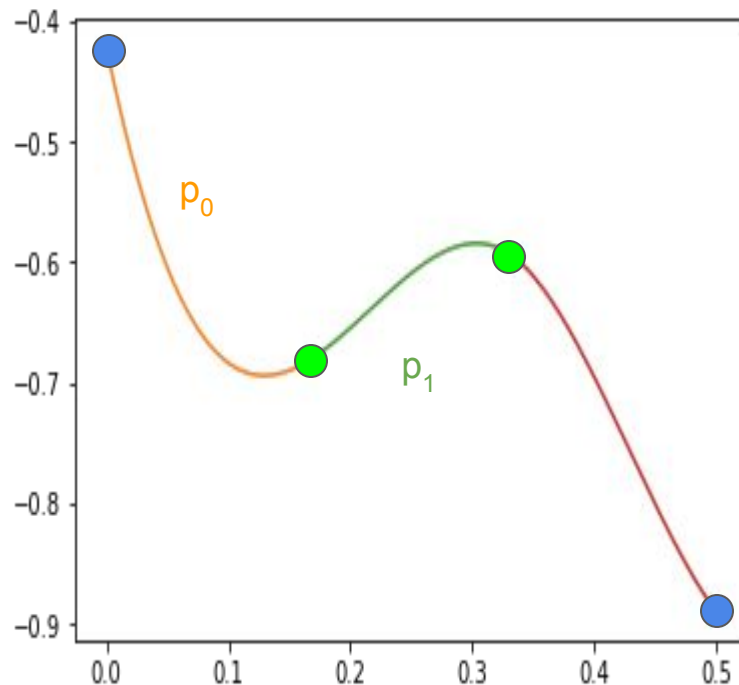
$$p_0(x_0) = y_0 \quad ; \quad p_2(x_3) = y_3$$



Interpolation Methods:

Spline interpolation

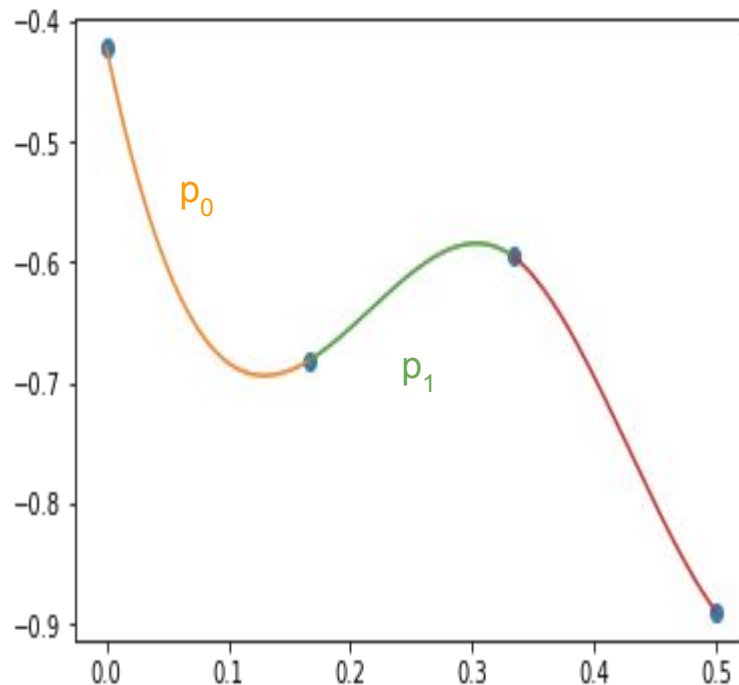
- **First and last point** must trivially satisfy the value of the data
 $p_0(x_0) = y_0$; $p_2(x_3) = y_3$
- This is now **10** constraints out of **12** in this example.



Interpolation Methods:

Spline interpolation

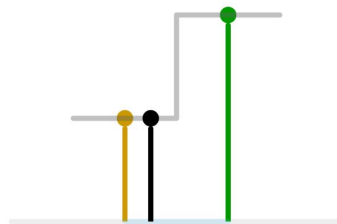
- First and last point must trivially satisfy the value of the data
 $p_0(x_0) = y_0$; $p_2(x_3) = y_3$
- This is now **10** constraints out of **12** in this example.
- For last two constraints often set second derivative of the first and last point to zero, or linearly extrapolate and set continuity to that line - or any other arbitrary slope.



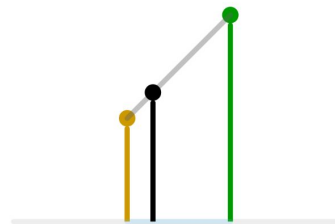
Interpolation Methods:

2D interpolation

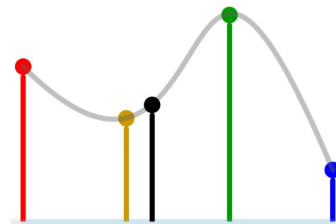
- We can extend some of these interpolation schemes easily to higher dimensions.
- Typically you will want to use some built-in routines to do this, but bi-linear or bi-cubic interpolation are conceptually and algorithmically easy to understand



