

Linear Methods

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Preliminaries

- We will go very deep into linear models.
- Most of you probably have seen linear models in some form, but we will start from scratch to further illustrate key concepts such as bias and variance.
- We will then discuss techniques such as regularization and transformation of inputs in the context of linear methods.

Notation

- Capital letters, e.g., X denote variables.
- Lower-case letters e.g., x , denote observations.
- Dummy index j denotes different variables, e.g., X_j
- Dummy index i denotes different observations, e.g., x_i
- Bolded variables are vector/matrices, e.g., \mathbf{y} , \mathbf{X}

Linear Regression

Linear Regression

Simplest possible model between target and feature

$$Y = f(X_1, X_2, \dots, X_p) = \beta_0 + \sum_{j=1}^p \beta_j X_j$$

X_j can be:

- Quantitative inputs
- Transformations of quantitative inputs, e.g., log, exp, powers, etc. Basis expansions, e.g., $X_2 = X_1^2$, $X_3 = X_1^3$
- Interactions between variables, e.g., $X_1 X_2$
- Encoding of levels of inputs

Supervised learning

- Given a set of paired observations $\{x_{ij}, y_i\}$, what are the model parameters (in this case, the coefficients β_j) that are “optimal”?
- “Optimal” is typically defined as minimization of some **loss function** (also known as **cost function**) that measures the error of the model.

Least squares regression

Consider the simple case of

$$Y = \beta_0 + \beta_1 X_1$$

In least squares regression, the loss function is defined as the sum squared error given the N observations:

$$\begin{aligned} L(Y, \hat{f}(X)) &= \sum_{i=1}^N (y_i - f(x_i))^2 \\ &= \sum_{i=1}^N (y_i - \beta_0 - \beta_1 x_{i1})^2 \end{aligned}$$

What are the optimal parameters β_0 and β_1 ?

$$\frac{\partial L}{\partial \beta_0} = \sum_{i=1}^N 2(y_i - \beta_0 - \beta_1 x_{i1})(-1) = 0$$

$$\Rightarrow \sum_{i=1}^N y_i = N\beta_0 + \sum_{i=1}^N \beta_1 x_{i1}$$

$$\Rightarrow \beta_0 = \bar{y} - \beta_1 \bar{x}_1$$

$$\frac{\partial L}{\partial \beta_1} = \sum_{i=1}^N 2(y_i - \beta_0 - \beta_1 x_{i1})(-x_{i1}) = 0$$

$$\Rightarrow \beta_1 = \frac{\sum_{i=1}^N x_{i1} y_i - N \bar{x}_1 \bar{y}}{\sum_{i=1}^N x_{i1}^2 - N \bar{x}_1^2}$$

Reformulating the general multiple linear regression as a vector equation...

Considering N observations of

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}$$

Let

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_p \end{pmatrix}, \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & & & & \\ 1 & x_{N1} & x_{N2} & \dots & x_{Np} \end{pmatrix},$$

So,

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}$$

Note that \mathbf{y} is a $N \times 1$ vector, $\boldsymbol{\beta}$ is a $(p+1) \times 1$ vector, and \mathbf{X} is a $N \times (p+1)$ matrix.

Reformulating the general multiple linear regression as a vector equation...

$$L = RSS = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Assuming (for the moment) that \mathbf{X} has full column rank, and hence $\mathbf{X}^T\mathbf{X}$ is positive definite, It can be shown using the same principles that the following unique solution for $\boldsymbol{\beta}$ is:

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\ \hat{\mathbf{y}} &= \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

Graphic representation of MLR with two dependent variables

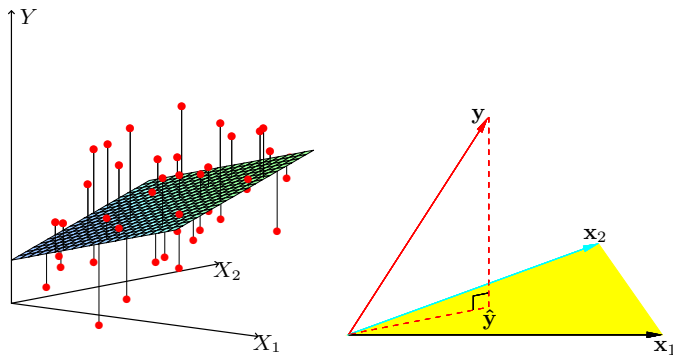


Figure: MLR minimizes sum square of residuals. The projection $\hat{\mathbf{y}}$ represents the vector of the least squares predictions onto the hyperplane spanned by the input vectors \mathbf{x}_1 and \mathbf{x}_2 . [1].

