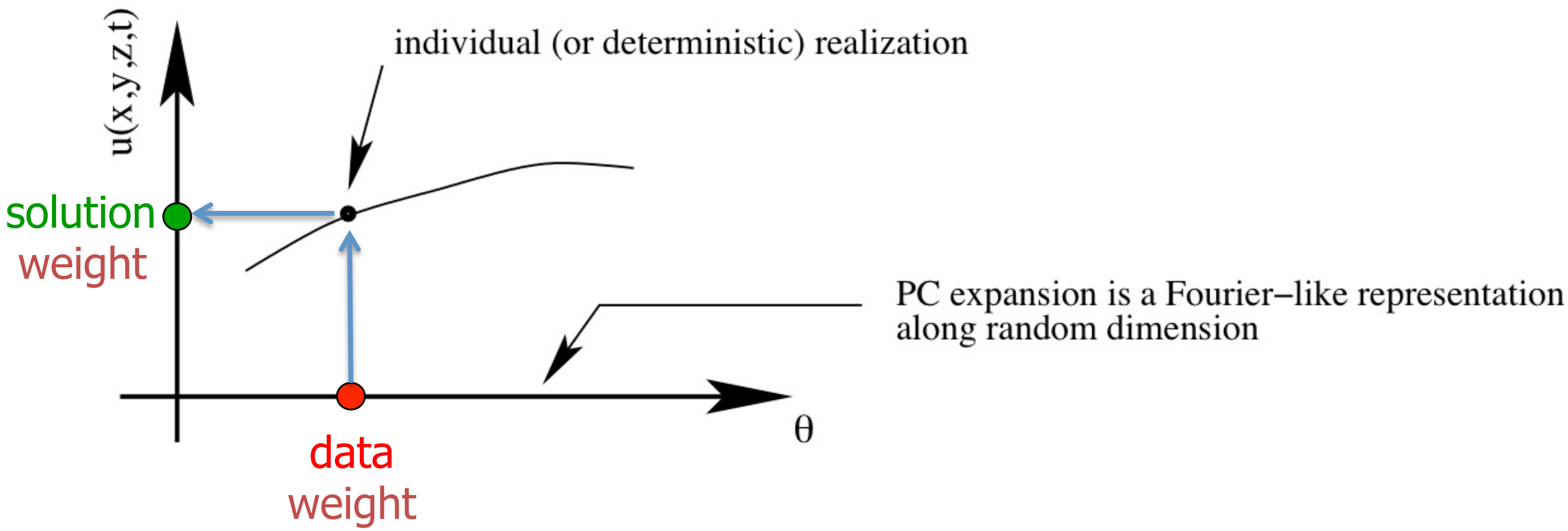
Spectral approach to UQ

- Probabilistic approach to UQ



- Stochastic solution is sought in a product space
  - probability space (x axis)
  - deterministic solution space (y axis)
  - both are assumed to have Hilbert space structure, with a countable orthogonal basis

Spectral Expansion

- mean-square convergent expansion in the space of random variables:

$$u(x,t;\boldsymbol{\xi}) = \sum_k u_k(x,t)\Psi_k(\boldsymbol{\xi})$$

  - solution mode
  - vector of canonical random variables that are suitably used to parametrize the uncertain inputs
  - orthogonal basis in the space of square integrable random functions
  - solution mode (coordinate in Hilbert space) is unknown to be determined

Examples

- Legendre:

$$Le_n(x) = \frac{1}{2^n} \sum_{l=0}^{[n/2]} (-1)^l \left(\begin{array}{c} n \\ l \end{array} \right) \left(\begin{array}{c} 2n-2l \\ n \end{array} \right) x^{n-2l}$$

  - orthogonal over [-1,1] with uniform measure

- Hermite:

$$He_n(x) = n! \sum_{m=0}^{[n/2]} (-1)^m \frac{1}{m!2^m(n-2m)!} x^{n-2m}$$

  - orthogonal over (-∞,∞) with Gaussian measure

Determination of coefficients

- Intrusive approach:
  - Generally Galerkin formalism – insert expansion into governing equations and derive governing equations for coefficients
- Non-intrusive approach:
  - Reconstruct functional relation based on discrete realizations
  - Regression approaches (including Bayesian regression)
  - Spectral projection (Gauss quadratures, sparse quadratures, adaptive quadratures, MC quadratures, …)
  - Compressing sensing (CS, BCS)
  - Etc…

Why spectral expansions?