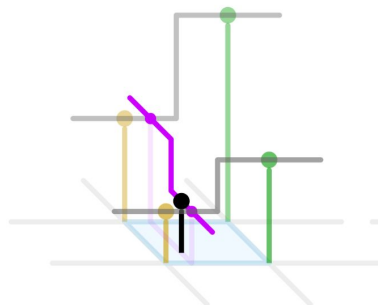
1D nearest-neighbour



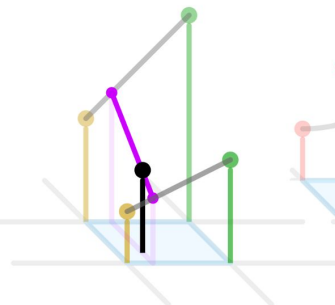
Linear



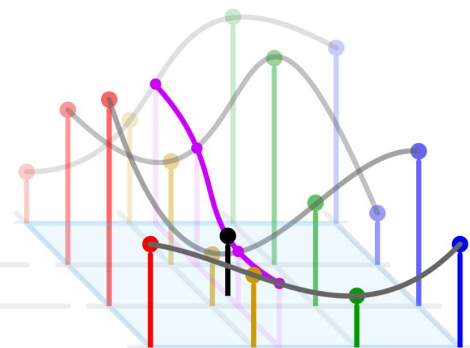
Cubic



2D nearest-neighbour



Bilinear

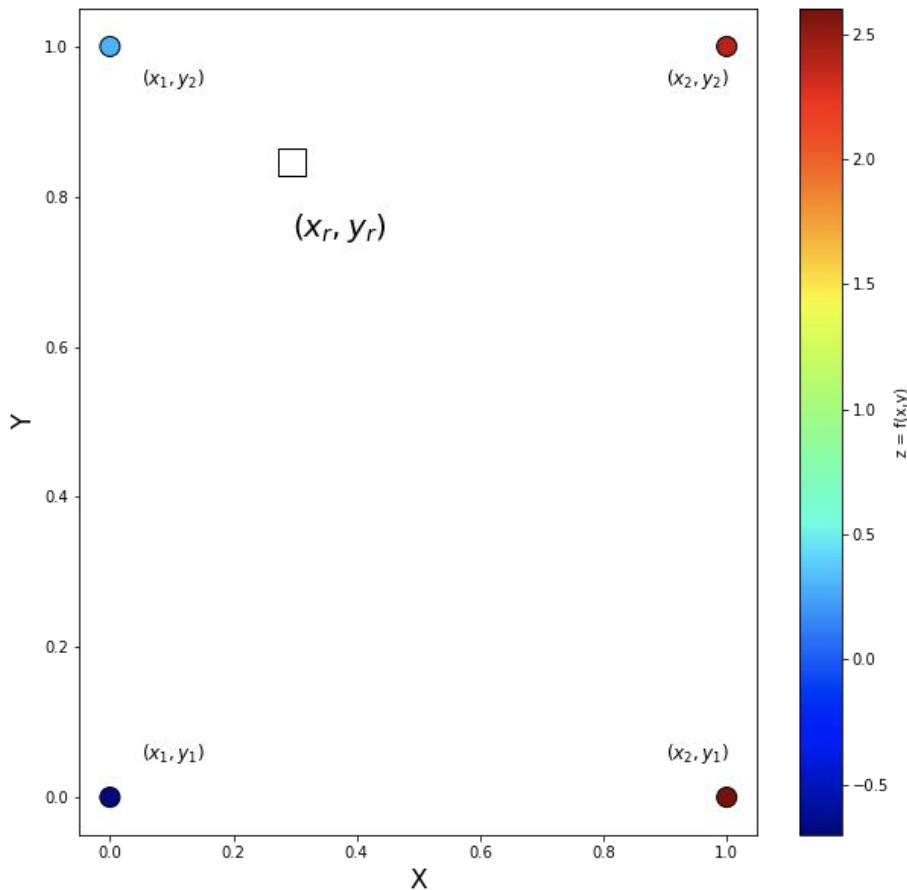


Bicubic

Interpolation Methods:

2D interpolation

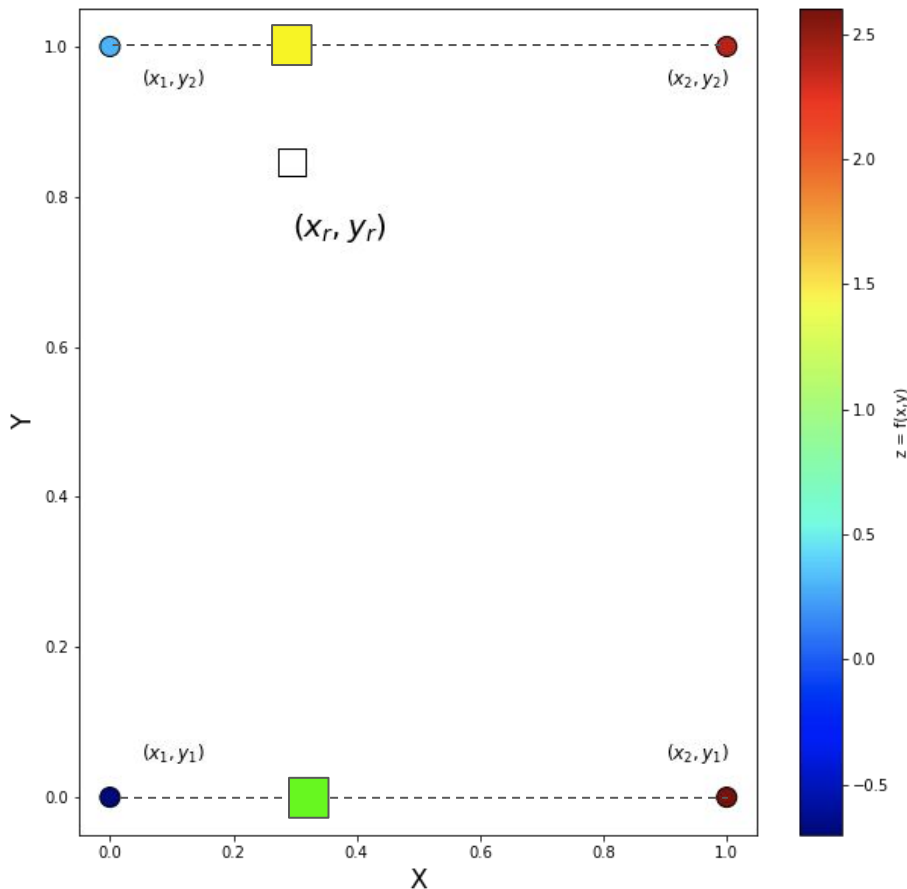
- Finding $f(x,y)$ at an arbitrary location based on known surrounding data is not a linear problem in general.



Interpolation Methods:

2D interpolation

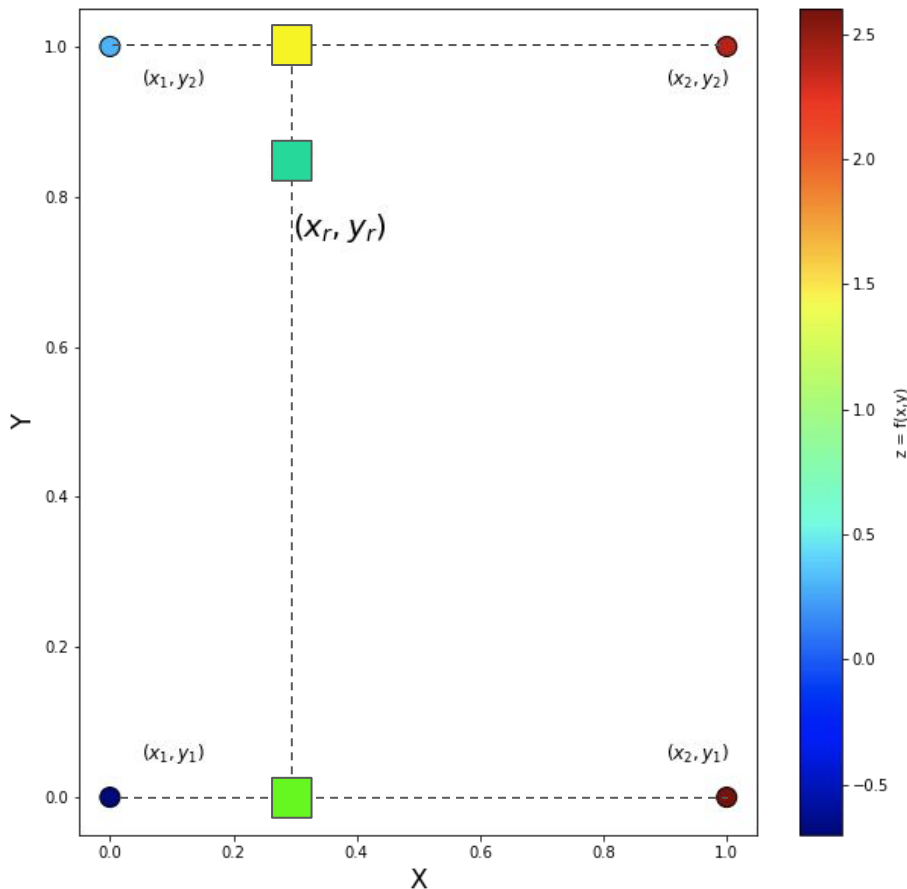
- Finding $f(x,y)$ at an arbitrary location based on known surrounding data is not a linear problem in general.
- However a direct approach is to approximate the parameter space as linear in x and y separately.



Interpolation Methods:

2D interpolation

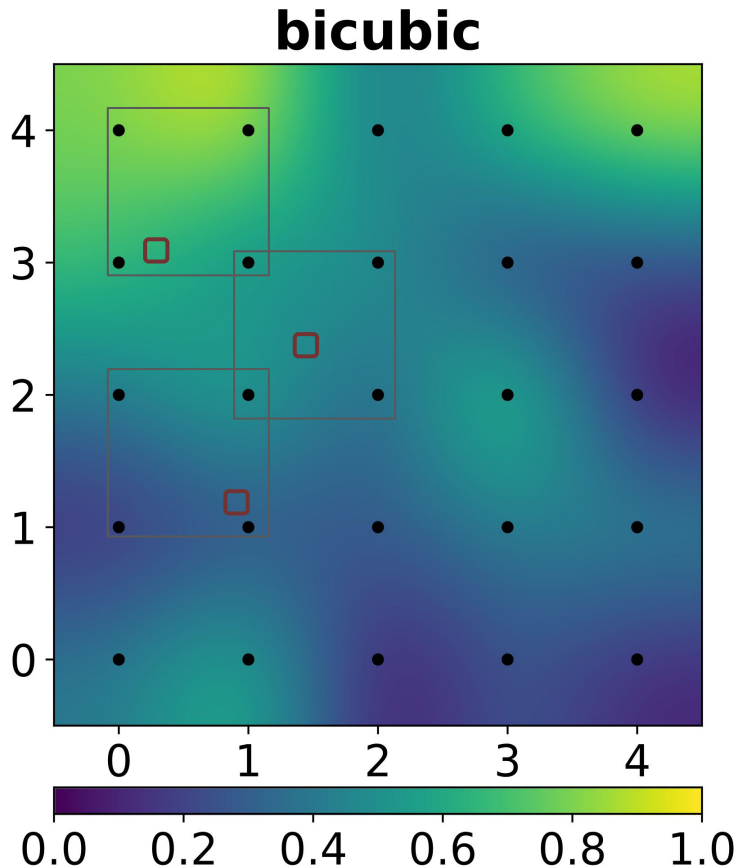
- Finding $f(x,y)$ at an arbitrary location based on known surrounding data is not a linear problem in general.
- However a direct approach is to approximate the parameter space as linear in x and y separately.



Interpolation Methods:

2D interpolation

- Whether bi-linear, or bi-cubic or 2D spline, most algorithms will do this piece-wise in 2D.
- Particularly common for image resampling and compression
- These would still be considered deterministic interpolation methods



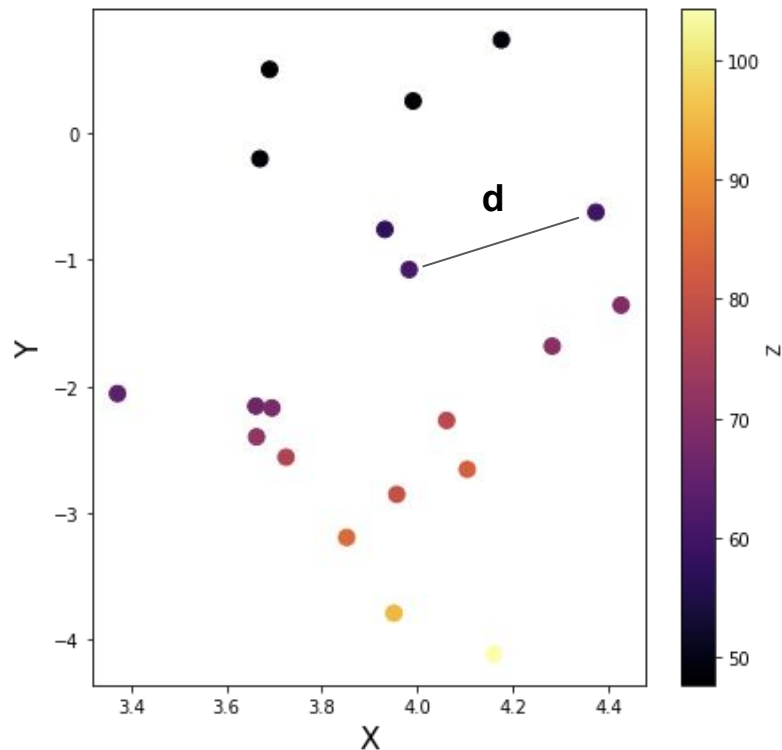
Interpolation Methods:

2D interpolation

- First, one computes a semivariogram - half the variance between data points as a function of their separation

$$\gamma(d) = \frac{1}{2} \text{mean}((z_i - z_j)^2)$$

- Typically bin in pair separation (d) and then compute the quantity γ for all points with roughly that pair separation



Interpolation Methods:

2D interpolation

- Plotting them gives you a sense of how the data are correlated at different spatial scales.
- Typically an analytic function is fit to the semivariogram data
- This helps provide a smooth computation of the weights which go into interpolating a 2D data set

$$z(x_{new}, y_{new}) = \sum_i^N \lambda_i z(x_i, y_i)$$

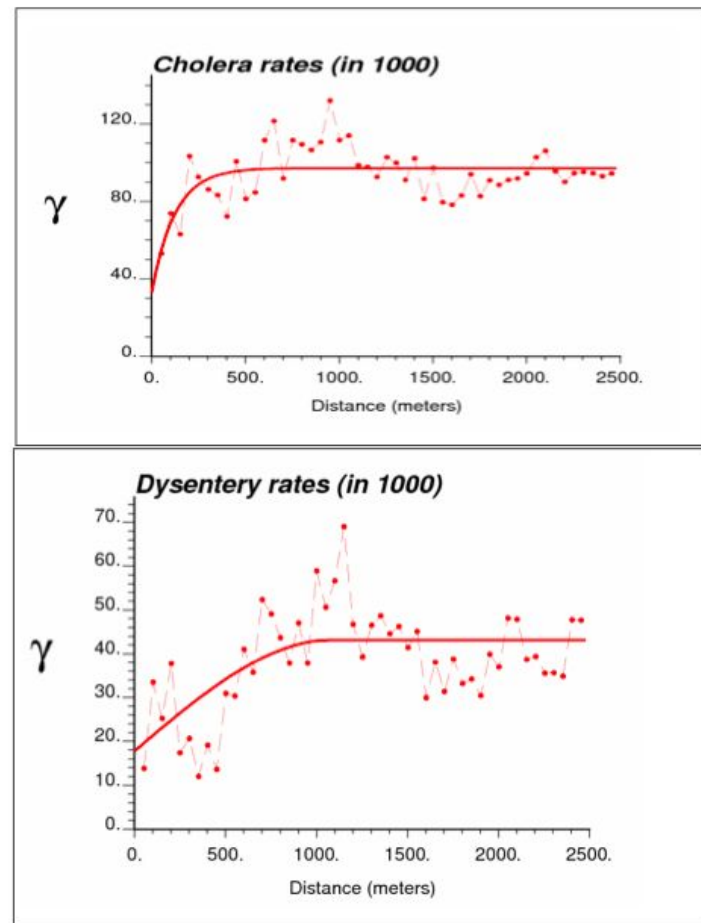
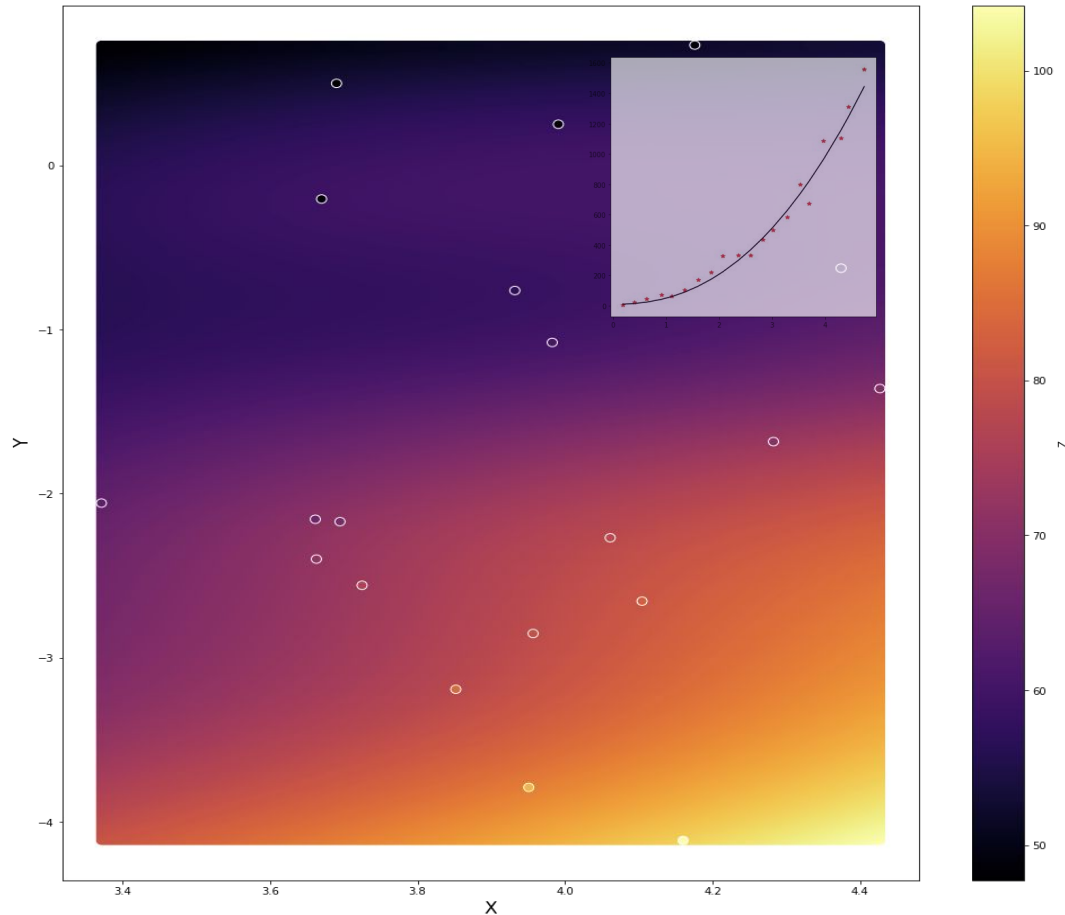


Figure 3
Omnidirectional semivariograms of cholera and dysentery incidence rates, with the model fitted.