Validity of least squares criterion

- Observations are independently drawn at random.
- Variance of \mathbf{y} is constant given by σ^2 .

$$\text{var}(\hat{\beta}) = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2$$

- and σ is estimated using:

$$\sigma^2 = \frac{1}{N - p - 1} \sum_{i=1}^N (y_i - \hat{y}_i)^2$$

Example materials data

- Target: Bulk modulus of elements (from Materials Project)
- Candidate features:
 - Melting point (MP)
 - Boiling point (BP)
 - Atomic number (Z)
 - Electronegativity (χ)
 - Atomic radius (r)
- Question: Why these features?
- We will add some transformations of these inputs as well, i.e., the square and square root of the electronegativity and atomic radius.

Element	MP	BP	Z	X	r
Ac	29	1323	3573	89	1.1
Ag	88	1234.93	2435	47	1.93
Al	83	933.47	2792	13	1.61
As	40	1090	887	33	2.18
Au	137	1337.33	3129	79	2.54
B	211	2349	4200	5	2.04
Ba	9	1000	2143	56	0.89
Be	122	1560	2742	4	1.57
Bi	29	544.4	1837	83	2.02
Br	4	265.8	332	35	2.96
C	118	3800	4300	6	2.55
Ca	17	1115	1757	20	1
Cd	42	594.22	1040	48	1.69
Ce	37	1068	3633	58	1.12
Cl	2	171.6	239.11	17	3.16
Co	212	1768	3200	27	1.86
Cr	259	2180	2944	24	1.66
Cs	2	301.59	944	55	0.79
Cu	145	1357.77	3200	29	1.9
Dy	41	1680	2840	66	1.22
Er	44	1802	3141	68	1.24
Eu	13	1099	1800	63	1.2
F	2	53.53	85.03	9	3.98
Fe	182	1811	3134	26	1.83
Ga	50	302.91	2477	31	1.81
Gd	37	1585	3523	64	1.2
Ge	59	1211.4	3093	32	2.01
H	1	14.01	20.28	1	2.2
Hf	108	2506	4876	72	1.3
Hg	8	234.32	629.88	80	2

Using pandas for easy data manipulation

```
import pandas as pd
# Read in data and set first column as index.
data = pd.read_csv("element_data.csv", index_col=0)
# Generate transformations as additional columns.
data["X^2"] = data["X"] ** 2
data["sqrt(X)"] = data["X"] ** 0.5
data["r^2"] = data["r"] ** 2
data["sqrt(r)"] = data["r"] ** 0.5
# Define our features, which is all the columns
# excluding K, which is the target.
features = [c for c in data.columns if c != "K"]
x = data[features]
y = data["K"]
```

MLR in scikit-learn

```
from sklearn import linear_model
reg = linear_model.LinearRegression()
reg.fit(x, y)
print(ref.coef_)
print(reg.intercept_)
```

- Note that x should contain the features only - there is no need to add a 1 column for the intercept. By default, the parameter `fit_intercept` in `sklearn.linear_model.LinearRegression` is `True`. You can set it to `False` to do a MLR without intercept.
- Documentation: [link](#).

Hypothesis Testing for Coefficients

- To derive insights into a model, we often want to know which of the input parameters are the most relevant to the target.
- Under assumptions of the errors in y follow a Gaussian distribution $N(0, \sigma^2)$, the errors in $\hat{\beta}$ also have a Gaussian distribution $N(\beta, (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2)$
- Hypothesis testing can be carried out for whether a particular β_j is 0 using the following test statistic:

$$t_j = \frac{\hat{\beta}_j}{\sigma \sqrt{v_j}}$$

where v_j is the j th diagonal element of $(\mathbf{X}^T \mathbf{X})^{-1}$. t_j has a t distribution with $N - p - 1$ degrees of freedom (dof).

