3.3 Information richness and data missingness in clinical studies for Heart Failure

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Prospective clinical studies typically yield a rich set of patient parameters. This, however, also increases chances of missing some parameters for some patients. Our study into chronic heart failure also shows various patterns of data missingness. Preliminary results from our structured study of the efficacy of various data imputation techniques seem to indicate that there is limited added value of more sophisticated imputation techniques over the relatively simple techniques with respect to the performance of classifiers of 30-day readmission. Other challenges for successful application of such predictive methods in clinical practice include the inherent selection bias that occurs in prospective studies. We showed that this bias has large effect on the generalizability of predictive models and should not be overlooked in model development.

3.4 Feature extraction for x-ray scattering from biomolecules and nanoparticles.

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To obtain information about the structure of biological molecules in terms of atomic positions in the molecule, x-ray crystallography is the principal tool. But what happens if the circumstances are such that a crystal of the molecules of interest is not available? Here, x-ray scattering from a solution of the molecule of interest gives a one-dimensional scattering intensity $I(q)$, as an average scattering over all orientations of the molecule, expressed as a function of the scattering wave vector q defined in terms of the scattering angle, θ.

Features of the molecular structure may be extracted from this function by a variety of methods of which the simplest is the Guinier method which measures the radius of gyration, R_g of the molecule in terms of the Gaussian character of the scattering function at small scattering angles $I(q) \sim \exp(-q^2 R_g^2/3)$. This provides a model-free method for extraction of the feature parameter R_g by fitting the data to the Guinier function at sufficiently small scattering angles. The non-linear nature of this function makes this a "super-resolution" method in which the spatial resolution of the resulting R_g is 2-3 orders of magnitude more accurate than would be given by linear Fourier analysis of the data [1].

In the last few years, the advent of x-ray free electron lasers (xFELs) has now made possible a method to obtain 3-dimensional atomic structures from scattering data of a solution of molecules in the xFEL x-ray beam. In this technique, each flash of the laser beam provides a very high intensity of x-rays in a few 10s of femtoseconds. The scattered x-rays are captured on a 2-dimensional detector as an image which is azimuthally isotropic around the direction of the incoming x-ray beam.

Angular correlators of this image as a function of the azimuthal angle, ϕ, around scattering rings of fixed theta, define a 3-dimensional correlation function $C(q_1, q_2, \psi)$. Here q_1 and