Interpolation Methods:

2D interpolation

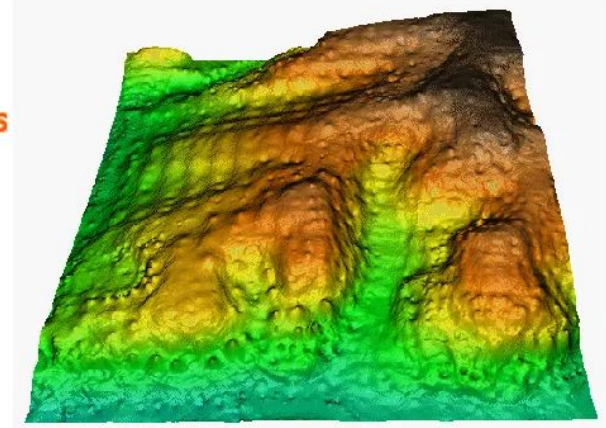
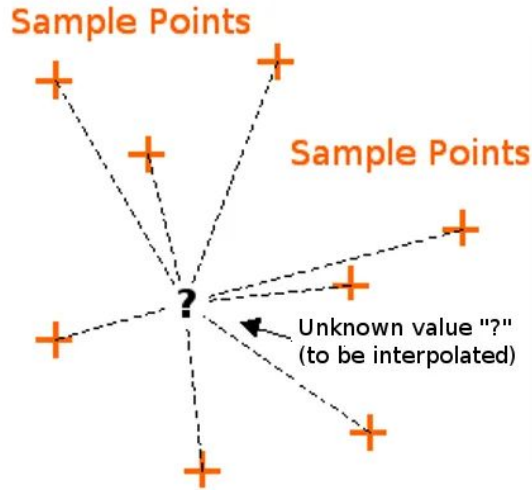
- These weights try to account for some covariance amongst the data during the interpolation.
- It can be extremely sensitive to the function fit to the the variogram data



Interpolation Methods:

2D interpolation

- A more stable but less flexible option is **Inverse Distance Weighting (IDW)**
- Here the weighting (λ) is of the form: $\lambda = d^{-p}$
- While closer points provide more weight you still have a subjective choice on how quickly this weighting falls off with distance



Interpolation Methods:

2D interpolation

- As with 1D interpolation you still have subjective choices which can significantly alter your final interpolated values
- E.g., why should weighting fall off linearly with distance? Quadratically? Which variogram model best represents the covariance in the data?
- **You can't separate most numerical algorithms from subjective choices**
- **Even things that are trained on data, have biases because of training sets or construction choices for the neural network, interpolation, or optimization routines.**
- **The best thing you can do is TEST parameter variations!**
Understand limitations and always consider the physical system.

Implementation in Python

| Interpolation Type | Function | Library | Description |
|-----------------------------------|--------------------------------------|--------------------|--|
| 1D Linear Interpolation | <code>interp1d</code> | <code>scipy</code> | Creates a linear interpolant over 1D data. Useful for filling gaps in evenly spaced data. |
| 1D Spline Interpolation | <code>UnivariateSpline</code> | <code>scipy</code> | Smooth spline interpolation over 1D data, with adjustable smoothing. Ideal for noisy data. |
| Cubic Spline | <code>CubicSpline</code> | <code>scipy</code> | Provides cubic spline interpolation, often producing smoother results. |
| 2D Interpolation | <code>interp2d</code> | <code>scipy</code> | Interpolates over 2D grids using linear, cubic, or quadratic methods. |
| Multidimensional Spline | <code>RectBivariateSpline</code> | <code>scipy</code> | Spline-based 2D interpolation for gridded data in two dimensions. |
| Regular Grid Interpolation | <code>RegularGridInterpolator</code> | <code>scipy</code> | Interpolates for N-dimensional data on a regular grid. Can handle more than 2 dimensions. |

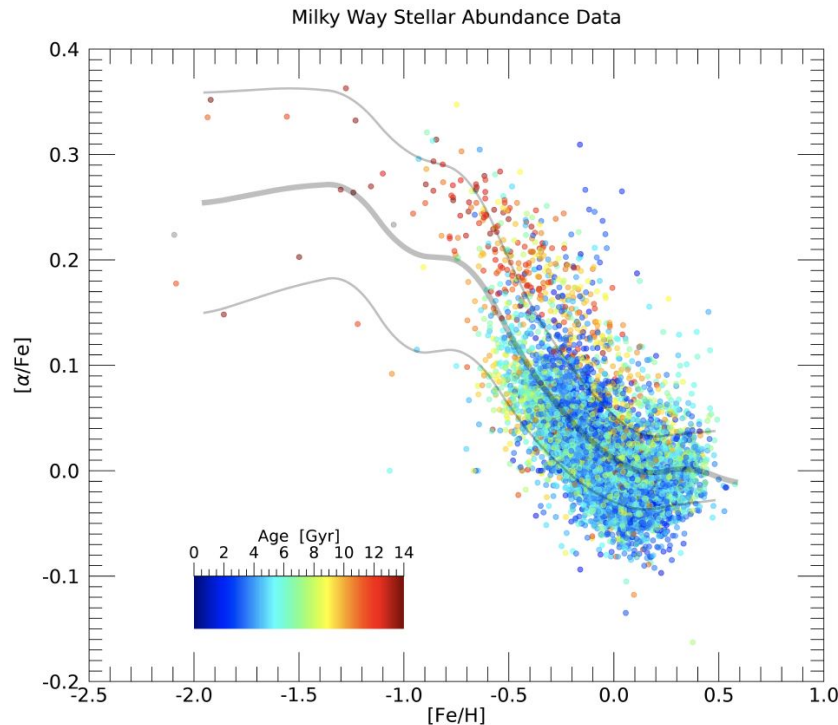
Implementation in Python

| | | | |
|--|------------------------------------|--------------------|---|
| Grid Interpolation for Scattered Data | <code>griddata</code> | <code>scipy</code> | Interpolates unstructured 2D or 3D data using linear, cubic, or nearest neighbor methods. |
| Nearest Neighbor Interpolation | <code>NearestNDInterpolator</code> | <code>scipy</code> | Interpolates nearest neighbors for multidimensional data, useful for irregular grids. |
| Radial Basis Function (RBF) | <code>Rbf</code> | <code>scipy</code> | Performs interpolation based on radial basis functions for scattered 1D, 2D, or 3D data. |
| Piecewise Polynomial | <code>PchipInterpolator</code> | <code>scipy</code> | Monotonic piecewise cubic Hermite interpolator, suitable for non-oscillatory data. |
| Polynomial Interpolation | <code>polyfit</code> | <code>numpy</code> | Fits a polynomial to the data, suitable for small datasets or low-degree polynomials. |
| Lagrange Interpolation | <code>lagrange</code> | <code>scipy</code> | Uses Lagrange polynomials for interpolation; can be unstable for high-degree polynomials. |

Approximation Methods:

Running averages

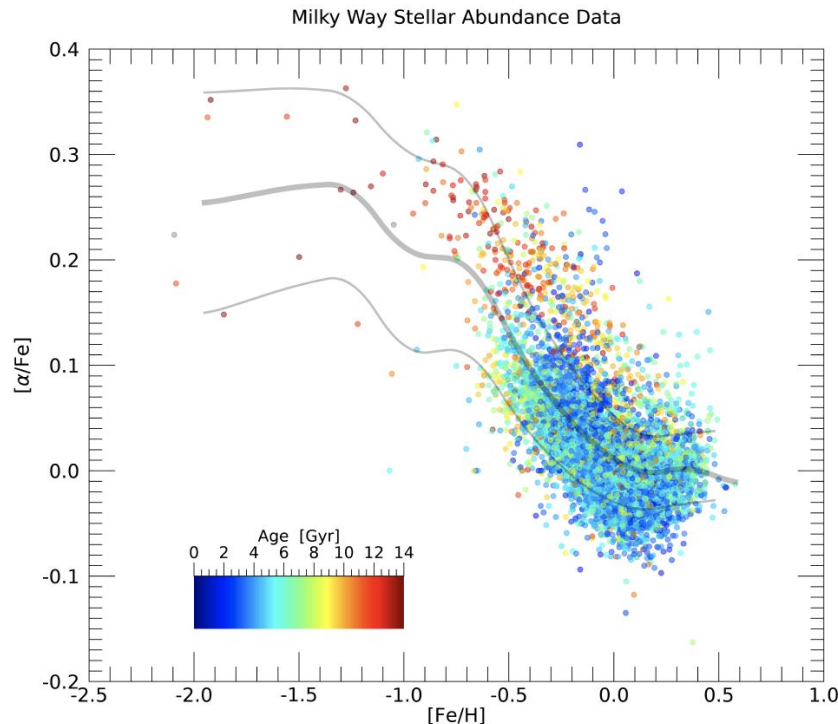
- In some cases we may want to highlight the smooth behaviour of a data set, rather than an instantaneous interpolation between two values.



Approximation Methods:

Running averages, confidence intervals

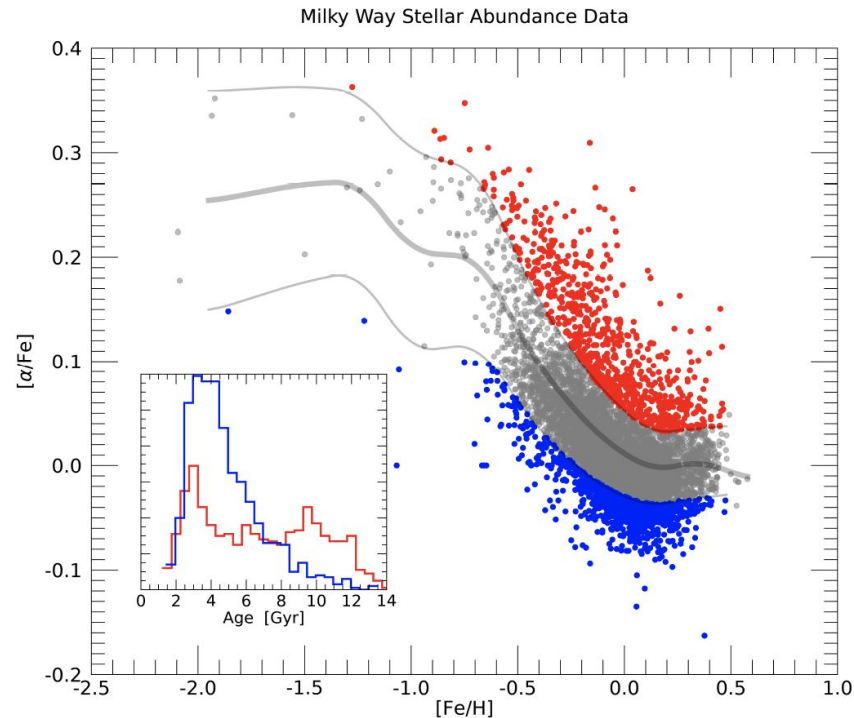
- In some cases we may want to highlight the smooth behaviour of a data set, rather than an instantaneous interpolation between two values.
- This can be sometimes useful for visualization and characterization purposes.



Approximation Methods:

Running averages, confidence intervals

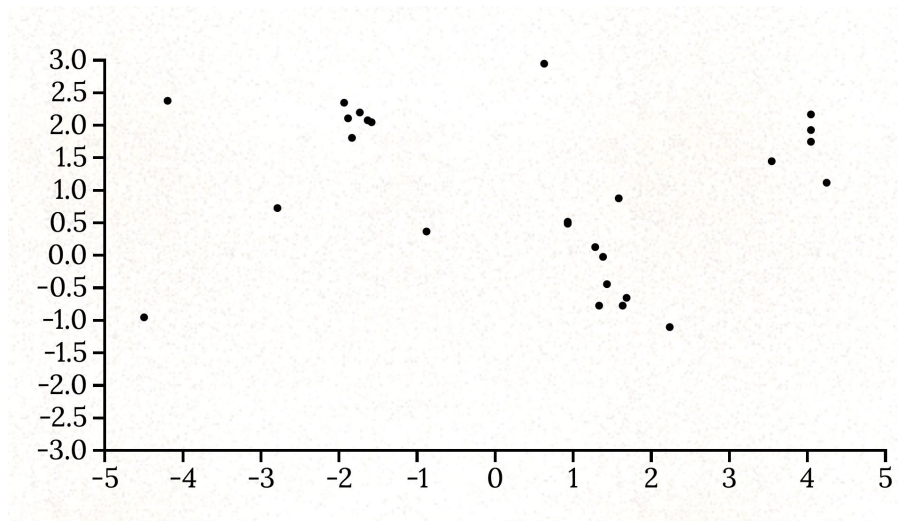
- In some cases we may want to highlight the smooth behaviour of a data set.
- This can be sometimes useful for visualization and characterization purposes.
- More often can help isolate influence/dependence of other variables in multi-dimensional data sets.