Hypothesis Testing for Groups of Coefficients

- More often, we want to test groups of coefficient for significance. E.g., to the k levels of a categorical variable.
- We will use the following F statistic:

$$F = \frac{(\text{RSS}_0 - \text{RSS}_1)/(p_1 - p_0)}{\text{RSS}_1/(N - p_1 - 1)}$$

where RSS_0 is the RSS of the larger model with $p_0 + 1$ parameters and RSS_1 is the RSS of the smaller model with $p_1 + 1$ parameters with $p_0 - p_1$ parameters set to zero. The F statistic has a distribution of $F_{p_1 - p_0, N - p_1 - 1}$.

Gauss-Markov Theorem

- Consider the estimator $\hat{\theta}$ for a variable θ .

$$\begin{aligned}\text{MSE} &= E(\hat{\theta} - \theta)^2 \\ &= \text{var}(\hat{\theta}) + [E(\hat{\theta}) - \theta]^2\end{aligned}$$

- The MSE can be broken down into the variance of the estimate itself and the square of the bias.

Gauss-Markov Theorem

The least squares estimator has the smallest variance among all linear *unbiased* estimators.

- However, there can be estimators that are biased with smaller MSE.

Model selection

Model selection

Model performance

- We will take a brief digression into model assessment and selection before continuing on to other linear methods.
- Model performance is related to its performance on *independent test data*, i.e., one cannot simply report a model's performance on training data alone.
- Note that this section is deliberately limited to high level concepts that are needed to continue further in exploration of linear methods. A more detailed discussion will be performed in later lectures.

Typical measures of model performance

- Mean squared error (MSE):

$$L(Y, \hat{f}(X)) = \frac{1}{N} \sum_{i=1}^N (y_i - f(x_i))^2$$

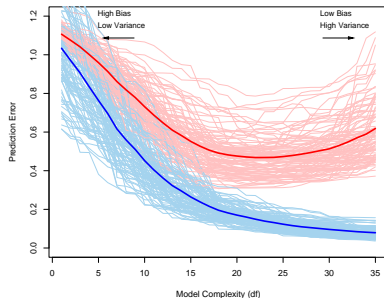
- Mean absolute error (MAE):

$$L(Y, \hat{f}(X)) = \frac{1}{N} \sum_{i=1}^N |y_i - f(x_i)|$$

- Test error: L over independent test set.
- Training error: L over training set.

Training and test errors with model complexity

- Model complexity increases as the number of parameters increases (e.g., number of independent variables in MLR).
- Training errors **always** decrease with increasing model complexity.
- However, test errors do not have a monotonic relationship with model complexity. Test errors are high when model complexity is too low (underfitting) or too high (overfitting).



Training, validation and test data

- Model selection: estimating the performance of different models in order to choose the best one.
- Model assessment: having chosen a final model, estimating its prediction error (generalization error) on new data.
- Ideal data-rich situation: Divide data into three parts:
 - Training set: For training the model.
 - Validation set: For estimating prediction error to select the model.
 - Test set: For assessing the generalization error of the final model.
- Typical training:validation:test split is 50:25:25 or 80:10:10, or in very data-poor situations, maybe even 90:5:5.
- Note that at no point in the model fitting process should the test set be “seen”.

K -fold cross validation (CV)

- Simplest and most widely used approach for model validation.
- Data set is split into K buckets (usually by random).
- Typical values of K is 5 or 10. $K = N$ is known as “leave-one-out” CV.

Train	Train	Validate	Train	Train
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- CV score is computed on the validate data set after training on the train data:

$$CV(\hat{f}^{-k(i)}, \alpha) = \frac{1}{N_{k(i)}} \sum_{i=1}^{N_{k(i)}} L(y_i, \hat{f}^{-k(i)}(x_i, \alpha))$$

- assuming the k^{th} data bucket has $N_{k(i)}$ data points and $\hat{f}^{-k(i)}$ refers to the model fitted with the k^{th} data left out ($N - N_{k(i)}$ data in fitting).