- Efficiency:
  - provided, generally, that sufficient smoothness is present
- Probabilistic framework:
  - provides fundamental tools for analyzing stochastic errors, convergence, etc…
- Format:
  - key to the machinery of approximation theory (optimization, sensitivity analysis, inverse design, etc…)

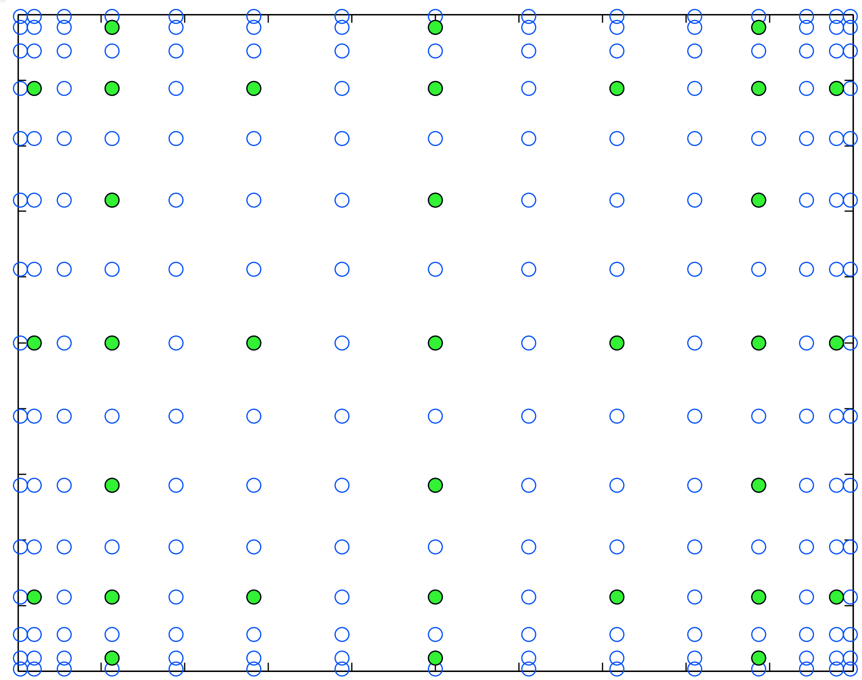
Non-Intrusive Spectral Projection (NISP)

- Alternative to Galerkin formalism in situations where modification of production or legacy codes is not feasible
- Essentially a collocation approach to the evaluation of probability integrals

uncertain inputs → Model → quantity of interest

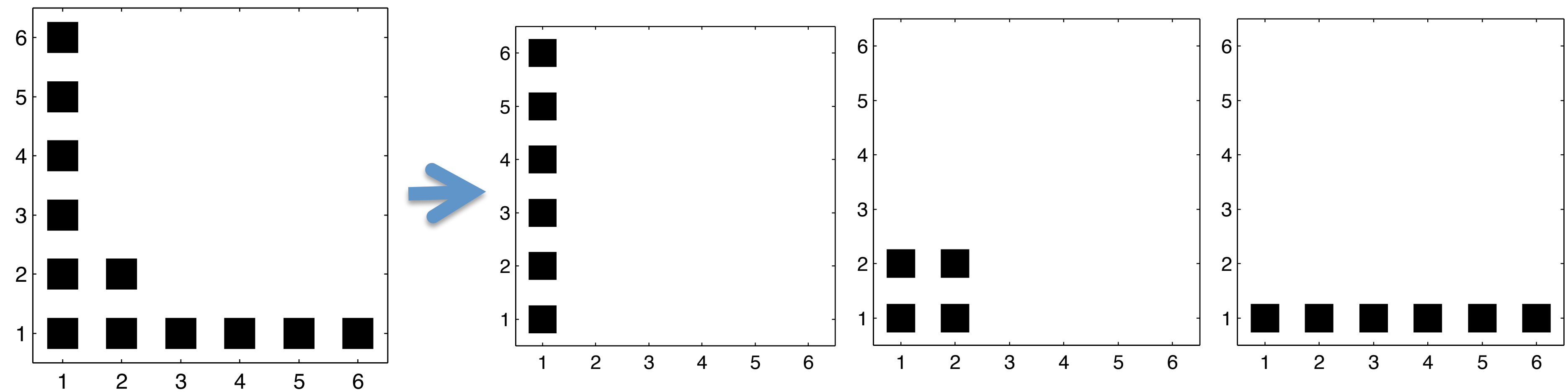
$$\langle \Psi_k^2 \rangle Q_k = \langle Q(\xi) \Psi_k(\xi) \rangle \approx \sum_{i=1}^{N} Q(x_i) w_i$$

Sparse quadratures



- Smolyak/Gauss Patterson
  - non-adaptive
  - nested grid
  - level p resolution ~ yields order p PC
- Adaptive extension
  - variance-based error indicators
  - “optimal” pseudo-spectral construction
- Both approaches well suited to moderate dimensionality

Smolyak pseudospectral construction



- New Smolyak pseudospectral approximation (Constantine et al., 2011; Conrad & Marzouk, 2012):
  - essentially a telescoping sum of pseudospectral projections (each internal-aliasing-free)
  - enables inclusion of all polynomials on general sparse grid that can be computed without internal aliasing
  - efficient use of data
  - adaptive variants avoid hand tuning

UQ Toolkit

- **UQ Toolkit** provides library of subroutines that implement moment formulas, approximate evaluations of various nonlinear transformations, post-processing functionals.

  Take-away: essential comfort in the machinery that transform f(u) into $[f(u)]_k$, without explicit need to manipulate moment expressions, yet keeping error control in mind.

- UQ Toolkit available as open source software at:

  http://www.sandia.gov/UQToolkit/