Approximation Methods:

Running averages, confidence intervals

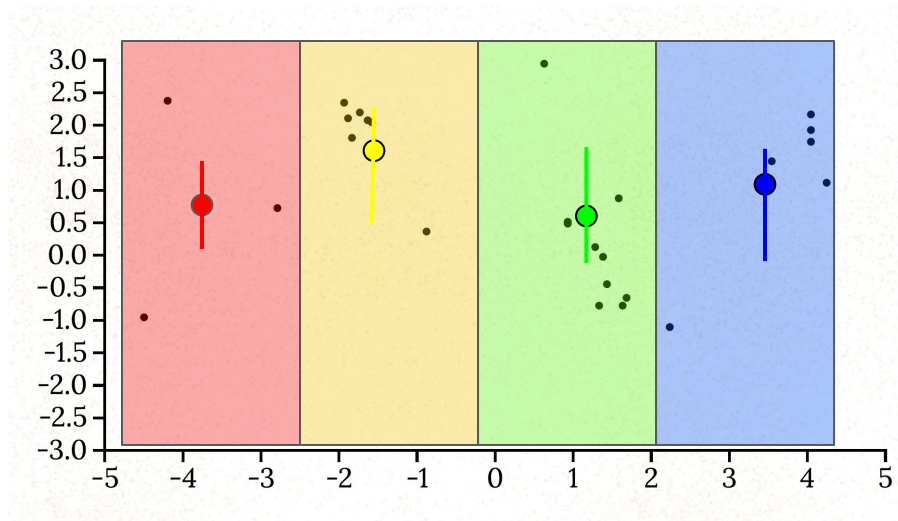
- Simplest boxcar estimates of mean and variance allow for smooth reconstructions at the cost of resolution.



Approximation Methods:

Running averages, confidence intervals

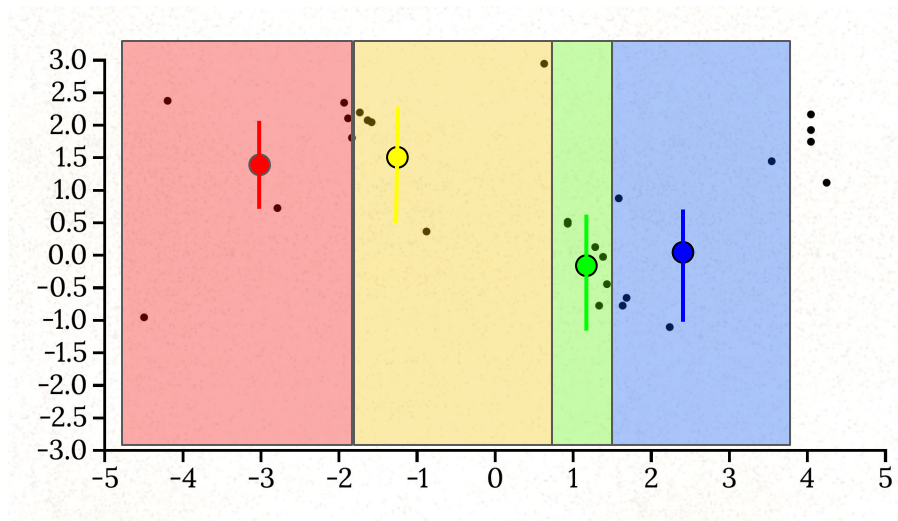
- Simplest boxcar estimates of mean and variance allow for smooth reconstructions at the cost of resolution.
- Divide data $[x_i, x_{i+1}, \dots, x_n]$ into subsets and compute statistics of interest within this window



Approximation Methods:

Running averages, confidence intervals

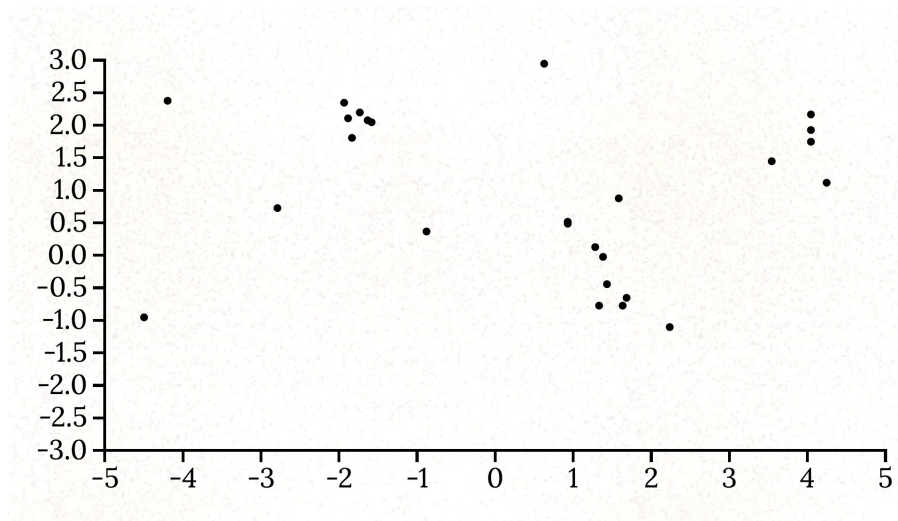
- Simplest boxcar estimates of mean and variance allow for smooth reconstructions at the cost of resolution.
- Divide data $[x_i, x_{i+1}, \dots, x_n]$ into subsets and compute statistics of interest within this window
- Often want to preserve \sim equal error in average estimates; can bin by i.e., equal number of points



Approximation Methods:

Running averages, confidence intervals

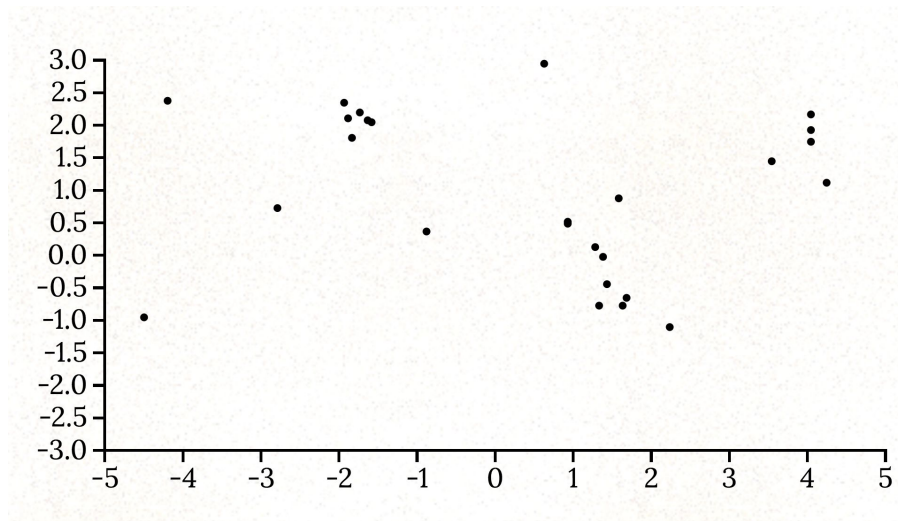
- Moving/running averages instead update the data set by replacing the last element of the window with the average from within the window