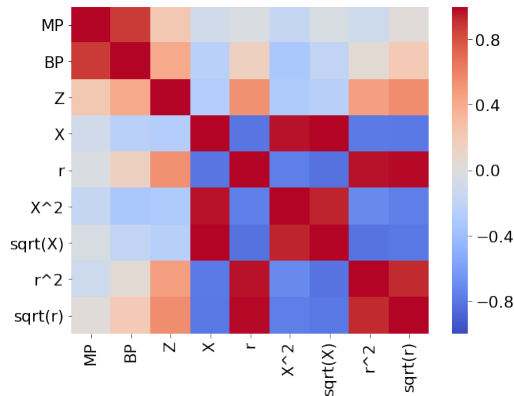
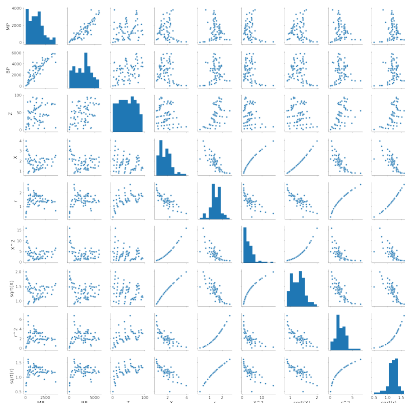
CV in scikit-learn

```
from sklearn.model_selection import cross_validate, KFold
kfold = KFold(n_splits=5, shuffle=True, random_state=42)
cv_results = cross_validate(ridge, z, y, cv=kfold)
```

- Note that we have customized the KFold object passed to the cross_validate method. The reason is that our element data is non-random by default. So we want to perform shuffling prior to doing the splits.
- Documentation: [link](#).

Characteristics of the example materials dataset

- Before proceeding further, let us try to tease out some aspects of the dataset.
- Quite clearly, there are correlations between some sets of variables.
- In other words, the input features are **non-orthonormal** with each other.



Beyond least squares

Beyond least squares

Model selection

- Often, we want to improve on the least squares model.
 - To improve prediction accuracy by sacrificing some bias for reduced variance.
 - To improve interpretability by reducing number of features or descriptors.
- Three main approaches:
 - 1 Subset selection
 - 2 Shrinkage methods
 - 3 Dimension reduction

Subset selection

Best subset selection

- Brute force approach.
- From p parameters, find the subset of k parameters that results in the smallest RSS.
- Combinatorially expensive for large p and large k .
- Note that the best subset for a larger k does not necessarily include the best subset for a smaller k .

Forward- or backward-stepwise selection

- Forward: Start with intercept, and iteratively add feature that most improves the fit.
- Backward: Start with full model, and sequentially deletes the feature with least impact on the fit.

Shrinkage methods

- Subset methods is discrete, i.e., retains/discards variables, and tends to exhibit high variance.
- Shrinkage methods are more continuous and do not suffer as much from high variability.
- Basic concept: instead of finding the parameters that minimizes the RSS only, we add a penalty term that penalizes more complex models, e.g., models with larger coefficients or larger number of coefficients. This “shrinks” the coefficients, in some cases, to 0.

Ridge regression (L_2 regularization)

$$\beta^{\hat{ridge}} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p \beta_j x_j)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

- $\lambda \geq 0$ is the shrinkage parameter. The larger the λ , the greater the shrinkage.
- Also equivalent to:

$$\begin{aligned} \beta^{\hat{ridge}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p \beta_j x_j)^2 \\ \text{subject to } \sum_{j=1}^p \beta_j^2 \leq t \end{aligned}$$

Ridge regression - Key details

- Intercept (β_0) is not part of penalty term.
- Inputs should be scaled prior to performing ridge regression, typically by centering to the mean and scaling to unit variance:

$$z_j = \frac{x_j - \mu_{x_j}}{s_{x_j}}$$

LASSO (L_1 regularization)

$$\beta^{L\hat{A}SSO} = \operatorname{argmin}_{\beta} \left\{ \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p \beta_j x_j)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\}$$

- Least Absolute Shrinkage and Selection Operator
- $\lambda \geq 0$ is the shrinkage parameter. The larger the λ , the greater the shrinkage.
- Also equivalent to:

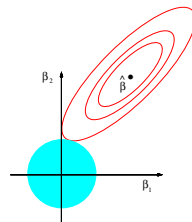
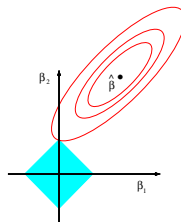
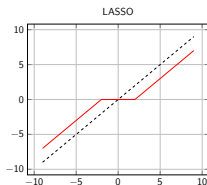
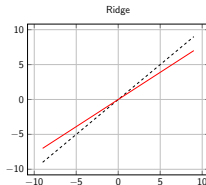
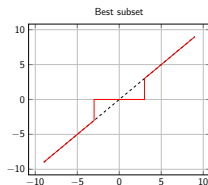
$$\begin{aligned} \beta^{L\hat{A}SSO} = \operatorname{argmin}_{\beta} \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p \beta_j x_j)^2 \\ \text{subject to } \sum_{j=1}^p |\beta_j| \leq t \end{aligned}$$

LASSO regression - Key details

- Intercept (β_0) is not part of penalty term.
- Inputs should be scaled prior to performing lasso regression, just as in ridge regression.

Subset vs ridge vs LASSO

- Consider a set of orthonormal features.
 - Ridge: proportional shrinkage. No coefficients are set to zero.
 - LASSO: “soft” thresholding. Translates coefficients by a factor, truncating at zero.
 - Best-subset: “hard” thresholding. Drops all coefficients below a certain threshold.



Other variants of shrinkage methods

- Elastic net penalty:

$$\lambda \left(\alpha \sum_{j=1}^p \beta_j^2 + (1 - \alpha) \sum_{j=1}^p |\beta_j| \right)$$

- Least angle regression

Derived input directions

- General concept: transforms input \mathbf{X} into a smaller subset of \mathbf{z}_m and regress on \mathbf{z}_m
- Principal component regression:
 - Transform non-orthonormal features into orthonormal directions using Principal Component Analysis (PCA).
 - Choose M directions that have the highest eigenvalues (explains the most variance) and discards the rest.
 - Will revisit at a later lecture.

Partial Least Squares (PLS)

- Algorithm:
 - ① Compute $\phi_{1j} = \langle \mathbf{x}_j, \mathbf{y} \rangle$ for each j .
 - ② First transformed direction $\mathbf{z}_1 = \sum_j \phi_{1j} \mathbf{x}_j$, i.e., each direction is weighted by strength of effect on \mathbf{y} .
 - ③ Regress \mathbf{y} on \mathbf{z}_1 to obtain θ_1 , orthogonalize $\mathbf{x}_1, \dots, \mathbf{x}_p$ wrt \mathbf{z}_1 via $x'_j = x_j - \frac{\langle \mathbf{z}_1, \mathbf{x}_j \rangle}{\langle \mathbf{z}_1, \mathbf{z}_1 \rangle} \mathbf{z}_1$.
 - ④ Repeat until $M \leq p$ coefficients are obtained.
- Finds directions with high variance and high correlation with response.

Preliminaries

- It is highly unlikely that the true function $f(X)$ is linear in X .
- In some cases, linearity is a reasonable assumption, e.g., a first order Taylor series expansion:

$$f(x) = f(a) + f'(a)(x - a) + f''(a)\frac{(x - a)^2}{2!} + f'''(a)\frac{(x - a)^3}{3!} + \dots$$

- Examples where this is used in materials science - linear elasticity (Hooke's law), etc.
- More frequently, we perform a transformation of inputs to create a linear basis expansion.

General concept

- Express:

$$f(X) = \sum_{m=1}^M \beta_m h_m(X)$$

where h_m is the m^{th} transformation of X .

- This is known as a linear basis expansion in X .
- The key lies in choice of the basis functions h_m .

Examples of basis expansions

- $h_m(X) = X_j^2, h_m(X) = X_i X_j$
 - Polynomial expansion to higher-order Taylor series terms.
 - No. of terms increases exponentially with degree of polynomial. For p variables, we have $O(p^2)$ square and cross-product terms in a quadratic model. For a degree d polynomial, we have $O(p^d)$.
- $h_m(X) = \log(X_j), \text{sqrt}(X_j), \exp(iX_j)$: non-linear transformations in X .
- $h_m(X) = I(L_m \leq X_k < U_m)$: Piece-wise division of regions of X . E.g., cubic splines.
- $h_m(X) = \text{RBF}(\|X - X_m\|)$: radial basis function, e.g., Gaussian.
- Typically, basis functions are used simply to allow a more flexible representation of the data. The basis functions can span a very large (sometimes infinite) set, from which a selection has to be made:
 - Restriction - Truncate the choice of basis functions using some criteria.
 - Selection - Choose basis functions that contribute significantly to the fit.
 - Regularization - Use the whole and/or very large subset and apply regularization techniques (e.g., ridge or LASSO) to restrict coefficients.