Approximation Methods:

Running averages, confidence intervals

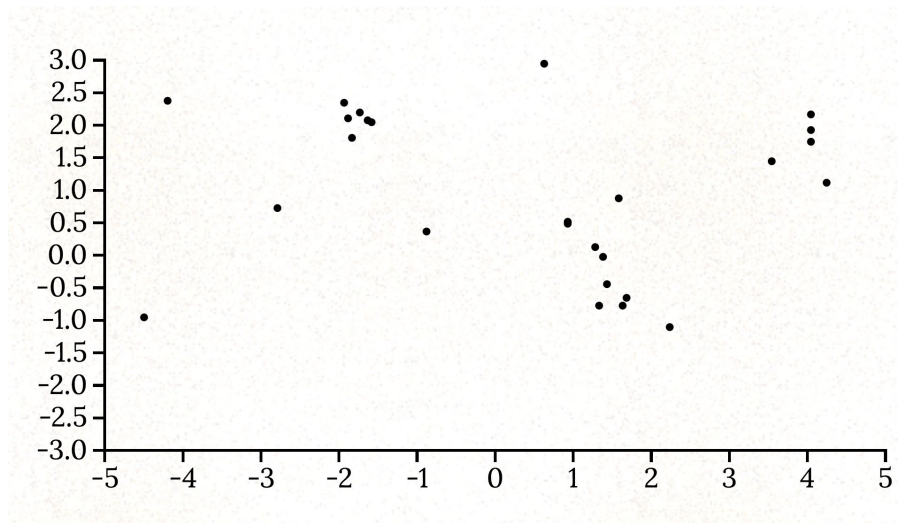
- Moving/running averages instead update the data set by replacing the last element of the window with the average from within the window
- E.g., $\mathbf{x}_{is} = \text{sum}(\mathbf{x}_i, \mathbf{x}_{i+1} \dots \mathbf{x}_j) / j$ for window size of j , over all data points $i < (n-j)$



Approximation Methods:

Running averages, confidence intervals

- Moving/running averages instead update the data set by replacing the last element of the window with the average from within the window
- E.g., $\mathbf{x}_{is} = \text{sum}(\mathbf{x}_i, \mathbf{x}_{i+1} \dots \mathbf{x}_j) / j$ for window size of j , over all data points $i < (n-j)$
- Has benefit of preserving resolution, but results qualitatively depend on window choice, and optionally, weighting choices



Summary on Interpolation/Approximation

- If you want smooth re-binning of simple data, representation of missing data for e.g., numerical integrals - **interpolation** can be helpful.
- If you want coarse trends of the data (including confidence intervals) in order to understand higher dimensional dependencies or role of outliers - **approximations/reconstructions** can be helpful
- Finally, remember that both interpolation and approximation are non-physical, can produce extrapolations or behaviours which are not necessarily the 'truth', and that subjective choices in e.g., order number or window size can change your interpretation.
- They are helpful methods - but **always**, consider the physical constraints of your system/question/data, and be aware that they all (even GPR) have subjective parameters which you should marginalize over.

Implementation in Python

| Approximation Type | Function | Library | Description |
|------------------------------|---|--------------------|--|
| Polynomial Approximation | <code>polyfit</code> | <code>numpy</code> | Fits a polynomial of a specified degree to data points; suitable for simple data or trends in smaller datasets. |
| Spline Approximation | <code>UnivariateSpline</code> , <code>LSQUnivariateSpline</code> , <code>CubicSpline</code> | <code>scipy</code> | Smooth curve fitting with splines, allowing for adjustable smoothing parameters. Great for 1D data. |
| Radial Basis Functions (RBF) | <code>Rbf</code> | <code>scipy</code> | Approximates scattered data in higher dimensions using radial basis functions, with various kernel options like Gaussian and Multiquadric. |

Implementation in Python

| | | | |
|--|---|----------------------|---|
| Least Squares Fitting | <code>curve_fit</code> | <code>scipy</code> | Fits arbitrary functions to data by minimizing the squared error; often used for nonlinear curve fitting. |
| Piecewise Linear Approximation | <code>interp1d</code> with <code>kind='linear'</code> | <code>scipy</code> | Provides a piecewise linear approximation, essentially connecting data points with straight lines. |
| Piecewise Polynomial (PCHIP) | <code>PchipInterpolator</code> | <code>scipy</code> | Monotonic, piecewise polynomial fit that prevents oscillations, ideal for strictly increasing or decreasing data. |
| Gaussian Process Regression (GPR) | <code>GaussianProcessRegressor</code>  | <code>sklearn</code> | Probabilistic model useful for high-dimensional function approximation, which provides uncertainty estimates. |

Implementation in Python

| | | | |
|---|--|-------------------------------|---|
| Chebyshev Polynomial Approximation | <code>Chebyshev.fit</code> | <code>numpy.polynomial</code> | Fits Chebyshev polynomials, which minimize approximation error in the least-squares sense and are useful for function approximation over intervals. |
| Fourier Series Approximation | <code>fft</code> or <code>irfft</code> | <code>numpy</code> | Approximates periodic data by decomposing it into a sum of sinusoids, useful for analyzing frequency components. |
| Linear Regression | <code>LinearRegression</code> | <code>sklearn</code> | Fits a linear model to data, often used as a baseline approximation for continuous or noisy data with a linear relationship. |

Implementation in Python

| | | | |
|--|--|----------------------|--|
| Polynomial Regression | <code>PolynomialFeatures</code> + <code>LinearRegression</code> | <code>sklearn</code> | Transforms data to include polynomial terms before applying linear regression, creating polynomial approximation. |
| k-Nearest Neighbors Regression | <code>KNeighborsRegressor</code> | <code>sklearn</code> | A non-parametric approximation that averages values from the nearest neighbors, useful for irregular data. |
| Support Vector Regression (SVR) | <code>SVR</code> | <code>sklearn</code> | Uses support vector machines for regression tasks, suitable for nonlinear relationships and higher-dimensional data. |

Implementation in Python

| | | | |
|--|---------------------------|--------------------------|--|
| Neural Network Approximation | <code>MLPRegressor</code> | <code>sklearn</code> | Multilayer Perceptron model for function approximation, suitable for complex and high-dimensional data patterns. |
| Local Polynomial Regression (LOESS) | <code>lowess</code> | <code>statsmodels</code> | Locally weighted regression that fits simple models around each data point, suitable for smooth approximation in 1D data with trends or seasonality. |