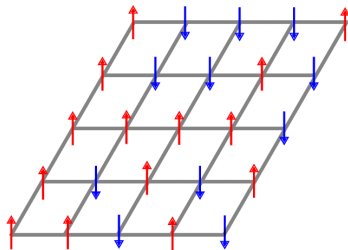
Linearization from physical laws

- Arrhenius law:

$$r = A \exp\left(-\frac{E_a}{RT}\right) \rightarrow \log(r) = \log(A) - \frac{E_a}{RT}$$

- Ising model:

$$H(\sigma) = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j - \mu \sum_j h_j \sigma_j$$

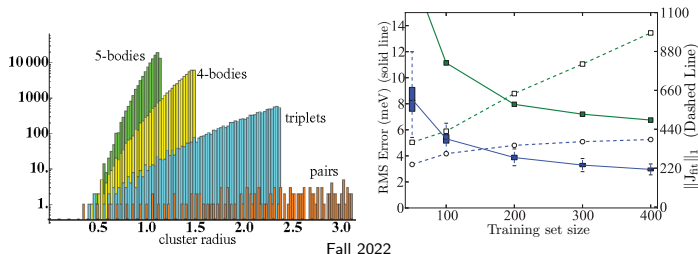


Compressive sensing for cluster expansions

- Cluster expansion of energy on lattice points:

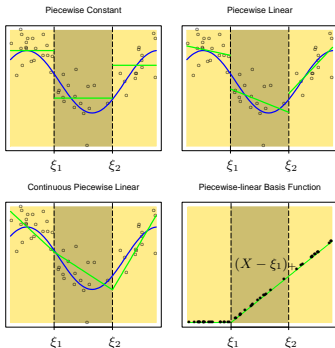
$$H(\sigma) = E_0 + \sum_f J_f \prod_f(\sigma)$$

- σ is the vector representing occupation of lattice sites, \prod_f are the cluster basis functions, J_f are effective cluster interactions (ECIs).
- Compressive sensing: essentially a LASSO to solve for ECIs.[2]



Piecewise polynomials

$$h_1(X) = I(X < \xi_1), h_2(X) = I(\xi_1 \leq X < \xi_2), h_3(X) = I(X \geq \xi_2)$$

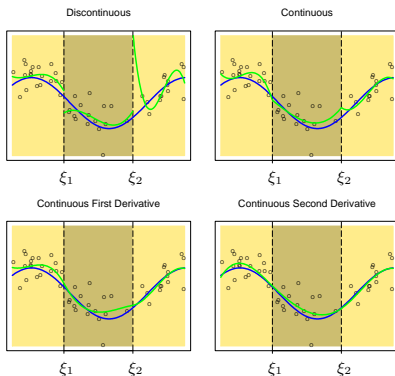


Parameters:

- No. of knots
- Order of polynomial
- Continuity at knots (value, first derivative, second derivative, etc.). For a polynomial of order N , we usually want all derivatives $< N$ to be continuous.

Cubic splines

Piecewise Cubic Polynomials



- Probably the most commonly used.
- Continuous 1st and 2nd derivatives.
- Natural cubic spline: polynomial is linear beyond boundaries.
- Smoothing spline: Use regularization to control complexity:

$$RSS(f, \lambda) = \sum_{i=1}^N \{y_i - f(x_i)\}^2 + \lambda \int \{f''(t)\}^2 dt$$

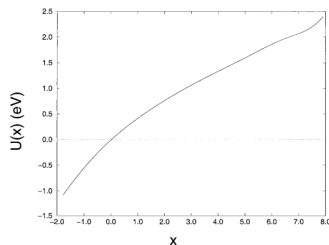
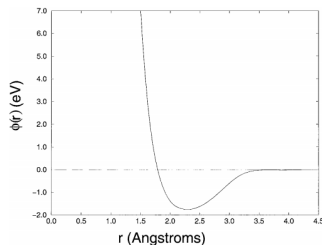
Examples of cubic spline fitting

- Spline-based Modified Embedded Atom Method (MEAM)

$$E = \sum_{i < j} \phi(r_{ij}) + \sum_i U(n_i),$$

$$n_i = \sum_j \rho(r_{ij}) + \sum_{i < k, j, k \neq i} f(r_{ij}) f(r_{ik}) g[\cos(\theta_{jik})]$$

where ϕ , U , ρ , f and g can be approximated by cubic splines.



Demo: Cubic spline fitting in scipy

```
import numpy as np
## Import CubicSpline from scipy
from scipy.interpolate import CubicSpline
## x, y data for generating the spline fitting
x = np.arange(10)
y = np.sin(x)
## Fit the spline
cs = CubicSpline(x, y)
## Generate new x values
xs = np.arange(-0.5, 9.6, 0.1)
## Perform the interpolation on the new points
ys = cs(xs)
```


Gaussian basis functions

$$h_m(x) = \exp(-k(x - x_m)^2)$$

- Gaussian functions centered at x_m .
- Other similar types of functions include Lorentzian ($h_m(x) = \frac{1}{1+kx^2}$), Gaussian-Lorentzian, Voigtian, Pearson type IV, and beta profiles.

Example: Rietveld refinement

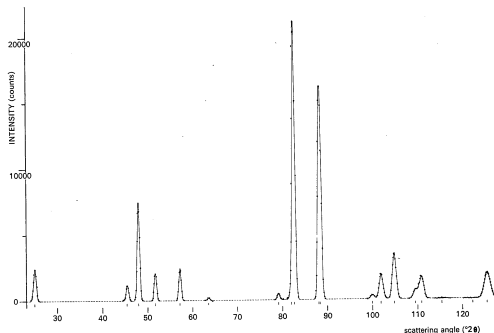


Figure: Neutron powder diffraction diagram of CaUO_4

- Least squares fitting of theoretical line profile to match a measured diffraction pattern (e.g., X-ray, neutron).[3]

Example: Rietveld refinement, contd.

- Peak shape function:

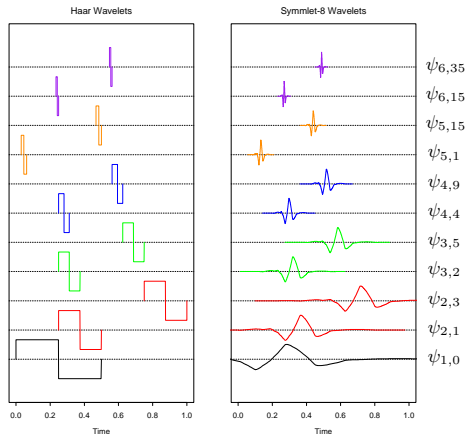
$$PSF(\theta) = \Omega(\theta) \otimes \Lambda(\theta) \otimes \Psi(\theta) + b(\theta)$$

- Ω : Instrument broadening, Λ : Wavelength dispersion, Ψ : Specimen function.
- For single phase, minimize:

$$\Phi = \sum_{i=1}^N w_i \left(Y_i^{obs} - \left(b_i + K \sum_{j=1}^m I_j y_j(x_j) \right) \right)^2$$

- where $y_j(x_j)$ is typically a pseudo-Voigt (mix of Gaussian and Lorentizan function) function.
- Note that the background (b_i) holds no useful structural information and should be minimized in experiments.

Wavelet smoothing



- Complete orthonormal basis
- Shrink and select toward **sparse** representation.
- Able to represent both time and frequency localization efficiently (Fourier basis can only do frequency localization).

Example: NMR Spectroscopy

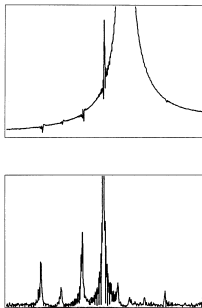
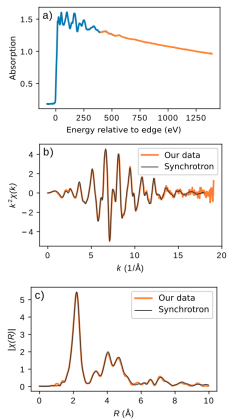


Figure: Subtraction of a large spectral line: (top) the original spectrum of polyethylene, (bottom) reconstructed spectrum after removal of CH_2 peak.[4]

Applications:

- Suppression of large unwanted spectral line (left).
- Rephasing spectrum perturbed by time-dependent magnetic field.
- Noise filtering
- Detecting phases in a mixture

Example: Fourier transform for analysis of extended X-ray absorption fine structure (EXAFS)



- (a) The extended edge (orange part) contains information of atom chemical environment.
- (b) Subtract the background, convert energy to k -space unit, and multiply the normalized intensity by k^2
- (c) Fourier transform k -space information to real space and obtain the first shell bond length.

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